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SURVEY PAPER

DIFFUSION AND FOKKER-PLANCK-SMOLUCHOWSKI EQUATIONS WITH GENERALIZED MEMORY KERNEL

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Abstract

We consider anomalous stochastic processes based on the renewal continuous time random walk model with different forms for the probability density of waiting times between individual jumps. In the corresponding continuum limit we derive the generalized diffusion and Fokker-Planck-Smoluchowski equations with the corresponding memory kernels. We calculate the q th order moments in the unbiased and biased cases, and demonstrate that the generalized Einstein relation for the considered dynamics remains valid. The relaxation of modes in the case of an external harmonic potential and the convergence of the mean squared displacement to the thermal plateau are analyzed.

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1. Introduction

Anomalous diffusion, the deviation of the mean squared displacement (MSD)

$$\langle x^2(t) \rangle = \int_{-\infty}^{\infty} x^2 W(x, t) dx \simeq K_{\alpha} t^{\alpha} \quad (1.1)$$

from the linear Brownian scaling with time is known from a wide range of systems - depending on the magnitude of the anomalous diffusion exponent α we distinguish subdiffusion ($0 < \alpha < 1$) and superdiffusion ($\alpha > 1$) [8, 75, 76, 77]. The anomalous diffusion constant K_α has the physical dimension $\text{cm}^2/\text{sec}^\alpha$. In Eq. (1.1), we calculate the spatial integral of x^2 over the probability density function $W(x, t)$ to find the test particle at position x at some given time t . Examples for such anomalous diffusion phenomena include subdiffusive phenomena or charge carrier motion in amorphous semiconductors [99, 102], tracer chemical dispersion in ground-water studies [6, 98], or the motion of submicron probes in living biological cells [9, 30, 51, 115] or in dense fluids [35, 50, 81, 87, 114]. Superdiffusion occurs in weakly chaotic systems [107], turbulence [52, 79, 86], or in active search processes [4, 31, 61, 63, 80, 108].

The Brownian motion is closely related to the Gaussian probability density function $W(x, t)$ to find the diffusing test particle at position x at some given time t . This Gaussian emerges *a fortiori* [27] by virtue of the central limit theorem. Anomalous diffusion loses this universal character, and instead comes about from different stochastic scenarios corresponding to the underlying physical setting. Popular models for anomalous diffusion include the famed Scher-Montroll continuous time random walk (CTRW), in which individual jumps are separated by independent, random waiting times t with distribution $\psi(t)$ [78, 99]. Scale-free distributions of these waiting times lead to subdiffusion [54]. Fractional Brownian motion and the closely related fractional Langevin equation motion are processes driven by power-law correlated Gaussian noise [33, 34, 38, 39, 57, 59, 58, 65, 66, 68]. A diffusion process on a matrix with a fractal dimension such as a Sierpinski gasket or a percolation cluster near criticality turns anomalous due to the abundance of bottlenecks and dead ends on all scales [48, 55, 56, 40, 70, 96, 97, 109]. Finally, stochastic processes with space or time dependent diffusivities give rise to anomalous diffusion [16, 17, 18, 19, 25, 26, 49, 60, 69, 117]. A contemporary summary of a rich variety of anomalous diffusion processes is provided in Ref. [75].

Here we concentrate on the description of anomalous diffusion processes governed by fractional transport equations and their generalizations. Fractional diffusion and Fokker-Planck-Smoluchowski type equations have been widely used to model anomalous diffusive processes in complex systems [37, 72, 76, 77]. The fractional Fokker-Planck-Smoluchowski equation was derived from a generalized master equation and the continuous time random walk (CTRW) model in the presence of an external potential [3, 73], and it corresponds to the velocity-averaged motion governed by generalized Klein-Kramers and Chapman Kolmogorov equations [71, 74]. We note that

subdiffusive CTRW processes and thus the motion encoded in the Fokker-Planck-Smoluchowski equation are weakly non-ergodic, that is, long time and ensemble averages of physical observables are disparate, in contrast to, for instance, Brownian motion [7, 42, 75].

