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Short note on the emergence of fractional kinetics

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HIGHLIGHTS

- The emergence of fractional kinetics is studied.
- A physical picture is proposed for processes governed by fractional differential equations.
- The fractional kinetics emerges from random timescales for particle trajectories.
- Probability distributions of random timescales for particle trajectories are computed.

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ABSTRACT

In the present Short Note an idea is proposed to explain the emergence and the observation of processes in complex media that are driven by fractional non-Markovian master equations. Particle trajectories are assumed to be solely Markovian and described by the Continuous Time Random Walk model. But, as a consequence of the complexity of the medium, each trajectory is supposed to scale in time according to a particular random timescale. The link from this framework to microscopic dynamics is discussed and the distribution of timescales is computed. In particular, when a stationary distribution is considered, the timescale distribution is uniquely determined as a function related to the fundamental solution of the space–time fractional diffusion equation. In contrast, when the non-stationary case is considered, the timescale distribution is no longer unique. Two distributions are here computed: one related to the M-Wright/Mainardi function, which is Green's function of the time-fractional diffusion equation, and another related to the Mittag-Leffler function, which is the solution of the fractional-relaxation equation.

1. Introduction

Fractional kinetics is associated to phenomena governed by equations built on fractional derivatives. This approach has turned out to be successful in modeling *anomalous diffusion* processes.

The label *anomalous diffusion* is used in contrast to *normal diffusion*, where the adjective *normal* has the double aim of highlighting that a Gaussian based process is considered (because of the correspondence between the Normal and the Gaussian density) and that it is a typical and usual diffusion process. The observation in nature of anomalous diffusion has been definitively established, see e.g. Refs. [1–3].

A number of stochastic approaches to explaining anomalous diffusion has been introduced in the literature. One of the most successful is the Continuous Time Random Walk (CTRW) [4–10].

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However, recalling the simplicity of physical laws, in the *Simple Lessons from Complexity* taught by Goldenfeld and Kadanoff [11], the authors' first reply to the question "*So why, if the laws are so simple, is the world so complicated?*" is

> "*To us, complexity means that we have structure with variations. Thus a living organism is complex because it has many different working parts, each formed by variations in the working out of the same genetic code*"

and finally that

> "*Complex systems form structures, and these structures vary widely in size and duration. Their probability distributions are rarely normal, so that exceptional events are not rare.*"

With this in mind, here solely the simplest CTRW model is considered, i.e. the Markovian one. However, notwithstanding this simplest framework, it is argued that anomalous diffusion emerges as a consequence of the underlying variations of the structures of the medium from which a *wide* range of random timescales follows. Hence, each particle trajectory is supposed to scale in time according to its own timescale. This because any trajectory realization is supposed to occur in a random configuration of the medium characterized by its own timescale. In other words, the main idea discussed in this Short Note is that processes can be in general simply Markovian, but, during the observation procedure, what is actually measured is the superposition of processes of the same type but with different reference scales, as a consequence of structure variations.

Randomness of the timescale can be re-phrased as fluctuations of the timescale. This latter concept can be linked with the pioneering work by Beck [12] that has led to so-called superstatistics [13]. However, the present research differs from that because it starts from a different explanatory idea and it is based on particle trajectories modeled by a CTRW rather than by the Langevin equation, even though in both cases a superposition integral is used. Moreover, through the velocity autocorrelation function, it has a connection with the microscopic dynamics described by a Hamiltonian approach for the Brownian motion [14] and by the so-called "semidynamical" *V-Langevin* approach [15,16].

The present research is quite close to a recent work by Pramukkul et al. [17]. In particular, since the CTRW is adopted, the present formalism can be related to the so-called stochastic central limit theorem [17]. But, again, in the present research, the superposition formalism is introduced by some arguments linked to microscopic dynamics and not as a mathematical tool. Moreover, with respect to the work by Pramukkul et al. [17], here some results concerning the timescale distribution function are also presented and discussed.

The main features of CTRW are the following. Let $p(\mathbf{r}, t)$ be the *pdf* for a particle to be at $\mathbf{r}$ at the time t. Moreover, let $\lambda(\delta\mathbf{r})$ be the *pdf* for a particle to make a jump of length $\delta\mathbf{r}$ after a waiting time τ whose *pdf* is denoted by $\psi(\tau)$. Since the integral $\int_0^\tau \psi(\xi)\,\mathrm{d}\xi$ represents the probability that at least one step is made in the temporal interval $(0, \tau)$ [8,18], the probability that a given waiting interval between two consecutive jumps is greater than or equal to τ is $\Psi(\tau) = 1 - \int_0^\tau \psi(\xi)\,\mathrm{d}\xi$ and the equation

$$\psi(\tau) = -\frac{\mathrm{d}\Psi}{\mathrm{d}\tau} \tag{1}$$

holds [8,18]. Hence $\Psi(t)$ is the probability that, after a jump, the diffusing quantity does not change during the temporal interval of duration τ and it is the *survival probability* at the initial position [6].

When jumps and waiting times are statistically independent, the master equation of the CTRW model is [8]

$$\int_0^t \Phi(t-\tau)\frac{\partial p}{\partial \tau}\,\mathrm{d}\tau = -p(\mathbf{r}, t) + \sum_{\mathbf{r}'} \lambda(\mathbf{r}-\mathbf{r}')p(\mathbf{r}', t), \tag{2}$$

where $\widetilde{\Phi}(s) = \widetilde{\Psi}(s)/\widetilde{\psi}(s)$ is a memory kernel and tilde symbol $\widetilde{\cdot}$ means the Laplace transform.

From Eq. (2) it follows that a Markovian process is obtained when $\Phi(\tau) = \delta(\tau)$, which implies that $\widetilde{\Phi}(s) = 1$ so that $\widetilde{\Psi}(s) = \widetilde{\psi}(s)$ and finally $\Psi(\tau) = \psi(\tau)$. Functions $\Psi(\tau)$ and $\psi(\tau)$ are related by (1), so then a CTRW model is Markovian if $\Psi(\tau) = \mathrm{e}^{-\tau}$. Equivalently, when $\Psi(\tau)$ is different from an exponential function, the resulting CTRW model is non-Markovian or, by using mathematical terminology, it belongs to the class of semi-Markov process.

Assume a complex medium is formed by randomly variable structures characterized by individual scales for each configuration. Hence, for any Markovian-CTRW trajectory, the time variable t and the waiting-time τ have to be scaled by a particular random timescale T. In particular, the survival probability $\Psi(\tau)$ turns out to be

$$\Psi(\tau) = \Psi(\tau/T) = \mathrm{e}^{-\tau/T}. \tag{3}$$

The ratio τ/T for any observation time is a random variable because T is a random variable.

In a pioneering paper by Hilfer and Anton in 1995 [6], it was shown that if the survival probability $\Psi(\tau)$ is

$$\Psi(\tau) = E_\beta(-\tau^\beta), \quad 0 < \beta < 1, \tag{4}$$

where $E_\beta(z)$ is the Mittag-Leffler function defined as [19,20, Appendix E]

$$E_\beta(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\beta n + 1)}, \quad z \in C, \tag{5}$$