

Inhomogeneous diffusion and ergodicity breaking induced by global memory effects

Adrián A. Budini

*Consejo Nacional de Investigaciones Científicas y Técnicas (CONICET), Centro Atómico Bariloche,
Avenida E. Bustillo Km 9.5, (8400) Bariloche, Argentina
and Universidad Tecnológica Nacional (UTN-FRBA), Fanny Newbery 111, (8400) Bariloche, Argentina*
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We introduce a class of discrete random-walk model driven by global memory effects. At any time, the right-left transitions depend on the whole previous history of the walker, being defined by an urnlike memory mechanism. The characteristic function is calculated in an exact way, which allows us to demonstrate that the ensemble of realizations is ballistic. Asymptotically, each realization is equivalent to that of a biased Markovian diffusion process with transition rates that strongly differs from one trajectory to another. Using this “inhomogeneous diffusion” feature, the ergodic properties of the dynamics are analytically studied through the time-averaged moments. Even in the long-time regime, they remain random objects. While their average over realizations recovers the corresponding ensemble averages, departure between time and ensemble averages is explicitly shown through their probability densities. For the density of the second time-averaged moment, an ergodic limit and the limit of infinite lag times do not commute. All these effects are induced by the memory effects. A generalized Einstein fluctuation-dissipation relation is also obtained for the time-averaged moments.

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Random-walk dynamics is one of the more simple nonequilibrium models that have been applied in diverse kinds of problems arising in physics, biology, economics, etc. In their standard Markovian formulation [1,2], the second moment of these diffusive processes grows linearly in time, a property shared by Brownian motion. Anomalous (sub and super) diffusive processes [3,4] depart from the linearity condition.

The temporal dependences of the moments of a random walk are defined from an ensemble of realizations. Nevertheless, single-particle tracking microscopy permits us to define the moments from an alternative temporal moving average performed with only one single trajectory [5–7]. From a physical point of view, this technique allows us to ask about the ergodic properties of a diffusion process, even when it does not have a stationary state.

In different tracking experiments performed with biophysical arrangements [7–10], it was found that the diffusion coefficient (which parametrizes the time-averaged second moment) becomes a random object that assumes different values for each realization. This distribution of diffusion coefficients renders the process *inhomogeneous* in the sense that in an ensemble of simple diffusers, each one has a different diffusion coefficient [11]. In addition to this feature, the time-averaged second moments are characterized by a subdiffusive behavior. Both properties lead to weak ergodicity breaking. That is, in contrast to strong ergodicity breaking, time and ensemble averages differ even when the system is able to visit the full available phase space. These striking experimental results can be captured through a continuous-time random-walk model with waiting time distributions characterized by power-law behaviors [11–13]. These results triggered the study of the ergodic properties of diverse anomalous diffusion processes [14–26] from a similar perspective.

The main goal of this paper is to explore whether the inhomogeneous property of a diffusion process (asymptotic randomness of the time-averaged moments) along with its associated weak ergodicity breaking [11,12] may also be

induced by the presence of strong memory effects in stochastic dynamics. Specifically, we are interested in globally correlated dynamics, where the walker transition depends on its whole previous history or trajectory.

It is known that globally correlated stochastic dynamics leads to anomalous diffusion processes [27–35]. On the other hand, we remark that the interplay between memory effects and weak ergodicity breaking was studied previously, such as, for example, in correlated continuous-time random-walk models [36,37], single-file diffusion [38], and fractional Brownian-Langevin motion [39]. Here, we consider a different kind of memory process. The model consists in a random walker whose transitions depend on the whole previous history of transitions. The right-left jump probabilities are defined by an urnlike mechanism [40–44], which does not fulfill the standard central limit theorem [44]. The ensemble dynamics becomes superdiffusive (ballistic). Furthermore, in contrast with other correlation mechanisms, here each realization is asymptotically equivalent to those of a biased Markovian walker but with (random) transition rates that assume different values for each realization. This property leads to random time averages and their associated ergodicity breaking.

We consider diffusive nonstationary dynamics (the statistics is not invariant under a time shift). Similarly to the case of continuous-time random walks (see, for example, Refs. [12] and [45]), the studied model yields statistical laws for ergodicity breaking that are different from those obtained from dynamics with a stationary state, case analyzed in Ref. [46]. In addition, here a generalized Einstein fluctuation-dissipation relation is established [12,47,48] for the time-averaged moments.

The paper is outlined as follows. In Sec. II, we introduce the stochastic dynamics that defines the globally correlated random walk. Its ensemble properties are studied through its characteristic function, which allows us to calculate its moments and probability evolution. In Sec. III, the time-averaged moments and the ergodic properties are analyzed. In Sec. IV, a generalized Einstein relation is obtained from the time-averaged moments. Section V is devoted to the

conclusions. Calculus details that support the main results are provided in the Appendixes.

II. GLOBAL CORRELATED RANDOM-WALK DYNAMICS

We consider a one-dimensional random walk where both the time and position coordinates are discrete. In each discrete time step ($t \rightarrow t + \delta t$), the walker perform a jump of length δx to the right or to the left. For simplicity, time is measured in units of δt . Then, $t = 0, 1, 2, \dots$. The stochastic position X_t at time t is

$$X_t = X_0 + \sum_{t'=1}^t \sigma_{t'}. \quad (1)$$

Here, X_0 is the initial position, and $\sigma_t = \pm \delta x$ is a random variable assigned to each step. The stochastic dynamics of the variables $\{\sigma_{t'}\}_{t'=1}^t$ is as follows. At $t = 1$ (first jump or transition), the two possible values are chosen with probability

$$P(\sigma_1 = \pm \delta x) = q_{\pm}, \quad (2)$$

where the weights satisfy $q_+ + q_- = 1$. The next values are determined by a conditional probability $\mathcal{T}(\sigma_1, \dots, \sigma_t | \sigma_{t+1})$ [49] that depends on the whole previous jump trajectory: $\sigma_1, \dots, \sigma_t$.

Different memory mechanisms can be introduced through $\mathcal{T}(\sigma_1, \dots, \sigma_t | \sigma_{t+1})$, such as, for example, in the elephant random-walk model [27–29]. Here, we analyze an alternative urnlike dynamics [46], where

$$\mathcal{T}(\sigma_1, \dots, \sigma_t | \sigma_{t+1} = \pm \delta x) = \frac{\lambda q_{\pm} + t_{\pm}}{t + \lambda}. \quad (3)$$

In this expression, λ is a positive free dimensionless parameter. Furthermore, t_+ and t_- are the number of times that the walker jumped (up to time t) to the right and to the left, respectively, $t = t_+ + t_-$. Hence, with probability $\lambda/(t + \lambda)$ the walker jumps to the right or to the left with weights q_+ and q_- , respectively. Complementarily, the jump is chosen in agreement with the weights $t_{\pm}/(t + \lambda)$, which gives the dependence of the dynamics over the whole previous jump trajectory.