We can write the Fokker-Planck-Smoluchowski equation in the form [76, 77] (see also Ref. [90])

$$\frac{\partial^\alpha}{\partial t^\alpha} W(x, t) = \mathcal{L}_{\text{FP}} W(x, t), \quad (1.2)$$

where the Fokker-Planck operator

$$\mathcal{L}_{\text{FP}} = \frac{\partial}{\partial x} \frac{V'(x)}{m\eta_\alpha} + K_\alpha \frac{\partial^2}{\partial x^2} \quad (1.3)$$

includes the diffusion term proportional to K_α and the drift term involving the particle mass m , the generalized friction constant η_α of physical dimension $\text{sec}^{\alpha-2}$, and the derivative of the external potential $V(x)$ [72, 76, 77]. When $V(x) = \text{const.}$, the Fokker-Planck-Smoluchowski equation (1.2) reduces to the fractional diffusion equation. The solution of the fractional partial differential equation (1.2) is unique for a given initial condition $W(x, 0+)$, usually taken as $W(x, 0+) = \delta(x)$, and boundary condition, for instance, the natural boundary condition $W(\pm\infty, t) = \frac{\partial}{\partial x} W(\pm\infty, t) = 0$. We expressed the fractional derivative in Eq. (1.2) in terms of the Caputo operator [83]

$$\frac{d^\alpha}{dt^\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{d}{dt'} f(t') (t-t')^{-\alpha} dt', \quad 0 < \alpha < 1. \quad (1.4)$$

Alternatively, we could have used the Riemann-Liouville operator ${}_0D_t^\alpha$, in case of which the initial condition is directly incorporated if used on the left hand side, ${}_0D_t^\alpha [W(x, t) - W_0(x)t^{-\alpha}/\Gamma(1-\alpha)]$ [76, 77, 90].

The fractional transport equation (1.2) is characterized by the single exponent α . It was shown that the Fokker-Planck-Smoluchowski equation and the corresponding fractional diffusion equation can be generalized by introduction of distributed order fractional operators [12, 14, 15]. The distributed order diffusion equation can be written as

$$\int_0^1 \tau^{\lambda-1} p(\lambda) \frac{\partial^\lambda}{\partial t^\lambda} W(x, t) d\lambda = K_1 \frac{\partial^2}{\partial x^2} W(x, t), \quad (1.5)$$

in which we have the diffusion coefficient K_1 on the right hand side, which has the conventional dimension cm^2/sec . Here, the expression $\frac{\partial^\lambda}{\partial t^\lambda}$ is the Caputo fractional derivative (1.4) of order $0 < \lambda < 1$, $p(\lambda)$ is a weight function, i.e., dimensionless non-negative function with $\int_0^1 p(\lambda) d\lambda = 1$, and τ is a time parameter with dimension of sec. In the presence of an external

potential, Eq. (1.5) includes the Fokker-Planck operator (1.3). For the sake of simplicity we present all results in dimensionless units.

We here consider generalizations of the fractional and distributed order diffusion and Fokker-Planck-Smoluchowski equations by introducing specific, concrete forms for the memory kernel. These generalized transport equations will be obtained from the CTRW theory with generalized waiting time probability density function (PDF). To this end, in Section 2 we consider a CTRW model with arbitrary waiting time PDF, and we derive the corresponding diffusion type equation. The generalized Fokker-Planck-Smoluchowski equation with memory kernel and external potential is analyzed in Section 3. The validity of the generalized Einstein relation is shown. General expressions of the moments of the fundamental solution are presented. The MSD for different forms of the memory kernel is investigated in Section 4, showing that the considered diffusion type equation with memory kernel is a suitable tool for modelling anomalous and ultraslow diffusive processes. In Section 5 we present results related to the relaxation of modes for different forms of the memory kernel. The case of an harmonic potential is considered in Section 6 and the corresponding first and second moments are derived. In Section 7 the q -th order moments are calculated and several special cases analyzed. In Section 8 definitions and some useful relations for the Mittag-Leffler functions are given. The conclusions are provided in Section 9.

