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Gaussian Processes in Complex Media: New Vistas on Anomalous Diffusion

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Normal or Brownian diffusion is historically identified by the linear growth in time of the variance and by a Gaussian shape of the displacement distribution. Processes departing from the at least one of the above conditions defines anomalous diffusion, thus a nonlinear growth in time of the variance and/or a non-Gaussian displacement distribution. Motivated by the idea that anomalous diffusion emerges from standard diffusion when it occurs in a complex medium, we discuss a number of anomalous diffusion models for strongly heterogeneous systems. These models are based on Gaussian processes and characterized by a population of scales, population that takes into account the medium heterogeneity. In particular, we discuss diffusion processes whose probability density function solves space- and time-fractional diffusion equations through a proper population of time-scales or a proper population of length-scales. The considered modeling approaches are: the continuous time random walk, the generalized gray Brownian motion, and the time-subordinated process. The results show that the same fractional diffusion follows from different populations when different Gaussian processes are considered. The different populations have the common feature of a large spreading in the scale values, related to power-law decay in the distribution of population itself. This suggests the key role of medium properties, embodied in the population of scales, in the determination of the proper stochastic process underlying the given heterogeneous medium.

Keywords: anomalous diffusion, fractional diffusion, complex medium, Gaussian process, heterogeneity, continuous time random walk, generalized gray Brownian motion, time-subordinated process

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1. INTRODUCTION

Normal diffusion has been widely investigated by means of different modeling approaches, such as:

conservation of mass, constitutive laws, random walks based on central limit theorem (CLT), stochastic models, i.e., Wiener process, Langevin equation, Fokker–Planck equation, and other Markovian Master equations [1–3]. The adjective *normal* highlights that a Gaussian-based process is considered.

However, many natural phenomena show a diffusive behavior that cannot be modeled by classical methods based on the CLT or linear and/or local constitutive laws. This is a ubiquitous observation in life sciences, soft condensed matter, geophysics and ecology, among others. These phenomena are generally labeled with the term *anomalous diffusion* in order to distinguish them from normal diffusion. In this last case, when assumptions of the CLT are satisfied, i.e., independence of random variables and finiteness of variances, the mean square displacement (MSD) of diffusing particles increases linearly in time. Conversely, departures from the CLT determine the emergence of anomalous diffusion. There are numerous experimental measurements in which the MSD scales with a non-linear power-law in time. These processes are successfully modeled through Fractional Calculus (see, e.g., [4–6]), so that the corresponding processes are referred to as *Fractional Diffusion* [7–16].

Anomalous diffusion is ubiquitously observed in many complex systems, ranging from turbulence [17, 18], plasma physics [19, 20] to soft matter, e.g., the cell cytoplasm, membrane, and nucleus [21–30] and neuro-physiological systems [31, 32]. In particular, the analysis of highly accurate data of single particle tracking (SPT), which are nowadays available thanks to the great instrumental advancement in fluorescence-based microscopy [33], has allowed to reveal the clear emergence of anomalous diffusion in many biological systems [27, 34–37].

As a consequence, the debate on the understanding of the most suitable microscopic model explaining the observed statistical features of SPT has taken momentum in the scientific community. The emergence of long-range correlations and anomalous diffusion asks for stochastic models departing from the classical Brownian motion based on the Gaussian-Wiener process and the standard random walk [1, 3]. At first, the main debate has been focused on whether the best stochastic approach should be one based on time-continuous trajectories, i.e., fractional Brownian motion (FBM), or to discontinuous trajectories characterized by jump events, i.e., continuous time random walk (CTRW) (see, e.g., [38] for a short discussion). However, both stochastic models, FBM and CTRW, do not describe the observed features of the SPT data. As a consequence, this implies that the above two minimal models (FBM and CTRW) do not take into account some microscopic dynamics affecting the particle motion and determining the emergence of long-range correlations, anomalous diffusion, non-Gaussian power-law distributions, ergodicity breaking, and aging [38].

For this reason, the scientific community is now focusing on the role of the system's heterogeneity, which was at first neglected in the above mentioned modeling approaches. Superstatistics [39–43] is probably the first model where heterogeneity is taken into account through a time modulation of a fast relaxing variable by a slow, adiabatic, variable. Many authors follow the main idea of superstatistics, developing stochastic models that try to go beyond superstatistics itself. This is obtained by developing an explicit stochastic dynamics for the adiabatic modulating variables characterizing the superstatistical models [44, 45]. Along this line, an interesting approach is the recently proposed diffusing diffusivity model (DDM) [46–50]. Approaches similar to superstatistics have also been proposed to model the inter-event times in point processes [51–54], which describe the intermittent events at the basis of event-driven diffusion processes, e.g., CTRWs where the inter-event time distribution is modulated by an external perturbation [41, 54, 55].

Other authors follow a somewhat different approach based on random-scaled Gaussian processes (RSGPs) [38, 56–59], which are physically based on a recently proposed model where inter-particle heterogeneity is explicity described through a population of scales characterizing the dynamical parameters of particle diffusive motion. This modeling approach has been denoted as heterogeneous ensemble of Brownian particles (HEBP) and has been developed on the basis of a Langevin model [57–59]. The HEBP model is then based on the Gaussian-Wiener process and, thus, on trajectories that are strongly continuous in the stochastic sense [60], while anomalous diffusion emerge as a consequence of heterogeneity. Fractional diffusion can be also interpreted as a consequence of complex heterogeneity in the underlying medium, where a classical diffusion takes place for the single particle. According to this approach, fractional diffusion emerges from the population of scales characterizing the medium. Interestingly, for a given stationary Gaussian process, the displacement distribution is uniquely related to the distribution of scales in the considered population. Thus, the observed diffusion properties can be used to guess the properties of the underlying diffusing medium.

All the above mentioned stochastic models where fractional diffusion follows from medium heterogeneity are essentially based on processes with continuous trajectories. Conversely, sudden transition events play a crucial role in the diffusing dynamics in many complex systems. Further, the role of microscopic models with smooth trajectories (Gaussian-based processes) and of event-based models with discontinuous trajectories in biological diffusion is not yet clear.