Notice that in the limit $\lambda \rightarrow \infty$, independent random variables with probability q_{\pm} are obtained. Hence, the stochastic dynamics becomes an usual memoryless random walk. In the limit $\lambda \rightarrow 0$, the random variables σ_t assume the same value as σ_1 . Therefore, a deterministic behavior follows after the first jump.

Given the transition probability (3), the set of random variables $\{\sigma_t\}$ is interchangeable [44]. Therefore, their joint probability density is invariant under arbitrary permutation of its arguments. In consequence, the probability of the variables σ_t (jump length) is independent of t , $P(\sigma_t = \pm \delta x) = q_{\pm}$. The average jump length reads

$$\langle \sigma \rangle \equiv \int d\sigma P(\sigma) \sigma = \delta x (q_+ - q_-). \quad (4)$$

Then, for $q_+ \neq q_-$ a biased random walk is obtained, $\langle \sigma \rangle \neq 0$. The second jump moment is

$$\langle \sigma^2 \rangle \equiv \int d\sigma P(\sigma) \sigma^2 = \delta x^2. \quad (5)$$

Notice that both statistical moments are finite.

The initial condition X_0 along with the transition probability (3) completely define the stochastic dynamics. Below, we characterize its statistical properties.

A. Characteristic function

The stochastic process X_t can be described through

$$x_t \equiv X_t - X_0 = \sum_{t'=1}^t \sigma_{t'}, \quad (6)$$

which measures the departure with respect to the initial condition X_0 . Its characteristic function is defined by

$$Q_t(k) \equiv \langle \exp(ikx_t) \rangle. \quad (7)$$

Here, $\langle \dots \rangle$ denotes an average over an ensemble of realizations. A close recursive relation for $Q_t(k)$ can be obtained as follows. At time $t + 1$, it can be written as

$$Q_{t+1}(k) = \left\langle e^{ikx_t} \sum_{\sigma = \pm \delta x} \mathcal{T}(\sigma_1, \dots, \sigma_t | \sigma) e^{ik\sigma} \right\rangle. \quad (8)$$

Here, we take into account that the random variable σ_{t+1} is chosen in agreement with $\mathcal{T}(\sigma_1, \dots, \sigma_t | \sigma_{t+1})$. Notice that the average includes all possible random values of $\{\sigma_i\}_{i=1}^t$, which in turn define all possible realizations of x_t . From Eq. (3), we get

$$Q_{t+1}(k) = Q_t(k) \frac{\lambda}{t + \lambda} \sum_{\mu = \pm} q_{\mu} e^{ik\delta x_{\mu}} + \frac{1}{t + \lambda} \sum_{\mu = \pm} \langle e^{ikx_t} t_{\mu} \rangle e^{ik\delta x_{\mu}}, \quad (9)$$

where for shortening the expression we defined $\delta x_{\pm} \equiv \pm \delta x$. Given that $x_t = \delta x (t_+ - t_-)$, the derivative of the characteristic function (7) can be written as

$$\frac{d}{dk} Q_t(k) = i \delta x \langle e^{ikx_t} (t_+ - t_-) \rangle. \quad (10)$$

Hence, after writing $e^{ik\delta x_{\mu}} = \cos(k\delta x_{\mu}) + i \sin(k\delta x_{\mu})$, by using that $t = t_+ + t_-$ and $q_+ + q_- = 1$ [50], Eq. (9) straightforwardly leads to the closed recursive relation

$$Q_{t+1}(k) = \cos(k\delta x) Q_t(k) + \frac{1}{t + \lambda} \sin(k\delta x) \frac{1}{\delta x} \frac{d}{dk} Q_t(k) + i(q_+ - q_-) \frac{\lambda}{t + \lambda} \sin(k\delta x) Q_t(k). \quad (11)$$

This is the main result of this section. It completely characterizes the probability and moments of x_t .

We notice that in the limit $\lambda \rightarrow 0$, the characteristic function is $Q_t(k) = \langle \exp(ikt\sigma_1) \rangle = q_+ \exp(ikt\delta x) + q_- \exp(-ikt\delta x)$, which consistently satisfies Eq. (11) with $\lambda = 0$. In fact, after the first event, the next ones assume the same value, $x_t = t\sigma_1$ [see Eq. (3)]. In the limit $\lambda \rightarrow \infty$, the solution of Eq. (11) is $Q_t(k) = \langle \exp(ik\sigma_1) \rangle^t = [q_+ \exp(ik\delta x) + q_- \exp(-ik\delta x)]^t$, which corresponds to the characteristic function of a Markovian random walk where the steps σ_t are independent random variables.

B. Moments behavior

From the characteristic function $Q_t(k)$, the moments can be obtained by differentiation as

$$\langle x_t \rangle = -i \frac{d}{dk} Q_t(k) \Big|_{k=0}, \quad \langle x_t^2 \rangle = -\frac{d^2}{dk^2} Q_t(k) \Big|_{k=0}. \quad (12)$$

For the *first moment*, Eq. (11) leads to the recursive relation

$$\langle x_{t+1} \rangle = \langle x_t \rangle \left[1 + \frac{1}{t + \lambda} \right] + \frac{\lambda}{t + \lambda} \langle \sigma \rangle, \quad (13)$$

where the average jump length $\langle \sigma \rangle$ is given by Eq. (4). The solution of this equation is

$$\langle x_t \rangle = \langle \sigma \rangle t = \delta x (q_+ - q_-) t. \quad (14)$$

Hence, the bias induced by $(q_+ - q_-)$ leads to a linear increasing of $\langle x_t \rangle$.

For the *second moment*, it follows the recursive relation

$$\langle x_{t+1}^2 \rangle = \langle x_t^2 \rangle \left[1 + \frac{2}{t + \lambda} \right] + \frac{2\lambda}{t + \lambda} \langle x_t \rangle \langle \sigma \rangle + \langle \sigma^2 \rangle, \quad (15)$$

whose solution is given by

$$\langle x_t^2 \rangle = \frac{\langle \sigma^2 \rangle}{1 + \lambda} (t^2 + t\lambda) + \frac{\langle \sigma \rangle^2 \lambda}{1 + \lambda} (t^2 - t). \quad (16)$$

From Eqs. (14) and (16), the second centered moment reads

$$\langle x_t^2 \rangle - \langle x_t \rangle^2 = \left[\frac{\langle \sigma^2 \rangle - \langle \sigma \rangle^2}{1 + \lambda} \right] (t^2 + t\lambda). \quad (17)$$

Hence, the memory effects lead to a *superdiffusive* behavior, which in the asymptotic time regime becomes ballistic. The ballistic regime is valid at any time when $\lambda \rightarrow 0$. Consistently, in the limit $\lambda \rightarrow \infty$ (memoryless case) it follows that

$$\langle x_t^2 \rangle - \langle x_t \rangle^2 = [\langle \sigma^2 \rangle - \langle \sigma \rangle^2] t, \quad (18)$$

which corresponds to an expected standard diffusive behavior.