2. CTRW model

Here we briefly review the fundamental results of the CTRW theory and derive the corresponding generalized diffusion equation in the case of an arbitrary form of the waiting time PDF ψ . For the PDF $W(x, t)$ we find the simple algebraic form for the Fourier-Laplace transform [76, 77, 99]

$$\tilde{W}(\kappa, s) = \frac{1 - \hat{\psi}(s)}{s} \frac{1}{1 - \hat{\psi}(s)(1 - \kappa^2)}. \quad (2.1)$$

Here $\hat{\psi}(s)$ is the Laplace transform of the waiting time PDF. For the distribution of jump lengths, we assumed a Gaussian form with variance σ^2 , whose small κ expansion in Fourier space reads $1 - \kappa^2$ [76, 77]. Here we note that the Laplace transform of a function $f(t)$ is given by $\mathcal{L}[f(t)] = \hat{F}(s) = \int_0^\infty f(t)e^{-st}dt$. The Fourier transform of $f(x)$ is given by $\tilde{F}(\kappa) = \mathcal{F}[f(x)] = \int_{-\infty}^\infty f(x)e^{i\kappa x}dx$. Consequently, the inverse Fourier transform is defined by $f(x) = \mathcal{F}^{-1}[\tilde{F}(\kappa)] = \frac{1}{2\pi} \int_{-\infty}^\infty \tilde{F}(\kappa)e^{-i\kappa x}d\kappa$. The physical dimensions of the space-conjugated Fourier variable can be restored by noting that the Fourier transform of the jump length distribution is $1 - \frac{1}{2}\sigma^2\kappa^2$ for

small κ , where σ^2 has the dimension of length. To avoid dimensions here, we set $\sigma^2 = 2$.

For a Poissonian waiting time PDF

$$\psi(t) = e^{-t}, \quad (2.2)$$

the mean waiting time

$$T = \int_0^\infty t\psi(t)dt \quad (2.3)$$

is finite and equal to unity. With dimensions this Poissonian waiting time PDF would read $\tau^{-1} \exp(-t/\tau)$, where τ is the mean time. Relation (2.1) then encodes the PDF for classical Brownian motion in Fourier-Laplace domain [76, 77],

$$\tilde{W}(\kappa, s) = \frac{1}{s + \kappa^2}, \quad (2.4)$$

from which by inverse Fourier-Laplace transform we retrieve the classical Gaussian

$$W(x, t) = \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{x^2}{4t}\right). \quad (2.5)$$

To get back to dimensional expressions, in this equation t should be replaced by $K_1 t$, where the diffusivity in the typical random walk sense is defined as $K_1 = \sigma^2/(2\tau)$.

If we consider a scale-free waiting time PDF of the power-law form $\psi(t) \simeq t^{-1-\alpha}$ with $0 < \alpha < 1$, for which the characteristic waiting time T diverges, it can be shown that the PDF in Fourier-Laplace space is given by the algebraic form [76, 77]

$$\tilde{W}(\kappa, s) = \frac{s^{\alpha-1}}{s^\alpha + \kappa^2}. \quad (2.6)$$

With dimensions, we would write $\psi(t) \simeq \tau^\alpha/t^{1+\alpha}$, and then in Eq. (2.6) we would replace κ^2 by $K_\alpha \kappa^2$, where $K_\alpha = \sigma^2/(2\tau^\alpha)$. By applying the inverse Fourier-Laplace transform, one can show that the PDF $W(x, t)$ obeys the fractional diffusion equation (1.2) [76, 77].

Here we introduce the generalized waiting time PDF

$$\hat{\psi}(s) = \frac{1}{1 + s\hat{\gamma}(s)} \quad (2.7)$$

in Laplace space, where $\gamma(t)$ has the property

$$\lim_{t \rightarrow \infty} \gamma(t) = \lim_{s \rightarrow 0} s\hat{\gamma}(s) = 0. \quad (2.8)$$