For this reason, we here propose, discuss, and review different models based on different Gaussian processes, whose parameters are characterized by a population of time or length scales. These models include stochastic processes with both time-continuous single particle trajectories and discontinuous trajectories with crucial jump events. We show that proper choices of the populations lead to space- or time-fractional diffusion. In this paper we propose and discuss a further development of the Master thesis by FDT [61].

The paper is organized as follows. In section 6 we propose and discuss two different Markovian CTRWs with population of time or length scales. In sections 3 and 4 we discuss RSGPs and subordination processes, respectively. Finally, in section 5 we give a brief discussion and draw some conclusions.

2. CONTINUOUS TIME RANDOM WALK (CTRW)

2.1. The Approach of Continuous Time Random Walk to Study Diffusion Processes

2.1.1. Basic Formulation of the CTRW

For the purposes of the present paper we briefly report some fundamentals on the CTRW. It is well-known that the CTRW is a successful approach to study diffusion processes. It considers the trajectories of discrete particles within a discrete space, according to the original formulation [7, 62, 63], or within a continuous underlying space, according to more recent studies [64, 65].

The trajectory of each particle is considered to be governed by the joint probability density function (PDF) $\varphi(\delta r, \delta t)$ of making a jump of length δr in the time interval δt. If the particle is located in r' at time t' and the position r is the particle position after a inter-event time (IET) δt, then: $r = r' + \delta r$, and $t = t' + \delta t$. The times t and t' are occurrence times of crucial jump events. In the basic theory of CTRW, these events are mutually independent and, thus, the IETs are statistically independent random variables whose features are described in the framework of renewal theory [51–54]. The marginal jump PDF $\lambda(\delta r)$ and the marginal waiting-time PDF $\psi(\tau)$ are, respectively

$$\lambda(\delta r) = \int_0^\infty \varphi(\delta r, \tau)\, d\tau\,, \qquad \psi(\tau) = \sum_{\delta r} \varphi(\delta r, \tau)\,. \quad (1)$$

The integral $\int_0^\tau \psi(\xi)\, d\xi$ is the probability that at least one step is made $(0, \tau)$ [64, 66]. Therefore, the probability that a given waiting time between two consecutive jumps is greater or equal to τ is:

$$\Psi(\tau) = 1 - \int_0^\tau \psi(\xi)\, d\xi = \int_\tau^\infty \psi(\xi)\, d\xi\,, \quad (2)$$

and upon differentiation: [64, 66]

$$\frac{d\Psi}{d\tau} = \frac{d}{d\tau}\left(1 - \int_0^\tau \psi(\xi)\, d\xi\right) = -\psi(\tau)\,. \quad (3)$$

Following Klafter et al. [62], the PDF $\eta(r, t)$ for a particle to arriving in r in the time interval from t to $t + \delta t$ is

$$\eta(r, t) = \sum_{r'} \int_0^t \eta(r', t')\varphi(r - r', t - t')\, dt' + \delta(t)\delta(r)\,, \quad (4)$$

where the initial condition is stated at $t = 0$ in $r = 0$. Hence, the PDF for a particle to be in r at time t is [62, 63]

$$p(r, t) = \int_0^t \eta(r, t - t')\Psi(t')\, dt' = \int_0^t \eta(r, \zeta)\Psi(t - \zeta)\, d\zeta\,. \quad (5)$$

Finally, by using (4), the PDF $p(r, t)$ is given by the following integral equation [62]

$$\begin{aligned} p(r; t) &= \delta(r)\Psi(t) + \sum_{r'} \int_0^t \int_0^\tau \eta(r', \tau - t')\varphi(r - r', t - \tau)\Psi(t')\, dt' d\tau \\ &= \delta(r)\Psi(t) + \sum_{r'} \int_0^t p(r', \tau)\varphi(r - r', t - \tau)\, d\tau\,. \end{aligned} \quad (6)$$

2.1.2. The Uncoupled Case and the Memory Effects

The simplest case of the CTRW modeling is the uncoupled case, i.e., the case when the jumps and the waiting times are statistically independent and it holds $\varphi(\delta r, \tau) = \lambda(\delta r)\psi(\tau)$. In this case Equation (6) can be re-arranged as [7]

$$p(r, t) = \delta(r)\Psi(t) + \int_0^t \psi(t - \tau) \sum_{r'} \lambda(r - r')p(r', \tau)\, d\tau\,. \quad (7)$$

For our purposes we rewrite Equation (7) in the Fourier–Laplace domain. The standard Laplace and Fourier transforms for sufficiently well-behaved functions are, respectively

$$\widetilde{g}(s) = \int_0^\infty e^{-st} g(t)\, dt\,, \quad \widehat{f}(k) = \sum_r e^{i\, k \cdot r} f(r)\,. \quad (8)$$

Then the Laplace transform of formula (6) is

$$\widetilde{p}(r, s) = \frac{1 - \tilde{\psi}(s)}{s} + \widetilde{\psi}(s) \sum_{r'} \lambda(r - r')\widetilde{p}(r', s)\,. \quad (9)$$

Now, after Fourier transform, we have that the Fourier–Laplace transform of the solution of (6) is

$$\widehat{\widetilde{p}}(k, s) = \frac{1 - \tilde{\psi}(s)}{s} + \widetilde{\psi}(s)\widehat{\lambda}(k)\widehat{\widetilde{p}}(k, s)\,, \quad (10)$$

and then, after re-arrangement, the above equation becomes

$$\widehat{\widetilde{p}}(k, s) = \frac{1 - \widetilde{\psi}(s)}{s\,[1 - \widehat{\lambda}(k)\widetilde{\psi}(s)]}\,. \quad (11)$$

According to Mainardi et al. [64], formula (11) can be written in the alternative form

$$\widetilde{\Phi}(s)\left[s\,\widehat{\widetilde{p}}(k, s) - 1\right] = \left[\widehat{\lambda}(k) - 1\right]\widehat{\widetilde{p}}(k, s)\,, \quad (12)$$

where

$$\widetilde{\Phi}(s) = \frac{1 - \widetilde{\psi}(s)}{s\, \widetilde{\psi}(s)} = \frac{\widetilde{\Psi}(s)}{\widetilde{\psi}(s)} = \frac{\widetilde{\Psi}(s)}{1 - s\, \widetilde{\Psi}(s)}\,. \quad (13)$$

After Fourier–Laplace anti-transforming, relation (12) gives

$$\int_0^t \Phi(t - \tau)\frac{\partial p}{\partial \tau}\, d\tau = -p(r, t) + \sum_{r'} \lambda(r - r')p(r', t)\,, \quad (14)$$

where it is evident the memory effect due to the auxiliary function $\Phi(\tau)$.