C. Probability evolution

After Fourier inversion, the characteristic function leads to a recursive relation for the probability $P_t(x)$ of x_t . We get [51]

$$P_{t+1}(x) = W_t^+ P_t(x - \delta x) + W_t^- P_t(x + \delta x), \quad (19)$$

where

$$W_t^\pm = \frac{1}{2} \left\{ 1 \pm \frac{1}{t + \lambda} \left[\left(\frac{x \mp \delta x}{\delta x} \right) + \lambda (q_+ - q_-) \right] \right\}. \quad (20)$$

The evolution (19), which is valid for $t \geq 1$, describes a hopping process with transitions W_t^\pm . In the limit $\lambda \rightarrow \infty$, it follows that $W_t^\pm = q_\pm$, recovering a standard random walk. For finite λ , the memory effects appear through W_t^\pm . Furthermore, for X_t the hopping also depends on the initial condition ($x \rightarrow X - X_0$), which is a non-Markovian property shared by the elephant random-walk model [27].

An interesting aspect of the evolution (19) is given by its *continuous limit*. It follows by taking the limits in which both the length jump ($\delta x \rightarrow 0$) and the time interval between jumps ($\delta t \rightarrow 0$) vanish. Then, we can approximate [for simplicity, the (dimensional) continuous time is also denoted by t]

$$P_t(x \mp \delta x) \rightarrow P_t(x) \mp \delta x \frac{\partial}{\partial x} P_t(x) + \frac{\delta x^2}{2} \frac{\partial^2}{\partial x^2} P_t(x), \quad (21)$$

along with

$$P_{t+1}(x) - P_t(x) \rightarrow \delta t \frac{\partial}{\partial t} P_t(x). \quad (22)$$

Introducing these approximations in Eq. (19), we obtain the equation

$$\begin{aligned} \frac{\partial}{\partial t} P_t(x) = & D \frac{\partial^2}{\partial x^2} P_t(x) - \frac{1}{t + t_\lambda} \frac{\partial}{\partial x} [x P_t(x)] \\ & - \frac{t_\lambda}{t + t_\lambda} V \frac{\partial}{\partial x} P_t(x), \end{aligned} \quad (23)$$

where the parameters are

$$D \equiv \frac{1}{2} \frac{\delta x^2}{\delta t}, \quad V \equiv (q_+ - q_-) \frac{\delta x}{\delta t}, \quad t_\lambda \equiv \lambda \delta t. \quad (24)$$

The Fokker-Planck equation (23) corresponds to a Brownian particle driven by a harmonic potential with spring constant $1/(t + t_\lambda)$. A similar result was obtained in Ref. [27] for the elephant random-walk model.

In the limit $\lambda \rightarrow \infty$, Eq. (23) becomes

$$\frac{\partial}{\partial t} P_t(x) = D \frac{\partial^2}{\partial x^2} P_t(x) - V \frac{\partial}{\partial x} P_t(x). \quad (25)$$

Consistently, this equation corresponds to the probability evolution of a Brownian particle with diffusion coefficient D and subjected to a constant force proportional to V .

The evolution Eq. (23) also leads to a superdiffusive ballistic process. Its solution can be written as [$P_{t=0}(x) = \delta(x)$]

$$P_t(x) = \sqrt{\frac{1}{2\pi\sigma_t^2}} \exp \left[-\frac{(x - Vt)^2}{2\sigma_t^2} \right], \quad \sigma_t^2 \equiv 2 \frac{D}{t_\lambda} t(t + t_\lambda). \quad (26)$$

Hence, the (time-dependent) harmonic potential is unable to induce a (time-independent) stationary state. In the limit $\lambda \rightarrow 0$, the previous solution reads $P_t(x) = \delta(x - Vt)$.

III. INHOMOGENEOUS DIFFUSION AND ERGODICITY BREAKING

The ergodic properties of a time series $X(t)$ associated with an arbitrary random walker can be analyzed through the *time-averaged moments* [11,12], which are defined by the following temporal moving average:

$$\delta_\kappa(t, \Delta) \equiv \frac{\int_0^{t-\Delta} dt' [X(t' + \Delta) - X(t')]^\kappa}{t - \Delta}. \quad (27)$$

Here, Δ is called the lag (or delay) time, and κ is a natural number, $\kappa = 1, 2, \dots$.

For *ergodic diffusion processes*, in the limit of increasing times, $\delta_\kappa(t, \Delta)$ recovers the ensemble behavior of the corresponding moments, that is,

$$\delta_\kappa(\Delta) \equiv \lim_{t \rightarrow \infty} \delta_\kappa(t, \Delta) = \langle [X(\Delta) - X(0)]^\kappa \rangle. \quad (28)$$

Here, the initial condition $X(0)$ follows from the translational invariance of Eq. (27). A weaker condition can be formulated by demanding the equality of the asymptotic behaviors ($\Delta \rightarrow \infty$) of both terms in Eq. (28).

Nonergodic processes do not fulfill Eq. (28). In particular, inhomogeneous diffusion corresponds to the case in which $\delta_\kappa(t, \Delta)$, even in the long-time limit, becomes a random object

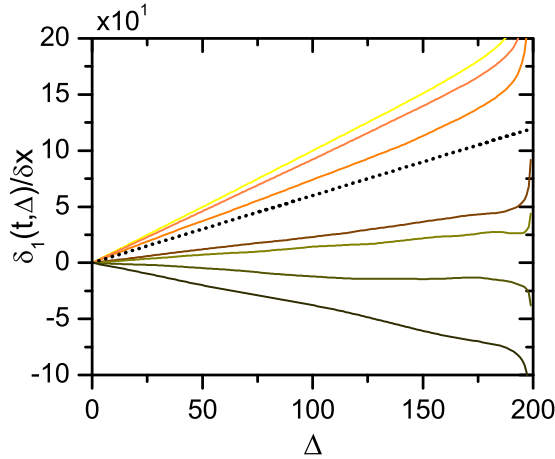


FIG. 1. Different realizations (full lines) of the first time-averaged moment $\delta_1(t, \Delta)$ [Eq. (27)] corresponding to the globally correlated random-walk dynamics defined by Eq. (3). The parameters are $\lambda = 2$, $q_+ = 0.8$, $q_- = 0.2$, and $t = 200$. The dotted (black) line corresponds to the analytical expression (34), which gives the ensemble mean value.

that assumes different values for each particular realization. Below we study the time-averaged moments $\delta_k(t, \Delta)$ for the random walk introduced in the previous section.

