# Correlated continuous-time random walks in external force fields

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We study the anomalous diffusion of a particle in an external force field whose motion is governed by nonrenewal continuous time random walks with correlated waiting times. In this model the current waiting time $T_i$ is equal to the previous waiting time $T_{i-1}$ plus a small increment. Based on the associated coupled Langevin equations the force field is systematically introduced. We show that in a confining potential the relaxation dynamics follows power-law or stretched exponential pattern, depending on the model parameters. The process obeys a generalized Einstein-Stokes-Smoluchowski relation and observes the second Einstein relation. The stationary solution is of Boltzmann-Gibbs form. The case of an harmonic potential is discussed in some detail. We also show that the process exhibits aging and ergodicity breaking.

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## I. INTRODUCTION

Over recent years, the physics community has shown growing interest in anomalous diffusion. A particularly important class are subdiffusion processes, characterized in terms of the mean-squared displacement (MSD) [1]:

$$\langle x^2(t)\rangle \simeq K_\gamma t^\gamma, \quad 0<\gamma<1. \tag{1}$$

Subdiffusion has been observed in a large variety of systems, starting with the seminal study of charge carrier transport in amorphous semiconductors by Scher and Montroll [2]. Other examples range from tracer dispersion in subsurface aquifers [3] over transport on critical percolation clusters [4], to the motion of bacteria in biofilms [5] and of tracers in living biological cells [6].

Classical diffusion processes with $\gamma = 1$ in absence or presence of an external force are typically described in terms of the Fokker-Planck equation [7] or, equivalently, by the Langevin equation [8]. The description of subdiffusion dynamics of the form of Eq. (1) involves other, more sophisticated methods. The three most widely used mathematical models effecting subdiffusion of the form of Eq. (1) are: (i) the continuous time random walk (CTRW) of Montroll and Weiss [9], in which after each jump an independent, random waiting time $T$ is drawn from a power-law distribution $\psi(t) \simeq \tau^\gamma/T^{1+\gamma}$ with diverging mean waiting time. Such CTRWs were the starting point to derive the fractional Fokker-Planck equation [1,10]. An alternative approach are coupled Langevin equations [11]. (ii) Fractional Brownian motion (FBM) is a Gaussian process powered by correlated noise of the form $\langle\xi_\gamma(t)\xi_\gamma(t')\rangle \simeq (\gamma-1)\,|t-t'|^{\gamma-2}$ [12]. For subdiffusion the noise is anticorrelated, and the walk dimension exceeds 2. (iii) The third model is diffusion on a fractal support such as a critical percolation cluster, causing subdiffusion by the scale-free topology (bottlenecks, dead ends) such that $\gamma = 2/d_w$, where $d_w > 2$ is the walk dimension [13].

Empirically, it turns out that many processes displaying anomalous diffusion are *correlated* in the sense that increments of the process are not independent of prior increments. Such correlations are expected when we deal with living creatures capable of decision-making, such as bacterial motion [5] or the movement ecology of animal motion [14]. In a recent study of human mobility, the inadequacy of renewal CTRW processes without correlations was explicitly discussed [15]. Correlations also occur in financial market dynamics [16] or chaotic and turbulent flows [17].

CTRW are renewal processes and therefore are not amenable to include such correlations. While FBM includes power-law correlations and has indeed been used to model financial data [18], it is confined to Gaussian processes and turns out to be mathematically cumbersome, in particular, with respect to first-passage properties [19]. Finally, diffusion on a fractal is confined to very particular topologies.

In this paper we study the dynamics of an alternative model of subdiffusion with intrinsic correlations, namely, correlated CTRW (CCTRW) processes. This approach is based on the picture of correlated waiting times [20], in which the $n$th waiting time $T_n$ explicitly depends on previous waiting times, $T_i$ with $0 < i < n$. Here we derive the continuous-time limit of CCTRW processes and apply this result to introduce coupled Langevin equations describing subdiffusion dynamics in the presence of an external force $F(x)$. We show that this process satisfies generalized Einstein relations and converges to the Boltzmann-Gibbs equilibrium distribution. The corresponding relaxation of modes follows either power-law or stretched exponential patterns. Additionally, we discuss phenomena of ergodicity breaking as well as aging in the form of decaying linear response.