2.1.3. The Markovian CTRW Model

A Markovian model is obtained from (14) when $\Phi(\tau) = \delta(\tau)$. This implies that $\widetilde{\Phi}(s) = 1$ and, from the second equality in (13), it holds $\widetilde{\Psi}(s) = \widetilde{\psi}(s)$ and $\Psi(\tau) = \psi(\tau)$. The functions $\Psi(\tau)$ and $\psi(\tau)$ are related by (3), then a CTRW model is Markovian if

$$\Psi(\tau) = e^{-\tau}\,, \quad (15)$$

and the resulting Markovian master equation is

$$\frac{\partial p}{\partial t} = -p(r, t) + \sum_{r'} \lambda(r - r')p(r', t)\,, \quad p(r, 0) = \delta(r)\,. \quad (16)$$

On the contrary, when $\Psi(\tau)$ is not an exponential function the resulting CTRW model is non-Markovian.

2.2. Markovian CTRW Model With a Population of Time-Scales

Let the functions $\lambda_n(\delta r)$ and $\psi_n(\tau)$ be the n-fold convolutions of the jump and of the waiting-time PDFs, respectively. The most general solution of (6) can be written as [63, 65]

$$p(r,t) = \sum_{n=0}^{\infty} P(n,t)\lambda_n(r)\,, \tag{17}$$

where $P(n,t)$ is the probability of n jumps occurring up to time t:

$$P(n,t) = \int_0^t \psi_n(t-\tau)\Psi(\tau)\,d\tau\,. \tag{18}$$

In particular, since $\Psi(\tau)$ is, by definition, the probability that the particle remains fixed $(0,\tau)$, then it holds $\psi_0(\tau) = \delta(\tau)$ and [63]

$$P(0,t) = \int_0^t \delta(\tau)\Psi(\tau)\,d\tau = \Psi(t)\,. \tag{19}$$

Let us consider a heterogeneous condition. Hence, for any Markovian trajectory, the waiting-time τ is scaled by a proper timescale T. This timescale is taken to be a random variable following a proper distribution. In particular, the survival probability $\Psi(\tau)$ for each single Markovian trajectory is:

$$\Psi_M(\tau/T) = \mathrm{e}^{-\tau/T}\,, \tag{20}$$

where the index M has been added to remark that it is the survival probability corresponding to the Markovian case. In this case the random walk goes on according to the standard iteration procedure with the same meaning for the symbols, but the random waiting time τ is driven by the rescaled PDF $\psi(\tau)$. The characteristic function of the particle PDF turns out to be

$$\widehat{p}(k,t/T_0) = \int_0^{\infty} \widehat{p}_M(k,t/T)f(T/T_0,t)\,dT/T_0\,, \tag{21}$$

where $p_M(r,t)$ refers to the Markovian PDF, and $f(T/T_0,t)/T_0$ is the distribution of the random timescale T such that $\int_0^{\infty} f(T/T_0,t)\,dT/T_0 = 1$ and T_0 is the effective observed timescale. The single timescale case is recovered when $f(T/T_0,t)/T_0 = \delta(T-T_0)$.

Hence, by Fourier inversion and by using formula (17) for the Markovian PDF $p_M(r,t)$, it follows

$$p(r,t/T_0) = \sum_{n=0}^{\infty}\left[\int_0^{\infty} P_M(n,t/T_0)f(T/T_0,t)\,dT/T_0\right]\lambda_n(r)\,. \tag{22}$$

To conclude, the combination of (17) and (22) gives

$$P(n,t/T_0) = \int_0^{\infty} P_M(n,t/T)f(T/T_0,t)\,dT/T_0\,, \tag{23}$$

and setting $n=0$ it holds the following

$$\begin{aligned} P(0,t/T_0) &= \int_0^{\infty} P_M(0,t/T)f(T/T_0,t)\,dT/T_0 \\ &= \int_0^{\infty}\int_0^t \psi_0(t-\tau)\Psi_M(t/T)d\tau f(T/T_0,t)\,dT/T_0 \\ &= \int_0^{\infty}\int_0^t \delta_0(t-\tau)\Psi_M(t/T)d\tau f(T/T_0,t)\,dT/T_0 \\ &= \int_0^{\infty} \Psi_M(t/T)f(T/T_0,t)\,dT/T_0 = \Psi(t/T_0)\,. \end{aligned} \tag{24}$$

Let hereinafter be $T_0 = 1$ for simplicity. In their pioneering work [7], derived the following fundamental result:
if the survival probability $\Psi(\tau)$ is a function of the Mittag–Leffler type, i.e.

$$\Psi(\tau) = E_\beta(-\tau^\beta) = \sum_{n=0}^{\infty}\frac{(-1)^n\tau^{\beta n}}{\Gamma(\beta n+1)}\,, \quad 0<\beta<1\,, \tag{25}$$

the particle PDF $p(r;t)$ solves the time-fractional diffusion equation, i.e., equation (A.1) with $\alpha = 2$. Therefore, from (24) and (25) it follows that, for any T-distribution $f(T,t)$ such that the following integral holds

$$\int_0^{\infty} \mathrm{e}^{-t/T} f(T,t)\,dT = E_\beta(-t^\beta)\,, \quad 0<\beta<1\,, \tag{26}$$

the resulting process is a time-fractional diffusion process.