A. Asymptotic randomness

For the proposed model, given that the permanence time in each state is finite, a central ingredient that determines its ergodic properties is the asymptotic behavior ($\lim_{t \rightarrow \infty}$) of the transition probability $\mathcal{T}(\sigma_1, \dots, \sigma_t | \sigma_{t+1} = \pm \delta x)$. For the urn model, Eq. (3), it is known that it converges to random values f_{\pm} [43,46], that is,

$$\lim_{t \rightarrow \infty} \mathcal{T}(\sigma_1, \dots, \sigma_t | \sigma_{t+1} = \pm \delta x) = f_{\pm}, \quad (29)$$

where $0 \leq f_{\pm} \leq 1$ and $f_+ + f_- = 1$. In each particular realization, f_{\pm} assume different random values. Their probability density $\mathcal{P}(f_{\pm})$ is a β distribution [43,46]

$$\mathcal{P}(f_{\pm}) = \frac{\Gamma(\lambda)}{\Gamma(\lambda_+) \Gamma(\lambda_-)} f_+^{\lambda_+ - 1} f_-^{\lambda_- - 1}, \quad (30)$$

where $\lambda_{\pm} \equiv \lambda q_{\pm}$, and $\Gamma(x)$ is the Gamma function. For clarity, these results are rederived in Appendix A. The average over realizations of f_{\pm} is $\langle f_{\pm} \rangle = \int_0^1 df_+ \mathcal{P}(f_{\pm}) f_{\pm} = q_{\pm}$. For alternative memory mechanisms, such as that associated with the elephant random-walk model [27–29], the previous randomness is absent [46].

The convergence of the transition probability to random values leads straightforwardly to an inhomogeneous diffusion process. In fact, each realization becomes equivalent to that of a biased Markovian random-walk process with transition rates f_{\pm} . The bias arises because (even when $q_+ = q_-$) in general $f_+ \neq f_-$.

In the limit $\lambda \rightarrow \infty$, from Eq. (30) it follows that $\mathcal{P}(f_{\pm}) = \delta(f_{\pm} - q_{\pm})$, implying that the fractions f_{\pm} , at any stage of the diffusion process, assume deterministically the values q_{\pm} . This case corresponds to the absence of memory and leads to a standard diffusion process [defined by Eq. (18)].

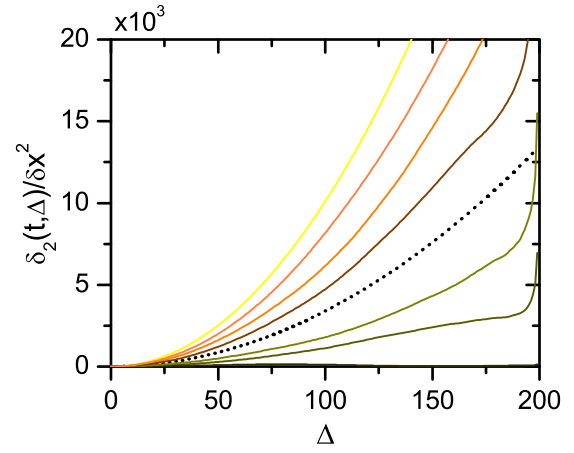


FIG. 2. Different realizations (full lines) of the second time-averaged moment $\delta_2(t, \Delta)$ [Eq. (27)] corresponding to an unbiased globally correlated random-walk dynamics. The parameters are $\lambda = 2$, $q_+ = q_- = 1/2$, and $t = 200$. The dotted (black) line corresponds to the analytical expression (35), which gives their ensemble mean value.

The asymptotic property (29) implies that at large times the time-averaged moment $\delta_k(\Delta) = \lim_{t \rightarrow \infty} \delta_k(t, \Delta)$ becomes a random variable. In fact, its average over realizations can be written as

$$\langle \delta_k(\Delta) \rangle = \langle \delta_k(\Delta, f_{\pm}) \rangle = \int_0^1 df_+ \mathcal{P}(f_{\pm}) \delta_k(\Delta, f_{\pm}). \quad (31)$$

In this expression, $\delta_k(\Delta, f_{\pm})$ corresponds to the (asymptotic) time-averaged moment corresponding to a memoryless random walk with transition rate $\mathcal{T}(\sigma_1, \dots, \sigma_t | \sigma_{t+1} = \pm \delta x) = f_{\pm}$. Given the ergodicity of this kind of dynamics, under the replacements $q_{\pm} \rightarrow f_{\pm}$, $t \rightarrow \Delta$, from Eqs. (28) and (14) we get

$$\delta_1(\Delta, f_{\pm}) = \Delta \delta x (f_+ - f_-). \quad (32)$$

Similarly, taking the limit $\lambda \rightarrow \infty$ (memoryless case) and under the same replacements, from Eq. (16) we get

$$\delta_2(\Delta, f_{\pm}) = \delta x^2 \{ (f_+ - f_-)^2 \Delta^2 + [1 - (f_+ - f_-)^2] \Delta \}. \quad (33)$$

Equations (32) and (33) define the random values (written in terms of f_{\pm}) that assume the time-averaged moments (27) in the long-time limit. To check these results, in Fig. 1 we plot $\delta_1(t, \Delta)$ for the global correlated random walk defined by Eq. (3). From each generated realization, $\delta_1(t, \Delta)$ is obtained from its definition [Eq. (27)]. Consistent with the analysis, each curve (for $\Delta < t$) can be very well fitted by the approximation (32), that is, a linear behavior in Δ is observed.

In Fig. 2, for an unbiased random walk ($q_+ = q_-$), we plot different realizations corresponding to the second time-averaged moment $\delta_2(t, \Delta)$. Consistent with Eq. (33), a quadratic behavior is observed for $\Delta < t$.

For both $\delta_1(t, \Delta)$ and $\delta_2(t, \Delta)$, the behaviors predicted by Eqs. (32) and (33) lose their validity when $\Delta \approx t$. In fact, in both figures an appreciable deviation can be observed in that regime. The fraction of (lag) time Δ over which that happens diminishes for increasing t .

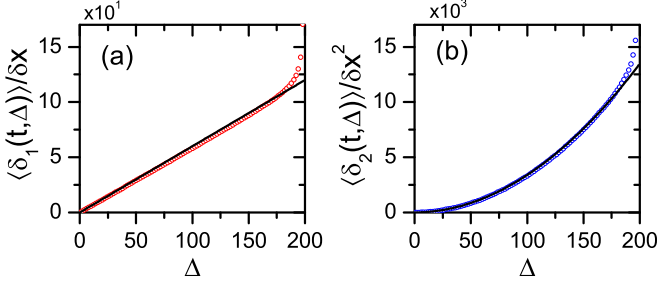


FIG. 3. Average over realizations of the first (a) and second (b) time-averaged moments $\delta_1(t, \Delta)$ and $\delta_2(t, \Delta)$. The parameters are the same as in Figs. 1 and 2, respectively. The circles correspond to a numerical average performed with 10^3 realizations. The full lines correspond to Eqs. (34) and (35), respectively.