## II. CORRELATED CTRW

Our starting point is the CTRW with correlated waiting times introduced in Refs. [20,21]. Thus, we assume that the

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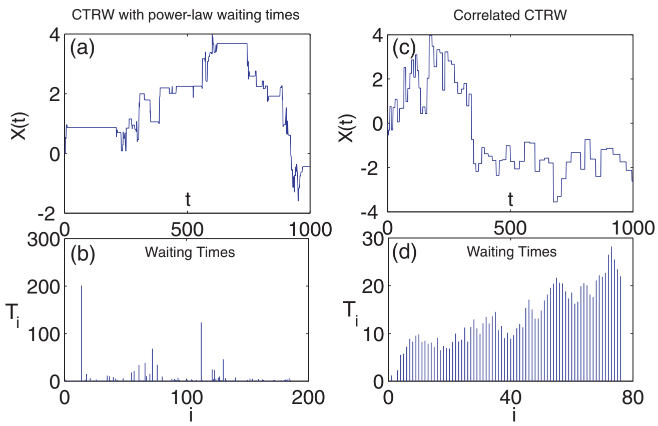


FIG. 1. (Color online) Typical trajectory of a renewal CTRW with power-law waiting times [$\alpha = 2/3$ (a)], compared to a trajectory of a CCTRW [$\alpha = 2$ (c)]. In (b) and (d) the corresponding waiting times are shown. For the renewal CTRW some of the waiting times are extremely long, leading to subdiffusion. In the CCTRW case with $\alpha = 2$, the mean of each increment $\xi_i$ is finite. However, $\langle T_i \rangle \to \infty$ as $i \to \infty$, producing subdiffusion; Eq. (1) with $\gamma = 2/3$.

waiting time $T_i$ equals

$$T_i = |\tau_i|, \tag{2}$$

where $\tau_i$ is the sum of random increments $\xi_j$:

$$\tau_i = \xi_1 + \cdots + \xi_i. \tag{3}$$

Thus, the waiting times may grow or decrease, while each waiting time $T_i$ is given by $T_i = |\tau_{i-1} + \xi_i|$. Here the absolute value guarantees positivity of the $T_i$, and thus the $T_i$ may be viewed as a random walk in the space of waiting times with a reflecting boundary condition at the origin [22]. We assume that the distribution of the iid random variables $\xi_j$ is symmetric and heavy-tailed ($\alpha$-stable) with Fourier transform:

$$\langle \exp(ik\xi_j)\rangle = \exp\left(-\tfrac{1}{2}|k|^{\alpha}\right), \quad 0 < \alpha \leqslant 2. \tag{4}$$

The average position of a particle diffusing symmetrically on a semi-infinite line grows indefinitely. In fact, for $1 < \alpha \leqslant 2$ the mean waiting time grows like $\langle T \rangle \simeq t^{1/\alpha}$. As shown below the process of Eq. (2) indeed leads to subdiffusive behavior of the type of Eq. (1). In Fig. 1 we compare a renewal CTRW with independent random waiting times with a CCTRW for $\alpha = 2$. For the renewal CTRW most waiting times are relatively small, with occasional large outliers giving rise to pronounced stalling events in the trajectory. In contrast, in the CCTRW process the waiting times develop smoothly, producing a trajectory reminiscent of a regular random walk albeit with, on average, continuously growing waiting times.

The Langevin equations for the position $x$ and the time $t$ corresponding to the continuous-time limit process of the above-defined CCTRW have the subordination form (details of the derivation are left to another paper [23])

$$\dot{x}(s) = \Gamma(s), \tag{5a}$$

$$\dot{t}(s) = |y(s)|, \quad \dot{y}(s) = \Gamma_{\alpha}(s). \tag{5b}$$

Here, $\Gamma(s)$ represents standard white Gaussian noise, formally $\Gamma(s) = dB(s)/ds$, where $B(s)$ is the Brownian motion with $\langle B^2(1)\rangle = 2D$. In Eq. (5a), $x$ as function of $s$ would thus represent the Wiener process, and the physical dimension of the diffusion constant is $[D] = \mathrm{cm}^2/\mathrm{sec}$. The variable $s$ can be viewed as a counting process (number of jumps) and is sometimes called operational time. The physical time of the process is related with $s$ through Eq. (5b): first, $\dot{y}(s)$ are time increments of the $\alpha$-stable kind, the noise $\Gamma_{\alpha}(s) = dL_{\alpha}(s)/ds$, being defined in terms of the *symmetric* distribution $L_{\alpha}$ with characteristic function

$$\langle \exp[ikL_{\alpha}(s)]\rangle = \exp\left(-s\tfrac{1}{2}|k|^{\alpha}\right), \quad 0 < \alpha \leqslant 2. \tag{6}$$

The process time $t$ is then defined as the absolute value of the series $y(s)$. Note that for regular CTRW the coupling between $s$ and $t$ occurs via a one-sided stable process. Also note that both noises $\Gamma$ and $\Gamma_{\alpha}$ are independent.