In particular, in the *stationary* case there is a unique the time-scale distribution, i.e., $f(T,t) = f_S(T)$. In fact, it is well-known that it holds [6]

$$\int_0^{\infty} \mathrm{e}^{-ty} K_\beta(y)\,dy = E_\beta(-t^\beta)\,, \quad 0<\beta<1\,, \tag{27}$$

where

$$K_\beta(y) = \frac{1}{\pi}\frac{y^{\beta-1}\sin(\beta\pi)}{1+2y^\beta\cos(\beta\pi)+y^{2\beta}}\,, \tag{28}$$

and, by comparing of (26) and (27), the *stationary* timescale distribution $f_S(T)$ turns out to be [67]

$$f_S(T) = \frac{1}{T^2}K_\beta\left(\frac{1}{T}\right)\,. \tag{29}$$

It is worth noting that the K_β, defined in (28), is the fundamental solution of the space-time fractional diffusion equation (A.1) when space and time fractional orders of derivation are equal each other and equal to β and when the asymmetry parameter assumes the extremal value, in which case the distribution has support solely on the positive real axis [11]. This case is also known as neutral diffusion [68, 69]. In the Markovian limit, i.e., $\beta = 1$, it holds $K_\beta(y) = \sin\pi/[\pi\,(y-1)^2] \to \delta(y-1)$ and a single timescale follows.

Concerning the waiting time PDF $\psi(t)$, we observe that, from formula (24) for the survival probability $\Psi(t)$ and from (3), we have

$$\psi(t) = -\frac{d\Psi(t)}{dt} = -\frac{d}{dt}\left(\int_0^\infty \Psi_M(t/T) f_s(T) dT\right). \quad (30)$$

By the fact that the involved functions are the exponential function Ψ_M and the normalized distribution $f_S(T)$, the following equality holds

$$\frac{d}{dt}\left(\int_0^\infty \Psi_M(t/T) f_S(T)\, dT\right) = \int_0^\infty \frac{d}{dt}\Psi_M(t/T) f_S(T)\, dT\,. \quad (31)$$

Finally, we can write the rescaled PDF $\psi(t)$ as.

$$\begin{aligned}\psi(t) &= -\frac{d\Psi(t)}{dt} = -\frac{d}{dt}\left(\int_0^\infty \Psi_M(t/T) f_S(T)\, dT\right) \\ &= -\int_0^\infty \frac{d}{dt}\Psi_M(t/T) f_S(T)\, dT = -\int_0^\infty \frac{d}{dt}\mathrm{e}^{-t/T} f_S(T)\, dT \\ &= \int_0^\infty \frac{1}{T}\mathrm{e}^{-t/T} f_S(T)\, dT \\ &= \int_0^\infty \Psi_M(t/T) f_S(T)\,\frac{dT}{T}\,. \end{aligned} \quad (32)$$

2.3. Markovian CTRW Model With a Population of Length-Scales

In this section we consider the case of a Markovian CTRW model with a population of length-scales. Hence, the space variable r is scaled by a proper distributed length-scale ℓ and the ratio r/ℓ is a distributed variable because ℓ is a distributed variable. The characteristic function of the particle PDF turns out to be

$$\widehat{p}(k/\ell_0, t) = \int_0^\infty \widehat{p}_G(k\ell, t) q(\ell/\ell_0)\, d\ell/\ell_0\,, \quad (33)$$

where $p_G(r,t)$ is the PDF of the Gaussian CTRW model and $q(\ell/\ell_0)/\ell_0$ is the distribution of the length-scale ℓ such that

$$\int_0^\infty q(\ell/\ell_0)\, d\ell/\ell_0 = 1\,, \quad (34)$$

and ℓ_0 is the effective observed length-scale. The case with a single length-scale is recovered when $q(\ell/\ell_0)/\ell_0 = \delta(\ell - \ell_0)$. Hereinafter we consider $\ell_0 = 1$.

Let the jump PDF be

$$\lambda(r - r') = \frac{\partial}{\partial r}\Lambda(r - r')\,, \quad (35)$$

where $\Lambda(r - r')$ is the cumulative distribution function of jumps, then we have

$$\Lambda(r - r') = \int_0^\infty \Lambda_G\left(\frac{r - r'}{\ell}\right) q(\ell)\, d\ell\,, \quad (36)$$

where $q(\ell)$ is the distribution of the length-scale and $\Lambda_G(r - r')$ is the cumulative distribution function of Gaussian jumps. Assuming $q(\ell)$ such that $\Lambda_G((r - r')/\ell)q(\ell)$ is integrable and differentiable and it holds $\left|\frac{\partial}{\partial r}\Lambda_G((r - r')/\ell)q(\ell)/\ell\right| \le g(\ell)$, with $g(\ell)$ integrable, then we have

$$\begin{aligned}\lambda(r - r') &= \frac{\partial}{\partial r}\Lambda(r - r') = \int_0^\infty \frac{\partial}{\partial r}\Lambda_G\left(\frac{r - r'}{\ell}\right) q(\ell)\, d\ell \\ &= \int_0^\infty \lambda_G\left(\frac{r - r'}{\ell}\right) q(\ell)\,\frac{d\ell}{\ell}\,. \end{aligned} \quad (37)$$

The PDF $p(r;\, t)$ of the process under consideration results to be

$$\begin{aligned} p(r;\, t) &= \delta(r)\Psi(t) + \sum_{r'}\int_0^t p(r', \tau)\lambda(r - r')\psi_M(t - \tau)\, d\tau \\ &= \delta(r)\Psi(t) + \sum_{r'}\int_0^t p(r', \tau)\left[\int_0^\infty \lambda_G\left(\frac{r - r'}{\ell}\right)\frac{q(\ell)}{\ell} d\ell\right]\psi_M(t - \tau)\, d\tau\,. \end{aligned} \quad (38)$$

Now, we want to find an explicit formula for $q(\ell)$ and we proceed considering the Fourier transform of the above equation, i.e.,

$$\widehat{p}(k, t) = \Psi_M(t) + \int_0^t \widehat{p}(k, \tau)\widehat{\lambda}(k)\psi_M(t - \tau)\, d\tau\,, \quad (39)$$

or analogously

$$\widehat{p}(k, t) = \Psi(t) + \int_0^t \widehat{p}(k, \tau)\left[\int_0^\infty \widehat{\lambda}_G(k\ell)\, q(\ell)\, d\ell\right]\psi_M(t - \tau)\, d\tau\,. \quad (40)$$