B. Ergodicity in mean value

The previous figures explicitly show that, contrary to ergodic dynamics, here the memory effects lead to a randomness of the time-averaged moments. Their average over an ensemble of realizations can be performed by using the probability distribution (30). Using that $\langle f_{\pm} \rangle = \int_0^1 df_+ \mathcal{P}(f_{\pm}) f_{\pm} = q_{\pm}$, Eq. (32) leads to

$$\langle \delta_1(\Delta) \rangle = \Delta \langle \sigma \rangle. \quad (34)$$

Furthermore, using that $\langle (f_+ - f_-)^2 \rangle = [1 + \lambda(q_+ - q_-)^2] / (1 + \lambda)$, from Eq. (33) it follows that

$$\langle \delta_2(\Delta) \rangle = \frac{\langle \sigma^2 \rangle}{1 + \lambda} (\Delta^2 + \Delta \lambda) + \frac{\langle \sigma \rangle^2 \lambda}{1 + \lambda} (\Delta^2 - \Delta). \quad (35)$$

The last two expressions, under the replacement $\Delta \rightarrow t$, recover Eqs. (14) and (16), respectively. Thus, the first two moments satisfy the ergodicity condition (28) only when averaged over realizations. The validity of both results, Eqs. (34) and (35), was checked numerically. In Fig. 3, the solid black lines are defined by these equations, while the circles correspond to an average over realizations, such as those shown in Figs. 1 and 2.

Interestingly, the previous property is also valid for higher time-averaged moments,

$$\langle \delta_{\kappa}(\Delta) \rangle = \lim_{t \rightarrow \infty} \langle \delta_{\kappa}(t, \Delta) \rangle = \langle [X(t) - X(0)]^{\kappa} \rangle_{t=\Delta}. \quad (36)$$

Thus, in terms of the characteristic function (7), they can be written as

$$\langle \delta_{\kappa}(\Delta) \rangle = i^{-\kappa} \frac{d^{\kappa}}{dk^{\kappa}} Q_{\Delta}(k) \Big|_{k=0}. \quad (37)$$

The equality (36) is demonstrated in Appendix B. We notice that for an arbitrary stochastic signal $X(t)$ we may consider the equality (36) as a definition of ergodicity in mean value.

C. Probability densities

While the asymptotic value $\delta_{\kappa}(\Delta) = \lim_{t \rightarrow \infty} \delta_{\kappa}(t, \Delta)$ of the time-averaged moments is random, Eq. (36) shows that their average over realizations recovers the ensemble behavior. Therefore, we can affirm that the random walker is ergodic on average. The lack of ergodicity is given by the random nature of $\delta_{\kappa}(\Delta)$. In fact, higher moments $\langle [\delta_{\kappa}(\Delta)]^n \rangle$ ($n \geq 2$) cannot

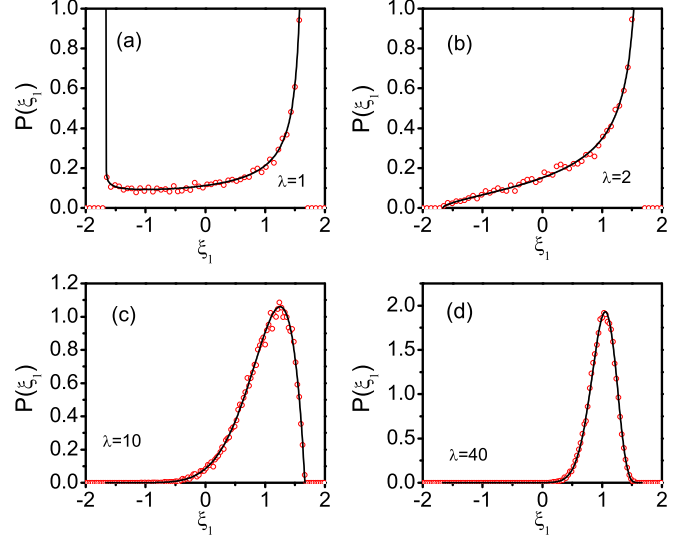


FIG. 4. Probability density $P(\xi_1)$ corresponding to the normalized first time-averaged moment, Eq. (38), with $\kappa = 1$. The full lines correspond to the analytical result [Eq. (41)]. The circles correspond to a numerical simulations with 10^4 realizations. The parameters are $q_+ = 0.8$, $q_- = 0.2$, $\Delta = 100$, and $t = 1000$. (a) $\lambda = 1$, (b) $\lambda = 2$, (c) $\lambda = 10$, and (d) $\lambda = 40$.

be related with the ensemble behavior. To characterize the lack of ergodicity, we introduce the *normalized (asymptotic) time-averaged moments*

$$\xi_{\kappa} \equiv \lim_{t \rightarrow \infty} \frac{\delta_{\kappa}(t, \Delta)}{\langle \delta_{\kappa}(t, \Delta) \rangle} = \frac{\delta_{\kappa}(\Delta, f_{\pm})}{\langle \delta_{\kappa}(\Delta) \rangle}, \quad (38)$$

their probability density being denoted by $P(\xi_{\kappa})$. Ergodicity in probability density corresponds to the absence of randomness,

$$P(\xi_{\kappa}) = \delta(\xi_{\kappa} - 1). \quad (39)$$

For $\kappa = 1$, from Eqs. (32) and (34) we get

$$\xi_1 = \frac{(f_+ - f_-)}{(q_+ - q_-)}, \quad (40)$$

which is a random variable independent of Δ . It characterizes the asymptotic (random) bias of the globally correlated random walk. Its probability distribution from Eq. (30) reads

$$P(\xi_1) = \frac{1}{\mathcal{N}} |\delta q| (1 + \delta q \xi_1)^{\lambda_+ - 1} (1 - \delta q \xi_1)^{\lambda_- - 1}. \quad (41)$$

Here, $\delta q \equiv q_+ - q_-$, and as before $\lambda_{\pm} = \lambda q_{\pm}$. The normalization constant is $\mathcal{N} = 2^{\lambda-1} \Gamma(\lambda_+) \Gamma(\lambda_-) / \Gamma(\lambda)$. The density has support in the interval defined by $|\xi_1| \leq 1/|\delta q|$, and consistently with the definition (38) it satisfies $\langle \xi_1 \rangle = \int_{-1/|\delta q|}^{+1/|\delta q|} P(\xi_1) \xi_1 d\xi_1 = 1$. Furthermore, for $\lambda < \infty$ it departs from Eq. (39).

In Fig. 4 we plot a set of probability densities $P(\xi_1)$ along with their numerical versions. They were determinate from a set of realizations such as those shown in Fig. 1. The analytical expressions fit very well the numerical results. Depending on the memory parameter λ , the density develops very different dependences. For increasing λ , the density is peaked around 1

[see Fig. 4(d)], which indicates that the ergodic regime is approached.

The second normalized moment [$\kappa = 2$ in Eq. (38)] from Eq. (33) can be written as

$$\xi_2 = a(f_+ - f_-)^2 + b, \quad (42)$$

where a and b are functions that also follow from Eq. (33) and only depend on Δ and λ . From Eq. (30) we get the probability density

$$P(\xi_2) = \frac{1}{\mathcal{N}} \frac{1}{|a|} \sqrt{\frac{a}{\xi_2 - b}} \left(1 - \frac{\xi_2 - b}{a}\right)^{\frac{\lambda}{2} - 1}. \quad (43)$$

The variable ξ_2 takes values in the interval $(b, a + b)$. Consistent with Eq. (38), it satisfies $\langle \xi_2 \rangle = \int_b^{a+b} P(\xi_2) \xi_2 d\xi_2 = b + a/(1 + \lambda) = 1$.