To solve the system of Eqs. (5a) and (5b), one first solves Eq. (5a), producing the driving process $x(s)$. Next, one solves Eq. (5b) to obtain the process $t(s)$, thus yielding the process $s(t)$, which is inverse to $t(s)$. Finally, one assembles both processes $x(s)$ and $s(t)$ to obtain the solution as the subordination

$$X(t) = x[s(t)]. \tag{7}$$

An external force $F(x)$ is included in our description by adding the drift term to Eq. (5a) in the usual way. Instead of Eq. (5a), this yields the Langevin equation

$$\dot{x}(s) = \frac{F(x(s))}{m\eta} + \Gamma(s), \tag{8}$$

with particle mass $m$ and friction coefficient $\eta$. Equations (8) and (5b) describe the dynamics of a particle performing a CCTRW under the influence of the external force $F(x)$.

In the explicit solution Eq. (7) of Eqs. (8) and (5b), the position $x$ satisfies the stochastic differential equation

$$dx(s) = \frac{F[x(s)]}{m\eta}ds + dB(s), \tag{9a}$$

and the subordinator $s(t)$ is the inverse of

$$t(s) = \int_0^s |L_{\alpha}(u)|du. \tag{9b}$$

Thus, $t(s)$ is the solution of Eq. (5b). The process $s(t)$ can also be represented as

$$s(t) = \inf\{s \geqslant 0 : t(s) > t\}. \tag{10}$$

Equation (8) together with Eq. (9b) is one of our central results.

### A. MSD in the force-free case

In the unbiased case with $F \equiv 0$, the solution to Eqs. (8) and (5b) has the simple form $X(t) = B[s(t)]$. It is not difficult to verify that $X(t)$ is $\alpha/[2(\alpha+1)]$-self-similar [23]. Thus, the MSD is

$$\langle X^2(t)\rangle = 2Dc_{\alpha}t^{\alpha/(\alpha+1)}. \tag{11}$$

The constant $c_{\alpha} = \langle s(1)\rangle$ depends on the specific distribution of the correlated waiting times and has physical dimension

$[c_\alpha] = \mathrm{sec}^{1-\alpha/(\alpha+1)}$. It can be represented as

$$c_\alpha = \frac{\alpha+1}{\alpha}\int_0^\infty \frac{1}{x^{(\alpha+1)/\alpha}} h\left[\frac{1}{x^{(\alpha+1)/\alpha}}\right] dx. \qquad (12)$$

Here, $h(x)$ is the probability density function of $t(1) = \int_0^1 |L_\alpha(u)|du$. In the limit $\alpha = 2$, $h(x)$ can be expressed in terms of a confluent hypergeometric function [24].

Thus, $X(t)$ satisfies subdiffusion of the kind of Eq. (1), with exponent $\gamma = \alpha/(\alpha+1)$, in agreement with the result derived in Ref. [20]. Interestingly, since $0 < \alpha \leqslant 2$, this exponent ranges exclusively between zero and 2/3. CCTRW processes can, therefore, not span the range between 2/3 and 1 [25]. Moreover, for $\alpha \ll 1$, the leading term of $\gamma = \alpha/(\alpha+1)$ is equal to $\alpha$. Thus, for small values of $\alpha$, the MSD of CCTRW behaves similarly to the MSD of CTRW with independent power-law waiting times.

### B. Stationary solution and Einstein relations

What happens in a confining external potential $V(x) = -\int^x F(x)dx$? Since $s(t)$ in Eq. (7) tends to infinity as $t \to \infty$, we obtain that the probability density function of the stationary solution of Eqs. (8) and (5b) equals

$$W_{\mathrm{st}}(x) \propto \exp\left(-\frac{V(x)}{Dm\eta}\right). \qquad (13)$$

Comparing this expression with the Gibbs-Boltzmann equilibrium distribution $W_{\mathrm{eq}} \propto \exp(-V(x)/[k_B T])$, we obtain a generalized Einstein or Einstein-Stokes-Smoluchowski relation,

$$D = \frac{k_B T}{m\eta}, \qquad (14)$$

connecting the noise strength $D$ with the dissipative parameter $\eta$ via the thermal energy $k_B T$.