Reminding that in the Markovian case the survival probability is $\Psi_M(t) = \mathrm{e}^{-t}$ and the waiting time PDF $\psi(t) = \mathrm{e}^{-t}$, Equation (40) becomes

$$\widehat{p}(k, t) = \mathrm{e}^{-t} + \widehat{\lambda}(k)\mathrm{e}^{-t}\int_0^t \mathrm{e}^{\tau}\widehat{p}(k, \tau)\, d\tau\,, \quad (41)$$

and the following relation holds

$$\widehat{\lambda}(k) = \frac{\widehat{p}(k, t) - \mathrm{e}^{-t}}{\mathrm{e}^{-t}\int_0^t \mathrm{e}^{\tau}\widehat{p}(k, \tau)\, d\tau}\,. \quad (42)$$

Considering Equation (11) in the Markovian case (that is $\beta = 1$), we have

$$\widehat{\widetilde{p}}(k, s) = \frac{1}{1 + s - \widehat{\lambda}(k)}\,, \quad (43)$$

and after Laplace anti-transforming we obtain

$$\widehat{p}(k, t) = \mathrm{e}^{-(1-\widehat{\lambda}(k))t}\,, \quad (44)$$

that is the general expression for $\widehat{p}(k, t)$. Since $|\widehat{\lambda_G}(k)| \le 1$ from the proprieties of characteristic functions, then also $|\widehat{\lambda}(k)| \le 1$, i.e.,

$$|\widehat{\lambda}(k)| \le \int_0^\infty |\widehat{\lambda}_G(k)| q(\ell)\, d\ell \le \int_0^\infty q(\ell)\, d\ell = 1\,. \quad (45)$$

Hence, the above general representation of $\widehat{p}(k,t)$ shows that $\widehat{p}(k,t)$ is a characteristic function for all $t \in \mathbb{R}^+$ and $k \in \mathbb{R}$ because it holds

$$\mathrm{e}^{-(1-\widehat{\lambda}(k))t} \le 1\,. \tag{46}$$

The explicit expression of $\widehat{\lambda}(k)$ can also be obtained. We know that the Gaussian density for jumps λ_G comes from an unbiased random walk in one-dimension. In this random walk, a particle starts from the origin and, at each time step Δt, makes a jump $\pm\Delta x$ to the left or the right with equal probability. We call $P_{h,n}$ the probability that the particle will be in point $x = h\sigma_G$ at the time $t = n\Delta t$. In this simple case we have

$$P_{h,n} = \frac{1}{2}P_{h-1,n-1} + \frac{1}{2}P_{h+1,n-1}\,, \tag{47}$$

assuming $P_{0,0} = 1$. The characteristic function for this binomial formulation is

$$\widehat{\lambda}_G(k) = \sum_{h=-n}^{n} \mathcal{P}(X = \sigma_G\, h)\, \mathrm{e}^{ik\sigma_G h}\,, \tag{48}$$

that n even becomes

$$\begin{aligned}
\widehat{\lambda}_G(k) &= \sum_{h=-\frac{n}{2}}^{n/2} \mathcal{P}(X = \sigma_G\, 2h)\mathrm{e}^{ik\sigma_G 2h} \\
&= \sum_{h=-\frac{n}{2}}^{n/2} \frac{n!}{(\frac{n+2h}{2})!(\frac{n-2h}{2})!}\left(\frac{1}{2}\right)^{\frac{n+2h}{2}}\left(\frac{1}{2}\right)^{\frac{n-2h}{2}} \mathrm{e}^{ik\sigma_G 2h} \\
&= \frac{1}{2^n}\sum_{h=-\frac{n}{2}}^{n/2}\binom{n}{\frac{n+2h}{2}}\mathrm{e}^{ik\sigma_G 2h} = \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k}\mathrm{e}^{ik\sigma_G(2k-n)} \\
&= \frac{1}{2^n}\sum_{k=0}^{n}\binom{n}{k}\mathrm{e}^{ik\sigma_G k}\mathrm{e}^{-ik\sigma_G(n-k)} = \left(\frac{\mathrm{e}^{ik\sigma_G} + \mathrm{e}^{-ik\sigma_G}}{2}\right)^n \\
&= \cos(\sigma_G k)^n\,.
\end{aligned} \tag{49}$$

Finally, the characteristic function $\widehat{\lambda}(k)$ turns out to be.

$$\widehat{\lambda}(k) = \int_0^\infty \cos(\sigma_G k\ell) q(\ell)\, d\ell = \int_0^\infty \cos(k\ell)\frac{1}{\sigma_G} q\left(\frac{\ell}{\sigma_G}\right) d\ell\,. \tag{50}$$

2.3.1. Comparison With the Green Function of the Space-Fractional Diffusion Equation

We recall that the Fourier transform of the Lévy stable density $L^0_\alpha(x;t)$ that solves the space-fractional diffusion equation, i.e., Equation (A.1) with $\beta = 1$, is

$$\begin{aligned}
\widehat{L}^0_\alpha(kt^{1/\alpha}) &= \int_{-\infty}^{\infty} \mathrm{e}^{ikt^{1/\alpha}\zeta} L^0_\alpha(\zeta)\, d\zeta \\
&= 2\int_0^\infty \cos(kt^{1/\alpha}\zeta) L^0_\alpha(\zeta)\, d\zeta = \mathrm{e}^{-|k|^\alpha t}\,.
\end{aligned} \tag{51}$$

If we compare the above relation with Equation (50), we obtain also the following consistent pair $\widehat{\lambda}(k)$ and $q(\ell)$:

$$\widehat{\lambda}(k) = \widehat{L}^0_\alpha(k)\,, \quad \frac{1}{\sigma_G} q\left(\frac{\ell}{\sigma_G}\right) = 2L^0_\alpha(\ell)\,. \tag{52}$$