For an unbiased random walk, $q_+ = q_- = 1/2$, we obtain $\mathcal{N} = 2^{\lambda-1} \Gamma^2(\lambda/2)/[\Gamma(\lambda)]$, while from Eq. (35) it follows that

$$a = \frac{(\Delta - 1)(1 + \lambda)}{\Delta + \lambda}, \quad b = \frac{1 + \lambda}{\Delta + \lambda}, \quad (44)$$

which satisfy the previous condition $b + a/(1 + \lambda) = 1$.

In the limit $\lambda \rightarrow \infty$ (with finite Δ), the density $P(\xi_2)$ becomes a δ Dirac function,

$$\lim_{\lambda \rightarrow \infty} P(\xi_2) = \delta(\xi_2 - 1), \quad (45)$$

which corresponds to the ergodic regime. This results follow straightforwardly from Eqs. (42) and (30). On the other hand, in the limit $\Delta \rightarrow \infty$ (with finite λ), the parameter a goes to $1 + \lambda$ while b vanishes. Hence,

$$\lim_{\Delta \rightarrow \infty} P(\xi_2) = \frac{1}{\mathcal{N}} \sqrt{\frac{1}{(1 + \lambda)\xi_2}} \left[1 - \frac{\xi_2}{1 + \lambda}\right]^{\frac{\lambda}{2} - 1}. \quad (46)$$

From here, it is simple to prove that both kinds of limits do not commute,

$$\lim_{\Delta \rightarrow \infty} \lim_{\lambda \rightarrow \infty} P(\xi_2) \neq \lim_{\lambda \rightarrow \infty} \lim_{\Delta \rightarrow \infty} P(\xi_2). \quad (47)$$

In fact,

$$\lim_{\Delta \rightarrow \infty} \lim_{\lambda \rightarrow \infty} P(\xi_2) = \delta(\xi_2 - 1), \quad (48)$$

while from Eq. (46) we get the Gamma density,

$$\lim_{\lambda \rightarrow \infty} \lim_{\Delta \rightarrow \infty} P(\xi_2) = \sqrt{\frac{1}{2\pi\xi_2}} \exp\left[-\frac{\xi_2}{2}\right]. \quad (49)$$

In spite of this difference, notice that the previous two probability densities lead to $\langle \xi_2 \rangle = 1$.

To check the previous results, in Fig. 5 we plot $P(\xi_2)$ obtained numerically from a set of realizations such as those shown in Fig. 2. For $\lambda \lesssim 1$, the distribution assumes a U -like form [Fig. 5(a)]. For higher values of λ , added to the power-law behavior predicted by Eq. (43) [Fig. 5(b)], $P(\xi_2)$ approaches a delta Dirac function [Fig. 5(c)] centered in $\xi_2 = 1$ [Eq. (45)]. When $\Delta \gg \lambda$, the distribution approaches the limit defined by Eq. (46), Fig. 5(d), which in the scale of the plot is almost indistinguishable from the behavior (49). Therefore, Figs. 5(c) and 5(d) explicitly show the fact that in general the ergodic limit and the limit of infinite delay times do not commute for the normalized moments.

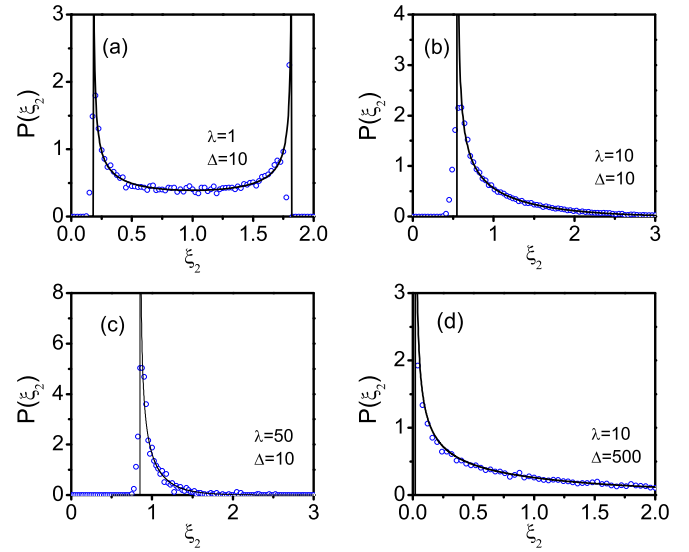


FIG. 5. Probability density $P(\xi_2)$ corresponding to the normalized second time-averaged moment, Eq. (38), with $\kappa = 2$. The full lines correspond to the analytical result [Eq. (43)]. The circles correspond to a numerical simulations with 5×10^4 realizations. The parameters are $q_+ = q_- = 1/2$ and $t = 1000$. (a) $\lambda = 1$, $\Delta = 10$; (b) $\lambda = 2$, $\Delta = 10$; (c) $\lambda = 10$, $\Delta = 10$; and (d) $\lambda = 40$, $\Delta = 500$.

D. Correlations between time-averaged moments

In the previous section, we characterized the probability densities of the asymptotic first and second time-averaged moments. It is interesting to note that these objects are correlated between them. In fact, from Eqs. (32) and (33) it is possible to obtain the relation $\delta_2(\Delta, f_{\pm}) = [\delta_1(\Delta, f_{\pm})]^2 (1 - 1/\Delta) + \delta x^2 \Delta$, which implies that

$$\lim_{t \rightarrow \infty} \delta_2(t, \Delta) = \lim_{t \rightarrow \infty} [\delta_1(t, \Delta)]^2 \left(1 - \frac{1}{\Delta}\right) + \delta x^2 \Delta. \quad (50)$$

Therefore, in the long-time limit, the realizations of $\delta_1(t, \Delta)$ and $\delta_2(t, \Delta)$ become proportional. The realizations shown in Figs. 1 and 2 are consistent with this relation, which is strictly valid in the limit $t \rightarrow \infty$. In spite of this fact, due to their different scaling with Δ , in the long-time regime their probability densities develop very different behaviors [see Eqs. (41) and (47)]. Relations such as that defined by Eq. (50) also appear in higher time-averaged moments. In fact, for all of them, their asymptotic behavior can always be written in terms of the random variables f_{\pm} .