To guarantee that this generalized function is a proper PDF its Laplace transform $\hat{\psi}(s)$ should be completely monotonic [100]. This requirement is fulfilled if the function $1 + s\hat{\gamma}(s)$ is a Bernstein function. We note that it can

be shown that if $f(s)$ is a complete Bernstein function then $g(s) = 1/f(s)$ is a completely monotonic function [5] which means that $s\hat{\gamma}(s)$ itself should be a Bernstein function. The waiting time PDF (2.7) together with a Gaussian jump length PDF with $\tilde{\lambda}(\kappa) \sim 1 - \kappa^2$ yield the Fourier-Laplace form

$$\tilde{W}(\kappa, s) = \frac{1}{s} \frac{1 - 1/[1 + s\hat{\gamma}(s)]}{1 - (1 - \kappa^2)/[1 + s\hat{\gamma}(s)]} = \frac{\hat{\gamma}(s)}{s\hat{\gamma}(s) + \kappa^2}, \quad (2.9)$$

of the PDF W . Relation (2.9) is valid for all times, not just in the long time limit, since the approximation $\hat{\psi}(s) \simeq 1 - s\hat{\gamma}(s)$ was not applied in the derivation of the PDF (2.9) in Fourier-Laplace space. Rewriting Eq. (2.9) as

$$\hat{\gamma}(s) \left[s\tilde{W}(\kappa, s) - 1 \right] = -\kappa^2 \tilde{W}(\kappa, s), \quad (2.10)$$

then from inverse Fourier-Laplace transform we obtain the generalized diffusion equation

$$\int_0^t \gamma(t-t') \frac{\partial}{\partial t'} W(x, t') dt' = \frac{\partial^2}{\partial x^2} W(x, t), \quad (2.11)$$

with the memory kernel $\gamma(t)$. The initial condition is again of form $W_0(x) = \delta(x)$, i.e. $\tilde{W}_0(\kappa) = 1$. Note that in the generalized diffusion equation (2.11) the memory kernel appears to the left of the time derivative in the integral such that for a power-law form of γ a Caputo fractional derivative emerges.

We note that in Ref. [106] an identical equation for the PDF was obtained in the analysis of anomalous diffusive process subordinated to normal diffusion by some operational time. There the memory kernel is connected to the cumulative distribution function of waiting times, i.e., one minus the probability to observe no step up to time t . Similar equations in Caputo or Riemann-Liouville form were considered in Refs. [23, 104, 116]. In Ref. [104] a thermodynamical interpretation of the Riemann-Liouville form is given. Anomalous processes with general waiting times were recently considered in [10]. A time-dependent Schrödinger equation with memory kernel was recently analyzed in [92].

We will consider the following specific forms for the memory kernel γ . In the simplest case we use the Dirac delta form $\gamma(t) = \delta(t)$, leading us back to an exponential (Poissonian) waiting time PDF underlying Brownian motion,

$$\psi(t) = \mathcal{L}^{-1} \left[\frac{1}{1+s} \right] = e^{-t}, \quad (2.12)$$

and Eq. (2.11) reduces to the classical diffusion equation. For a power-law memory kernel $\gamma(t) = t^{-\alpha}/\Gamma(1-\alpha)$ the waiting time PDF is represented by the generalized (two parameter) Mittag-Leffler (M-L) function (8.2) [44,

45, 46, 47]

$$\psi(t) = \mathcal{L}^{-1} \left[\frac{1}{1 + s^\alpha} \right] = t^{\alpha-1} E_{\alpha, \alpha}(-t^\alpha). \quad (2.13)$$

In this case Eq. (2.11) reduces to the fractional diffusion equation (1.2). For a memory function with two power-law terms, $\gamma(t) = a_1 \frac{t^{-\alpha_1}}{\Gamma(1-\alpha_1)} + a_2 \frac{t^{-\alpha_2}}{\Gamma(1-\alpha_2)}$ with $0 < \alpha_1 < \alpha_2 < 1$ the waiting time PDF is an infinite series in the three parameter M-L functions (8.3) [89],

$$\begin{aligned} \psi(t) &= \mathcal{L}^{-1} \left[\frac{1}{1 + a_1 s^{\alpha_1} + a_2 s^{\alpha_2}} \right] \\ &= \frac{t^{\alpha_2-1}}{a_2} \sum_{n=0}^{\infty} \frac{(-1)^n}{a_2^n} t^{\alpha_2 n} E_{\alpha_2-\alpha_1, \alpha_2 n + \alpha_2}^{n+1} \left(-\frac{a_1}{a_2} t^{\alpha_2-\alpha_1} \right). \end{aligned} \quad (2.14)$$

This case corresponds to the distributed order diffusion equation with two fractional exponents [89] (compare also Refs. [13, 105]), which can be obtained if we substitute $\gamma(t)$ in the generalized diffusion equation (2.11).