Another important relation for regular diffusion processes is the linear response behavior, often called the second Einstein relation. To see whether the CCTRW process fulfills this relation, we calculate the first moment of $X(t)$ in the presence of a constant force, $F_0$, obtaining

$$\langle X(t)\rangle_{F_0} = F_0 \frac{c_\alpha t^{\alpha/(\alpha+1)}}{m\eta}. \qquad (15)$$

Comparison of the above result with Eq. (11) indeed leads to the second generalized Einstein relation

$$\langle X(t)\rangle_{F_0} = \frac{F_0}{2}\frac{\langle X^2(t)\rangle}{k_B T}. \qquad (16)$$

Thus, the CCTRW process preserves the two fundamental physical properties of diffusion processes, in analogy to regular subdiffusive CTRW [1,10].

### C. Single-mode relaxation

Let us now determine the relaxation dynamics of CCTRW processes. To this end, we consider the Fourier transform of $X(t)$ in the force-free case. At given wave number $k$, the temporal behavior defines the mode relaxation. Denote by $W(x,t)$ the probability density function of $X(t)$ and by $W(k,t) = \langle \exp(-Dk^2 s(t))\rangle$ its Fourier transform. We consider

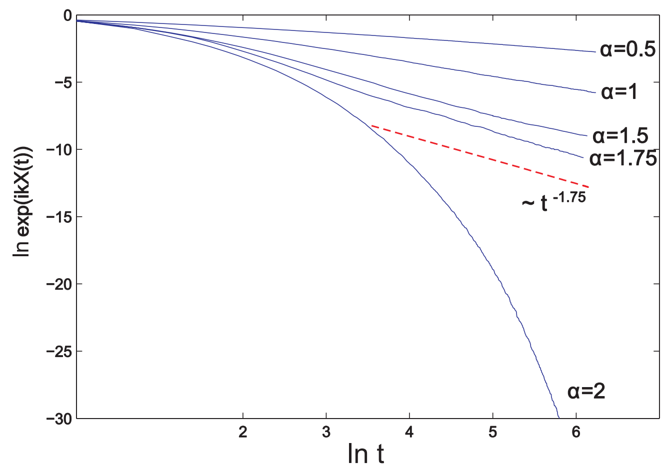


FIG. 2. (Color online) Single-mode relaxation corresponding of CCTRW subdiffusion for various exponents $\alpha$ (double-logarithmic scale) from simulations of the CCTRW process (solid lines). The dashed line is the theoretically predicted asymptotic behavior of the single mode for $\alpha = 1.75$. For $0 < \alpha < 2$, we observe power-law type relaxation, whereas for $\alpha = 2$ the model displays stretched exponential pattern. In each case $k = 1$.

two cases. The first case is $0 < \alpha < 2$, for which we observe the following upper and lower bounds for the process $t(s)$ in Eq. (9b). Denote by $A_s = |\int_0^s L_\alpha(u)du|$ and $B_s = s \times \sup_{u\in[0,s]} |L_\alpha(u)|$. Then we have $A_s \leqslant \int_0^s |L_\alpha(u)|du = t(s)$. Moreover, $t(s) \leqslant s \times \sup_{u\in[0,s]} |L_\alpha(u)| = B_s$. Consequently, since all three processes $A_s \leqslant t(s) \leqslant B_s$ are nondecreasing, we see that $\exp[-Dk^2(A_t)^{-1}] \leqslant \exp[-Dk^2 s(t)] \leqslant \exp[-Dk^2(B_t)^{-1}]$, where $(A_t)^{-1}$ and $(B_t)^{-1}$ are the respective inverse of $A_s$ and $B_s$ [26]. Now, using the fact that both $A_s$ and $B_s$ are $(\alpha+1)/\alpha$-self-similar and heavy-tailed with index $\alpha$, by the Tauberian theorem we obtain

$$W(k,t) \simeq 1/t^\alpha \qquad (17)$$

at long times $t$. Here, the notation $W(k,t) \simeq t^{-\alpha}$ means that $c_1 t^{-\alpha} < W(k,t) < c_2 t^{-\alpha}$ for appropriate positive constants $c_1$ and $c_2$, which depend only on the parameters $\alpha$ and $k$. Thus, for $0 < \alpha < 2$, we obtain asymptotic power-law single-mode relaxation, as demonstrated in Fig. 2 based on numerical simulations. However, note that the relaxation exponent $\alpha$ differs from the exponent $\gamma = \alpha/(1+\alpha)$ of the MSD, unlike for renewal CTRW [1].