Moreover, this choice is consistent also with the proprieties of unitary initial value for the characteristic function and of normalization for the PDF, i.e.,

$$\widehat{\lambda}(k)\Big|_{k=0} = \mathrm{e}^{-|k|^\alpha}\Big|_{k=0} = 1\,, \tag{53}$$

and

$$\begin{aligned}
\widehat{\lambda}(k)\Big|_{k=0} &= \int_0^\infty \cos(\sigma_G k\ell) q(\ell) d\ell\Big|_{k=0} = \int_0^\infty q(\ell) d\ell \\
&= \int_0^\infty \cos(k\ell)\frac{1}{\sigma_G} q\left(\frac{\ell}{\sigma_G}\right) d\ell\Big|_{k=0} = \int_0^\infty \frac{1}{\sigma_G} q\left(\frac{\ell}{\sigma_G}\right) d\ell \\
&= 2\int_0^\infty L^0_\alpha(x) = \int_{-\infty}^{\infty} L^0_\alpha(x) = 1\,.
\end{aligned} \tag{54}$$

In general for $k \in \mathbb{R}$ it holds

$$\begin{aligned}
\widehat{p}(k,t) &= \mathrm{e}^{-(1-\widehat{\lambda}(k))t} = \mathrm{e}^{-(1-\mathrm{e}^{-|k|^\alpha})t} \\
&= \exp\left\{t\sum_{n=1}^{\infty}\frac{(-1)^n}{n!}|k|^{\alpha n}\right\} = \prod_{n=1}^{\infty}\mathrm{e}^{\frac{(-1)^n}{n!}|k|^{\alpha n} t}\,.
\end{aligned} \tag{55}$$

In the limit $|k| \ll 1$ the characteristic function $\widehat{p}(k,t)$ results to be

$$\begin{aligned}
\widehat{p}(k,t) &= \mathrm{e}^{-(1-\widehat{\lambda}(k))t} \\
&= \mathrm{e}^{-(|k|^\alpha - \frac{|k|^{2\alpha}}{2} + \frac{|k|^{3\alpha}}{6} + \ldots)t} \simeq \mathrm{e}^{-|k|^\alpha t}(1 + O(t|k|^{2\alpha})).
\end{aligned} \tag{56}$$

Then, for $|k| \ll 1$, it holds

$$\widehat{p}(k;t) \simeq \widehat{L}^0_\alpha(kt^{1/\alpha}). \tag{57}$$

Hence the characteristic function of the considered process is a Lévy stable density, that is the fundamental solution of the space-fractional diffusion equation. To conclude, since a characteristic function corresponds to a unique distribution and *vice versa*, in the considered limit ($k \ll 1$) the PDF $p(r - r';t)$ is a Lévy stable density.

3. RANDOMLY-SCALED GAUSSIAN PROCESSES

Let us denote a randomly-scaled Gaussian process (RSGP) as a stochastic process defined by the product of a Gaussian process times a non-negative random variable. In general, the one-point one-time PDF is not sufficient to characterize a stochastic process. There are infinitely many stochastic processes that follow the same one-dimensional distribution and, thus, solve the same Cauchy problem for the associated diffusion/master equation describing the time evolution of the PDF. However, in RSGPs, this indeterminacy is solved by the choice of the Gaussian process that is fully characterized for given first and second moments.

In this paper we consider a special class of RSGPs called generalized gray Brownian motion (ggBm), that is defined by using the fractional Brownian motion as Gaussian process [70–75]. For other form of randomly-scaled Gaussian process we refer the reader to Sliusarenko et al. [59]. Hence, we consider the following class of processes:

$$X_{\alpha,\beta}(t) = \ell\, B^H(t)\,, \quad 0 < \beta \le 1\,, \quad 0 < \alpha \le 2\,, \tag{58}$$

where $B^H(t)$ is the fBm process with Hurst exponent $0 < H < 1$, and then with power law variance t^{2H}.

The application of this approach to fractional diffusion is based on the correspondence of the PDFs resulting from the product of two independent random variables with the PDFs resulting from the integral representation formula (A.10).

Let define Z_1 and Z_2 as two real independent random variables: $z_1 \in \mathbb{R}$ and $z_2 \in \mathbb{R}^+$. The associated PDFs are $p_1(z_1)$ and $p_2(z_2)$, respectively. Let Z be the random variable obtained by the product of Z_1 and Z_2^γ, i.e., $Z = Z_1 Z_2^\gamma$. Denoting with $p(z)$ the PDF of Z, it results:

$$p(z) = \int_0^\infty p_1\left(\frac{z}{\lambda^\gamma}\right) p_2(\lambda)\, \frac{d\lambda}{\lambda^\gamma}\,. \tag{59}$$

Comparing the above formula with the integral representation formula (A.10), and applying the change of variables $z = xt^{-\gamma\omega}$ and $\lambda = \tau t^{-\omega}$, the integral representation (71) is recovered from (59) by setting:

$$\begin{aligned} &\frac{1}{t^{\gamma\omega}} p \left(\frac{x}{t^{\gamma\omega}}\right) \equiv p(x;t)\,, \quad \frac{1}{\tau^\gamma} p_1\left(\frac{x}{\tau^\gamma}\right) \equiv \psi(x;\tau) \\ &\frac{1}{t^\omega} p_2 \left(\frac{\tau}{t^\omega}\right) \equiv \varphi(\tau;t)\,. \end{aligned} \tag{60}$$