IV. GENERALIZED EINSTEIN RELATION

The diffusion coefficient of a normal random-walk process can be related to its mobility. This last coefficient gives the proportionality between the force and the average velocity of the walker when submitted to an external field. This is the well-known Einstein (fluctuation-dissipation) relation [1–3]. For the present model, it is not possible to establish a similar relation in terms of the ensemble behavior. In fact, the different time dependences of the first two moments [see Eqs. (14) and (17)] confirm this limitation. Given the ergodicity in mean value defined by Eq. (36), the same drawback applies to the

asymptotic time-averaged moments. Nevertheless, from the correlation defined by Eq. (50) we realize that such a relation can be obtained by introducing a centered (second) time-averaged moment (second time-averaged cumulant), defined as

$$\delta_2^*(t, \Delta) \equiv \delta_2(t, \Delta) - [\delta_1(t, \Delta)]^2. \quad (51)$$

Here, $\delta_\kappa(t, \Delta)$ ($\kappa = 1, 2$) are the usual time-averaged moments [Eq. (27)]. Denoting its asymptotic value as

$$\delta_2^*(\Delta) \equiv \lim_{t \rightarrow \infty} \delta_2^*(t, \Delta), \quad (52)$$

its average over an ensemble of realizations can be written as

$$\langle \delta_2^*(\Delta) \rangle = \langle \delta_2^*(\Delta, f_\pm) \rangle, \quad (53)$$

where $\delta_2^*(\Delta, f_\pm)$ from Eqs. (32) and (33) reads

$$\delta_2^*(\Delta, f_\pm) = \delta x^2 [1 - (f_+ - f_-)^2] \Delta. \quad (54)$$

In contrast to $\delta_2(\Delta, f_\pm)$ [Eq. (33)], here a linear dependence with Δ is obtained. Similarly, using that $\langle (f_+ - f_-)^2 \rangle = [1 + \lambda(q_+ - q_-)^2]/(1 + \lambda)$, the average over realizations becomes

$$\langle \delta_2^*(\Delta) \rangle = \delta x^2 \frac{\lambda}{1 + \lambda} [1 - (q_+ - q_-)^2] \Delta. \quad (55)$$

The case $q_+ = q_-$ and $q_+ \neq q_-$ define the unforced and forced (driven) dynamics, respectively. Taking a dimensional delay time ($\Delta \rightarrow \Delta/\delta t$), from the previous expression and Eq. (34) it follows that

$$\langle \delta_2^*(\Delta) \rangle_{q_+ = q_-} = 2D_* \Delta, \quad \langle \delta_1(\Delta) \rangle_{q_+ \neq q_-} = V \Delta, \quad (56)$$

where the (average) diffusion and (average) velocity coefficients are [compare with Eq. (24)]

$$D_* \equiv \frac{1}{2} \frac{\delta x^2}{\delta t} \frac{\lambda}{1 + \lambda}, \quad V \equiv \frac{\delta x}{\delta t} (q_+ - q_-). \quad (57)$$

They can be related as

$$D_* = \frac{\lambda}{1 + \lambda} \frac{\delta x}{2} \frac{V}{(q_+ - q_-)}, \quad (58)$$

which defines an Einstein-like relation. In fact, it relates the diffusion coefficient corresponding to the centered (second) time-averaged moment of the unforced dynamics with the velocity of the first time-averaged moment for the forced case [Eq. (56)].

The standard Einstein relation involves a thermodynamic temperature [1–3]. Here, this dependence can be introduced by assuming that the probabilities q_\pm are given by a Boltzmann exponential factor (activated process) $q_\pm = \exp[\pm \delta x F / 2kT] / Z$ [3], where F is the external force, T is the temperature, k is the Boltzmann constant, while Z guarantees the normalization $q_+ + q_- = 1$. Thus,

$$q_+ - q_- = \tanh \left[\frac{\delta x F}{2kT} \right]. \quad (59)$$

In the limit $F \rightarrow 0$, Eqs. (58) and (59) lead to

$$D_* = \frac{\lambda}{1 + \lambda} kT \left(\frac{V}{F} \right). \quad (60)$$

In the limit $\lambda \rightarrow \infty$, we obtain the standard Einstein relation [see, for example, Eq. (5.3) in Ref. [3]]. In fact, V/F is the

(average) mobility. For finite λ , the standard result is modified by the memory of the dynamics, which introduces the factor $\lambda/(1 + \lambda)$. Furthermore, notice that the generalized relation (60) does not characterize the ensemble dynamics. In fact, it can only be established in terms of the time-averaged moments [Eq. (56)], which satisfy

$$\langle \delta_1(\Delta) \rangle_{q_+ \neq q_-} = \frac{1 + \lambda}{\lambda} \frac{(q_+ - q_-)}{\delta x} \langle \delta_2^*(\Delta) \rangle_{q_+ = q_-}. \quad (61)$$

From Eq. (59) this relation can be written as ($F \rightarrow 0$)

$$\langle \delta_1(\Delta) \rangle_{F \neq 0} = \frac{1 + \lambda}{\lambda} \frac{F}{2kT} \langle \delta_2^*(\Delta) \rangle_{F=0}. \quad (62)$$

A similar property was also found for subdiffusive continuous-time random-walk models [12] and others anomalous diffusion processes [47,48].

V. SUMMARY AND CONCLUSIONS

We introduced a discrete random-walk model driven by global memory effects, where each walker step depends on the previous number of performed left-right transitions [Eq. (3)]. After obtaining a recursive relation for its characteristic function, we obtained its first moments. Given that the memory mechanism may induce a bias, the first moment has a linear dependence with time [Eq. (14)]. The second moment, event in the absence of bias, develops a superdiffusive ballistic behavior [Eq. (16)]. In a continuous time-space limit, the probability density is governed by a (non-Markovian) local in-time Fokker-Planck equation [Eq. (23)], being defined by an effective harmonic-oscillator potential with a strength constant inversely proportional to the elapsed time.

In the long-time regime, each realization is equivalent to that of a biased Markovian walker with transitions rates that differs from realization to realization. This kind of asymptotic inhomogeneous diffusion is induced by the memory effects. Consequently, and similarly to the case of subdiffusive continuous-time random walks, the time-averaged moments [Eq. (27)] become random objects (Figs. 1 and 2) with a time-independent statistics. Their average over realizations recovers the ensemble behavior obtained from the characteristic function (Fig. 3). Nevertheless, due to their intrinsic randomness, characterized through their probability densities (Figs. 4 and 5), the diffusion process is nonergodic. For the second-averaged moment, we find that the ergodic limit and the limit of large delay times do not commute [Eq. (47)]. Added to their randomness, we showed that in general the time-averaged moments are correlated between all of them.

Due to the different time dependences of the first and second moments, it is not possible to establish an Einstein-like relation for the ensemble dynamics. Nevertheless, we showed that a generalized relation can be formulated after introducing a centered (second) time-averaged moment (second time-averaged cumulant) [Eq. (51)]. In contrast with the standard result, the relation between the corresponding (average) diffusion and (average) mobility coefficients is modified by the memory control parameter [Eqs. (58) and (60)].