For the case $\alpha = 2$, application of the self-similarity property of $s(t)$ together with the fact that the integral $\int_0^1 L_2(u)du$ is normally distributed with mean 0 and variance 1/3, yields another set of inequalities, $d_1 Z_3^{3/2}[Dk^2(3/2)^{1/3}t^{2/3}] \leqslant W(k,t) \leqslant d_2 Z_3^{3/2}[Dk^2(3/2)^{1/3}t^{2/3}]$. Similar to before, $d_1$ and $d_2$ are appropriate positive constants, and $Z_q^v(x) = \int_0^\infty y^{v-1}e^{-y^q}e^{-x/y}dy$ is the Krätzel function [27]. The asymptotic behavior of the Krätzel function [27] yields

$$W(k,t) \simeq \exp(-ct^{1/2}), \qquad (18)$$

for long times $t$. Here, $c = D^{3/4}|k|^{3/2}2^{7/4}3^{-1/2}$. Remarkably, in the case of $\alpha = 2$, we obtain a stretched exponential decay of single modes (compare Fig. 2).

### D. Harmonic potential

Let us now address the case of an external harmonic potential, $V(x) = \kappa x^2/2$. Then, the explicit solution Eq. (7) of Eqs. (8) and (5b) has the form

$$X(t) = x_0 \exp\left[-\frac{\kappa s(t)}{m\eta}\right] + \int_0^{s(t)} \exp\left\{\frac{\kappa[u - s(t)]}{m\eta}\right\}\Gamma(u)du, \tag{19}$$

where $x_0$ is the initial condition. It follows that the first moment of $X(t)$ satisfies

$$\langle X(t)\rangle = \left\langle x_0 \exp\left[-\frac{\kappa s(t)}{m\eta}\right]\right\rangle. \tag{20}$$

Thus, for $0 < \alpha < 2$ it decays to zero as $\frac{1}{t^\alpha}$, whereas for $\alpha = 2$ the decay is stretched exponential. The variance of $X(t)$ is given by [using relation (16)]

$$\mathrm{Var}[X(t)] = \frac{k_B T}{\kappa}\left(1 - \left\langle \exp\left[-\frac{2\kappa s(t)}{m\eta}\right]\right\rangle\right), \tag{21}$$

converging to the thermal value $\lim_{t\to\infty} \mathrm{Var}[X(t)] = k_B T/\kappa$. Similar to before, the average $\langle \exp[-\frac{\kappa s(t)}{m\eta}]\rangle$ decays to zero as $\frac{1}{t^\alpha}$ for $0 < \alpha < 2$, while for $\alpha = 2$ the decay is stretched exponential.

### E. Weak ergodicity breaking and aging

To further characterize the CCTRW process we address the question of whether it obeys ergodicity in the Boltzmann sense, i.e., whether for a sufficiently long time the time average MSD $X(t)$ equals the ensemble averaged MSD (11). For subdiffusive renewal CTRW this property is violated and so-called weak ergodicity breaking observed due to the diverging characteristic waiting time [28,29]. Generally, the time-averaged MSD is defined as

$$\overline{\delta^2(\Delta,t)} = \frac{1}{t-\Delta}\int_0^{t-\Delta} [X(t'+\Delta) - X(t')]^2 dt', \tag{22}$$

where $\Delta$ is the so-called lag time and $t$ represents the length of the time series $X(t')$. For Brownian motion, $\overline{\delta^2(\Delta,t)} \to 2D\Delta$ for sufficiently long $t$, matching the ensemble average $\langle x^2(\Delta)\rangle$ as expected for an ergodic process. From Eq. (11) we see that

$$\langle [X(t'+\Delta) - X(t')]^2\rangle = 2Dc_\alpha[(t'+\Delta)^{\alpha/(\alpha+1)} - (t'+\Delta)^{\alpha/(\alpha+1)}]. \tag{23}$$