Then, by identifying functions and parameters as

$$p(z) \equiv K^0_{\alpha,\beta}(z)\,, \qquad p_1(z_1) \equiv G(z_1)\,, \qquad p_2(z_2) \equiv K^{-\alpha/2}_{\alpha/2,\beta}(z_2)\,, \tag{61}$$

$$\gamma = \frac{1}{2}\,, \qquad \omega = \frac{2\beta}{\alpha}\,, \qquad \gamma\omega = \frac{\beta}{\alpha}\,, \tag{62}$$

formula (59) reduces to the integral formula (A.10) for the symmetric space-time fractional diffusion equation. In terms of random variables it follows that [56]

$$Z = Xt^{-\beta/\alpha} \quad \text{and} \quad Z = Z_1 Z_2^{1/2}\,, \tag{63}$$

hence it holds

$$X = Zt^{\beta/\alpha} = Z_1 t^{\beta/\alpha} Z_2^{1/2}\,. \tag{64}$$

Since $p_1(z_1) \equiv G(z_1)$, Z_1 is a Gaussian random variable. Consequently, the variable $Z_1 t^{\beta/\alpha}$ is Gaussian with variance proportional to $t^{2\beta/\alpha}$. Hence, we chose the fBm with $0 < H = \beta/\alpha < 1$ as a Gaussian process with consistent power law variance. Furthermore, the random variable $Z_2 = \Lambda_{\alpha/2,\beta}$ is distributed according to $p_2(z_2) \equiv K^{-\alpha/2}_{\alpha/2,\beta}(z_2)$. Finally, we have the process

$$\begin{aligned} &X_{\alpha,\beta}(t) = \sqrt{\Lambda_{\alpha/2,\beta}}\, B^H(t)\,, \quad 0 < \beta < 1\,, \quad 0 < \alpha < 2\,, \\ &0 < H = \beta/\alpha < 1\,. \end{aligned} \tag{65}$$

where $\ell = \sqrt{\Lambda_{\alpha/2,\beta}}$ is an independent constant non-negative random variable distributed according to the PDF $K^{-\alpha/2}_{\alpha/2,\beta}(\lambda)$, $\lambda \ge 0$, that is a special case of (A.7). The process defined above is the solution of the space-time fractional diffusion Equation (A.1) in the symmetric case. This means that the one-time one-point PDF of $X_{\alpha,\beta}(t)$ is the fundamental solution of Equation (A.1) in the symmetric case, namely the PDF $K^0_{\alpha,\beta}(x;t)$ defined in (A.10).

The space-fractional diffusion is recovered when $\beta = 1$, in fact by using formula (A.7) with $t = 1$, we have

$$\begin{aligned} K^{-\alpha/2}_{\alpha/2,1}(\lambda) &= \int_0^\infty M_1(\tau) L^{-\alpha/2}_{\alpha/2}(\lambda;\tau)\, d\tau \\ &= \int_0^\infty \delta(1-\tau) L^{-\alpha/2}_{\alpha/2}(\lambda;\tau)\, d\tau = L^{-\alpha/2}_{\alpha/2}(\lambda)\,. \end{aligned} \tag{66}$$

Here we are interested in the distribution of $\ell = \sqrt{\Lambda_{\alpha/2,1}}$ then, by normalization condition, the PDF of ℓ results to be

$$q(\ell) = 2\ell L^{-\alpha/2}_{\alpha/2}(\ell^2)\,. \tag{67}$$

Analogously, the time-fractional diffusion is recovered when $\alpha = 2$, in fact by using formula (A.7) with $t = 1$, we have

$$\begin{aligned} K^{-1}_{1,\beta}(\lambda) &= \int_0^\infty M_\beta(\tau) L^{-1}_1(\lambda;\tau)\, d\tau \\ &= \int_0^\infty M_\beta(\tau)\delta(\lambda-\tau)\, d\tau = M_\beta(\lambda)\,, \end{aligned} \tag{68}$$

and the corresponding PDF of ℓ is

$$q(\ell) = 2\ell M_\beta(\ell^2)\,. \tag{69}$$

4. TIME-SUBORDINATION FOR GAUSSIAN PROCESSES

Another approach proposed to model the emergence of fractional and, more in general, anomalous diffusion in complex media is the time-subordination of a otherwise standard diffusion process (see, e.g., [15, 76, 77]). Even when the time-subordination procedure is applied to a Gaussian process, the PDF of the resulting process is no longer Gaussian, and the particle MSD has a non-linear time dependence. Let $Y(\tau)$, $\tau > 0$, be a stochastic process. Time-subordination is defined by the following expression:

$$X(t) = Y(Q(t))\,. \tag{70}$$

Thus, time-subordination follows from the randomization of the time clock in a stochastic process $Y(\tau)$, i.e., by using a new clock $\tau = Q(t)$, being $Q(t)$ a random process with non-negative increments. The resulting process $Y(Q(t))$ is said to be subordinated to $Y(\tau)$. This is called the *parent process*, while $Q(t)$ is called the *directing process*, so that it is said that $Y(\tau)$ it is directed by $Q(t)$ [78].

In diffusion processes, the parameter τ is named *operational time*. The process $t = t(\tau)$, which is the inverse of $\tau = Q(t)$, is called the *leading process* [15, 79]. It is worth noting that, in general, $X(t)$ is non-Markovian, even when the parent process $Y(\tau)$ is Markovian. At the macroscopic level, i.e., in terms of the particle PDF, the subordination process $X(t)$ is described by the following expression:

$$p(x;t) = \int_0^\infty \psi(x;\tau)\varphi(\tau;t)\,d\tau\,, \tag{71}$$

where $p(x;t)$ is the PDF of $X(t)$, $\psi(x;\tau)$ the PDF of $Y(\tau)$ and $\varphi(\tau;t)$ the PDF of $Q(t)$. In the following, the PDFs are self-similar, i.e., have a scaling property. Similarly to the approaches previously described, we introduce a population of time-scales T with distribution function $f(T)$ for the subordinated process $Y(\tau)$. Then parameter τ is now determined by the process $Q(t/T)$.