The present results, as well as the analyses performed in Refs. [36–39], confirm that different kinds of memory processes may lead to weak ergodicity breaking, in

particular that characterized by random time-averaged moments (inhomogeneous diffusion). It is expected that the same kind of results arise in continuous (time and space) random-walk models with finite residence times and finite average jump lengths. On the other hand, conditions that guarantee that a memory mechanism leads (or not) to ergodicity breaking are not known. General criteria for solving this issue, as well as the interplay between global memory effects and divergent residence times, jointly with the validity of the Einstein relation, are interesting questions that emerge from the present analysis.

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APPENDIX A: PROBABILITY DENSITY OF THE ASYMPTOTIC TRANSITION PROBABILITIES

Here, we derive the probability density (30) of the asymptotic transition probabilities, $f_{\pm} = \lim_{t \rightarrow \infty} \mathcal{T}(\sigma_1, \dots, \sigma_t | \sigma_{t+1} = \pm \delta x)$ [Eq. (29)].

The joint probability $P(\sigma_1, \dots, \sigma_t)$ of obtaining the random values $\sigma_1, \dots, \sigma_t$ by using Bayes rule can be written as

$$P(\sigma_1, \dots, \sigma_t) = P(\sigma_1) \mathcal{T}(\sigma_1 | \sigma_2) \cdots \mathcal{T}(\sigma_t | \sigma_{t+1}). \quad (\text{A1})$$

Given the transition probability Eq. (3), it is simple to check that $P(\sigma_1, \dots, \sigma_t)$ only depends on the number of times t_{\pm} that the values $\pm \delta x$ were chosen. From this interchangeability property, the probability $P_t(t_+, t_-)$ of getting t_{\pm} times the values $\pm \delta x$ after t steps ($t = t_+ + t_-$) can be written as

$$P_t(t_+, t_-) = \frac{t!}{t_+! t_-!} \frac{\Gamma(\lambda)}{\Gamma(t + \lambda)} \frac{\Gamma(t_+ + \lambda_+)}{\Gamma(\lambda_+)} \frac{\Gamma(t_- + \lambda_-)}{\Gamma(\lambda_-)}, \quad (\text{A2})$$

where the property $\Gamma(n + x)/\Gamma(x) = x(1 + x)(2 + x) \cdots (n - 1 + x)$ was used. The combinatorial factor takes into account all realizations with the same numbers t_{\pm} .

In the limit $x \rightarrow \infty$, the Stirling approximation $\Gamma(x) \approx \sqrt{2\pi/x} e^{-x} x^x$, which in the same limit leads to $\Gamma(x + \alpha)/\Gamma(x) \approx x^{\alpha}$, is valid. Using that $n! = \Gamma(n + 1)$, and applying the previous approximations to Eq. (A2), in the limit $t \rightarrow \infty$ it follows that

$$P_t(t_+, t_-) \approx \frac{\Gamma(\lambda)}{t^{\lambda-1}} \frac{t_+^{\lambda_+-1}}{\Gamma(\lambda_+)} \frac{t_-^{\lambda_--1}}{\Gamma(\lambda_-)}. \quad (\text{A3})$$

By performing the change of variables $t_{\pm} \rightarrow t f_{\pm}$, and by using the fact that, due to normalization $t = t_+ + t_-$ there is only one

independent variable ($f_+ + f_- = 1$), the previous expression leads straightforwardly to the β distribution Eq. (30).

APPENDIX B: ERGODICITY IN MEAN VALUE

Here, we demonstrate the validity of Eqs. (36) and (37). Their fulfillment implies that the random walk is ergodic in mean value. The demonstration is closely related to the de Finetti representation theorem for dichotomic variables [40,44]. In the present context, we notice that the probability $P_t(t_+, t_-)$ [Eq. (A2)] can be written as

$$P_t(t_+, t_-) = \int_0^1 df_+ \mathcal{P}(f_{\pm}) P_t(t_+, t_-, f_{\pm}). \quad (\text{B1})$$

Here, $\mathcal{P}(f_{\pm})$ is given by Eq. (30) while $P_t(t_+, t_-, f_{\pm})$ is the counting probability for independent variables $\sigma_i = \pm \delta x$ with transition probability $\mathcal{T}(\sigma_1, \dots, \sigma_t | \sigma_{t+1} = \pm \delta x) = f_{\pm}$. Therefore, it is

$$P_t(t_+, t_-, f_{\pm}) \equiv \frac{t!}{t_+! t_-!} f_+^{t_+} f_-^{t_-}. \quad (\text{B2})$$

Given that the characteristic function $Q_t(k)$ [Eq. (7)] can be written as

$$Q_t(k) = \sum_{t_{\pm}=0}^t P_t(t_+, t_-) \exp[ik\delta x(t_+ - t_-)], \quad (\text{B3})$$

where $t_+ + t_- = t$, Eq. (B1) allows us to write $Q_t(k)$ as an average over the variables f_{\pm} ,

$$Q_t(k) = \int_0^1 df_+ \mathcal{P}(f_{\pm}) Q_t(k, f_{\pm}), \quad (\text{B4})$$

where $Q_t(k, f_{\pm})$ is the characteristic function for independent variables with transition probabilities f_{\pm} ,

$$Q_t(k, f_{\pm}) = [f_+ e^{+ik\delta x} + f_- e^{-ik\delta x}]^t. \quad (\text{B5})$$

Given that *asymptotically* the realizations of the random walk converge to that of a memoryless process with transition rate $\mathcal{T}(\sigma_1, \dots, \sigma_t | \sigma_{t+1}) = f_{\pm}$ [Eq. (29)], in each realization the (asymptotic) statistics of $[x(t' + \Delta) - x(t')]$, which define the integral defining $\delta_{\kappa}(t, \Delta)$ [Eq. (27)], does not depend on t and is defined by Eq. (B5) under the replacement $t \rightarrow \Delta$. The relation Eq. (37) is a straightforward consequence on this result and Eq. (B4).

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- [49] Consistently with the notation of Ref. [46], here $\mathcal{T}(A|B)$ denotes the conditional probability of B given A .
- [50] The sum contributions in Eq. (9) can be rewritten as $\sum_{\mu=\pm} q_{\mu} e^{ik\delta x_{\mu}} = \cos(k\delta x) + i(q_{+} - q_{-}) \sin(k\delta x)$, and as $\sum_{\mu=\pm} \langle e^{ikx_{\mu}} t_{\mu} \rangle e^{ik\delta x_{\mu}} = t Q_t(k) \cos(k\delta x) + i \langle e^{ikx_{\mu}} (t_{+} - t_{-}) \rangle \sin(k\delta x)$.
- [51] We used that, given the Fourier transform $\tilde{f}(k) = \cos(ka) f(k)$, then $\tilde{f}(x) = [f(x-a) + f(x+a)]/2$. When $\tilde{f}(k) = i \sin(ka) f(k)$, it follows that $\tilde{f}(x) = [f(x-a) - f(x+a)]/2$. If $\tilde{f}(k) = \frac{\sin(ka)}{a} \frac{df(k)}{dk}$, then $\tilde{f}(x) = \frac{(x-a)}{2a} f(x-a) - \frac{(x+a)}{2a} f(x+a)$.