This in turn implies a *linear* scaling with the lag time

$$\langle \overline{\delta^2(\Delta,t)}\rangle \sim 2Dc_\alpha \frac{\Delta}{t^{1-\alpha/(\alpha+1)}}, \tag{24}$$

for $\Delta \ll t$. Thus, the model displays weak ergodicity breaking for any $0 < \alpha \leqslant 2$. Interestingly the form of relation Eq. (24) is equivalent to the one obtained for subdiffusive renewal CTRW with power-law waiting time distribution $\psi(T) \simeq \tau^\gamma/T^{1+\gamma}$, with the substitution $\gamma \to \alpha/(1+\alpha)$, compare Refs. [28,29].

Another manifestation of a dynamic anomaly in the CCTRW model is aging, i.e., the dependence of the process dynamics on the time elapsing since system initiation. More precisely, we investigate the response of the process to a sinusoidal, time-dependent external field. In the case of such a time-dependent force $F(t)$, the CCTRW process has the form

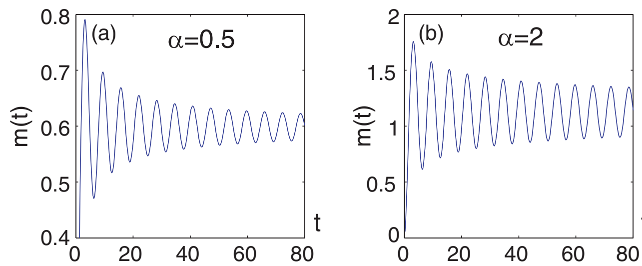


FIG. 3. (Color online) First moment of a CCTRW process with sinusoidal external force. As time proceeds, the response to the force diminishes, a manifestation of aging. In (a) we have the case $\alpha = 0.5$, whereas in (b) the Gaussian case $\alpha = 2$ is depicted.

$$X(t) = \frac{1}{m\eta}\int_0^t F(\tau)ds(\tau) + B[s(t)]. \tag{25}$$

This is the consequence of the subordination method applied carefully to systems under the influence of time-dependent forces [30–32]. Consequently, the first moment of $X(t)$ for the force $F(t) = F_0 \sin(\omega t)$ equals [23]

$$m(t) = \langle X(t)\rangle = \frac{c_\alpha \alpha}{\alpha+1}\frac{F_0}{m\eta}\int_0^t u^{-1/(\alpha+1)}\sin(\omega u)du. \tag{26}$$

Due to the factor $u^{-1/(\alpha+1)}$, the response to $F(t)$ decays as time proceeds for any $0 < \alpha \leqslant 2$, as demonstrated in Fig. 3. This result shows that the correlated waiting times lead to significant deviations when compared to the classical Markovian case. A similar behavior was reported in Ref. [30] for subdiffusive renewal CTRW with heavy-tailed waiting times.

## III. CONCLUSIONS

We studied a model of subdiffusion in external force fields, which originates from a CTRW process with correlated waiting times. This CCTRW model was rephrased in terms of coupled Langevin equations, equivalent to the definition within the framework of subordination, the random time change using the operational time of the system. We showed that the stationary solution of the model equals the Boltzmann distribution, and that the model satisfies the generalized Einstein relations in consistency with the fluctuation-dissipation relation. The relaxation dynamics of single modes, depending on the parameter value of the exponent $\alpha$, is either of power-law or stretched-exponential form. Similar to renewal CTRW processes with heavy-tailed waiting times, our model displays weak ergodicity breaking. Moreover, the response to time-dependent fluctuating forces stagnates at long times, a manifestation of aging.

We believe that the introduced CCTRW model is an interesting alternative in the modeling of complex systems showing anomalous diffusion under the influence of external force fields. It relaxes the renewal property of standard CTRW theory and is thus of interest in all those cases, where the nonrenewal behavior is relevant: search strategies in movement ecology, human motion patterns, or financial market dynamics, but also various physical processes such as turbulent flows or complex systems with strong inhomogeneities.

There are numerous open lines to be pursued for CCTRW processes. Thus, we may ask for the shape of the corresponding Fokker-Planck-type dynamic equation, how correlations in the jump length are consistently introduced in the presence of an external force, or how the stochasticity of time averages in the CCTRW model can be quantified.


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