By comparing (71) and (A.10) we have

$$p(x;t) \equiv K^0_{\alpha,\beta}(x;t)\,, \quad \psi(x;\tau) \equiv G(x;\tau) = \frac{1}{\tau^{1/2}} G\left(\frac{x}{\tau^{1/2}}\right)\,,$$
$$\varphi(\tau;t) \equiv K^{-\alpha/2}_{\alpha/2,\beta}(\tau;t)\,. \tag{72}$$

Hence, the integral representation (71) turns out to be

$$K^0_{2,\beta}(x;t) = \int_0^\infty \frac{1}{Q(t/T)^{1/2}} G\left(\frac{x}{Q(t/T)^{1/2}}\right) K^{-\alpha/2}_{\alpha/2,\beta}(Q(t/\tau);t)\frac{dQ}{dT}\,dT\,. \tag{73}$$

In the case of space-fractional diffusion, from formula (A.11) we observe that the scaling property gives $Q(t/T) = (t/T)^{1/\alpha}$, and $f(T)$ results to be

$$f(T) = L^{-\alpha/2}_{\alpha/2}\left(\frac{1}{T^{1/\alpha}}\right)\frac{1}{\alpha T^{1/\alpha+1}}\,. \tag{74}$$

Analogously, in the case of time-fractional diffusion, from formula (A.12) we observe that the scaling

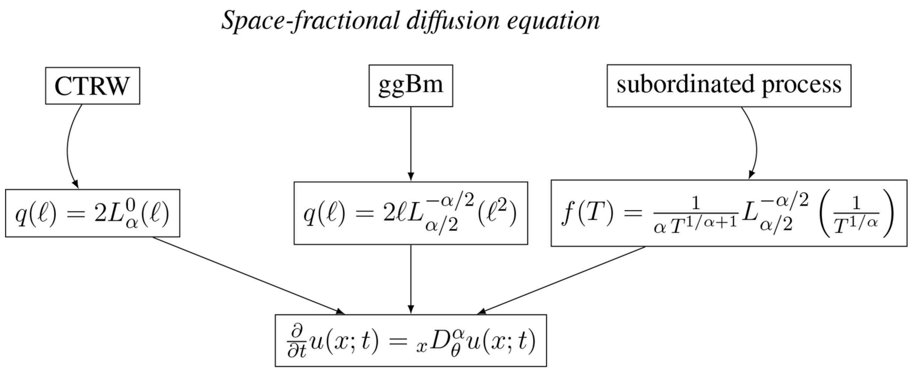

FIGURE 1 | Schematic picture of the three stochastic processes in heterogenous media leading to the same space-fractional diffusion equation for the 1-point 1-time PDF.

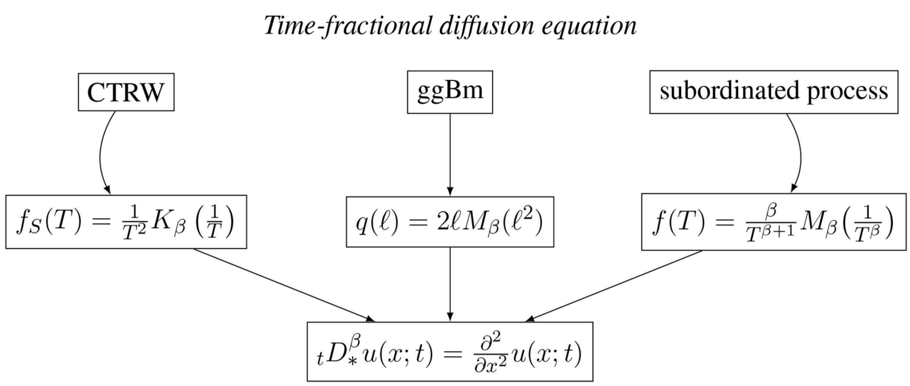

FIGURE 2 | Schematic picture of the three stochastic processes in heterogenous media leading to the same time-fractional diffusion equation for the 1-point 1-time PDF.

property gives $Q(t/T) = (t/T)^{\beta}$, and $f(T)$ results to be

$$f(T) = M_{\beta}\left(\frac{1}{T^{\beta}}\right)\frac{\beta}{T^{\beta+1}}\,. \qquad (75)$$

5. CONCLUSIONS

In this paper we studied a framework for explaining the emergence of anomalous diffusion in media characterized by random structures. In particular, we considered three different modeling approaches based on Gaussian processes but displaying a population of scales. The main idea is that the deviation from Gaussianity is indeed an indirect estimation of the population of the scales that characterize the medium where the diffusion takes place. We discussed the cases of space- and time-fractional diffusion through the CTRW, the ggBm and time-subordinated process.

The introduction of a population of scales significantly affects the particle PDF. The same fractional diffusion follows from different populations of scales when different Gaussian processes are considered. This suggests that the same macroscopic fractional process can be experimentally observed in different systems displaying different populations of scales and, consequently, driven by different underlying mesoscopic Gaussian processes. In **Figures 1**, **2** we give a synthetic picture of the three processes here described, all leading to the macroscopic space- or time-fractional diffusion equations.

When a macroscopic fractional process is experimentally observed, the simultaneous measurement of the population of scales embodies a selection criterion for the corresponding mesoscopic (and maybe not experimentally detectable) underlying Gaussian process. The same holds in the other way round, when a macroscopic fractional process is experimentally observed in place of a specific Gaussian process theoretically and/or experimentally expected, and then the deviation from Gaussianity embodies an indirect measurement of the population of the scales.

In general, this framework can be adopted for studying the presence and the characterization of impurities, as well as of obstacles, in a given complex medium. These results highlight the key role of the properties of the medium, embodied by the population of the scales, in the determination of the proper stochastic process for a given medium. The present research and our final claim aim to analyze and provide an explanation to the role and the effects of the system's configuration (environment plus particles) on the emergence of deviations from Gaussianity. In this respect, the present results add a contribution to similar existing literature concerning, for example, the dependence on system's configuration of the emergence of nonextensive statistical mechanics in confined granular media [80], or the emergence of processes modeled by fractional linear diffusion or by integer non-linear diffusion accordingly to different settings of CTRW simulations [81].

DATA AVAILABILITY

All datasets generated for this study are included in the manuscript and the **Supplementary Files**.

AUTHOR CONTRIBUTIONS

GP, PP, FD, and RS discussed the main ideas and took care of the text. The research presented in this paper and, in particular, the mathematical derivation of the models has been carried out at BCAM, Bilbao, and was developed by FD for his Master Thesis in Mathematics, Roma Tre University, under the supervision of GP and RS. GP wrote the Appendix in **Supplementary Material**.

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SUPPLEMENTARY MATERIAL

The Supplementary Material for this article can be found online at: https://www.frontiersin.org/articles/10.3389/fphy.2019.00123/full#supplementary-material

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