Finally, the case of a memory function with N power-law functions

$$\gamma(t) = \sum_{i=1}^N a_i \frac{t^{-\alpha_i}}{\Gamma(1-\alpha_i)}, \quad (2.15)$$

corresponds to a distributed order diffusion equation with N different exponents of the fractional operator. It can be solved in terms of the multinomial M-L function (8.7). The waiting time PDF is then given by

$$\begin{aligned} \psi(t) &= t^{\alpha_N-1} E_{(\alpha_N, \alpha_N-\alpha_1, \dots, \alpha_N-\alpha_{N-1}), \alpha_N} \left(-\frac{t^{\alpha_N}}{a_N}, \right. \\ &\quad \left. -\frac{a_1}{a_N} t^{\alpha_N-\alpha_1}, \dots, -\frac{a_{N-1}}{a_N} t^{\alpha_N-\alpha_{N-1}} \right). \end{aligned} \quad (2.16)$$

Note that for $N = 1$ ($\alpha_1 = \alpha$, $a_1 = 1$), from Eq. (2.16) we retrieve Eq. (2.13) for the simple fractional diffusion equation. We now consider three specific cases in more detail, in particular, a truncated M-L kernel.

2.1. Dirac delta and power-law memory kernel. Let us first consider a memory composed of a power-law and a Dirac delta function,

$$\gamma(t) = a_1 \frac{t^{-\alpha}}{\Gamma(1-\alpha)} + a_2 \delta(t), \quad (2.17)$$

with $0 < \alpha < 1$, and where a_1 and a_2 are constants. From Laplace transform of Eq. (2.17) it then follows that

$$\hat{\gamma}(s) = a_1 s^{\alpha-1} + a_2, \quad (2.18)$$

from where we can conclude that assumption (2.8) is satisfied. For the waiting time PDF we find

$$\psi(t) = \frac{1}{a_2} \sum_{n=0}^{\infty} \frac{(-1)^n}{a_2^n} t^n E_{1-\alpha, n+1}^{n+1} \left(-\frac{a_1}{a_2} t^{1-\alpha} \right), \quad (2.19)$$

where $E_{\alpha, \beta}^{\delta}(z)$ is the three parameter M-L function (8.3). The infinite series in the three parameter M-L functions of the form (2.19) are convergent [82, 94]. From the definition of three parameter M-L function (8.3) for the short time limit we then obtain

$$\psi(t) \simeq \frac{1}{a_2} \left(1 - \frac{a_1}{a_2} \frac{t^{1-\alpha}}{\Gamma(2-\alpha)} \right). \quad (2.20)$$

In the long time limit by help of formula (8.5) we find

$$\psi(t) \simeq a_1 \alpha \frac{t^{-\alpha-1}}{\Gamma(1-\alpha)}. \quad (2.21)$$

2.2. Distributed order memory kernel. We now turn to the case of a distributed order memory kernel,

$$\gamma(t) = \int_0^1 p(\lambda) \frac{t^{-\lambda}}{\Gamma(1-\lambda)} d\lambda, \quad (2.22)$$

where $p(\lambda)$ is a weight function with $\int_0^1 p(\lambda) d\lambda = 1$. The Laplace transform of Eq. (2.22) yields

$$\hat{\gamma}(s) = \int_0^1 p(\lambda) s^{\lambda-1} d\lambda. \quad (2.23)$$

Thus, a memory kernel of this form satisfies the assumption (2.8) since $\lim_{s \rightarrow 0} \int_0^1 p(\lambda) s^{\lambda} d\lambda = 0$. Inserting the memory kernel (2.22) into relation (2.11) and exchanging the order of integration we recover the distributed order diffusion equation (1.5). The waiting time PDF (2.7) thus becomes

$$\hat{\psi}(s) = \frac{1}{1 + \int_0^1 p(\lambda) s^{\lambda} d\lambda}. \quad (2.24)$$

A special case of Eq. (2.22) is the uniformly distributed order memory kernel with $p(\lambda) = 1$, which implies that

$$\hat{\gamma}(s) = \frac{s-1}{s \log(s)}. \quad (2.25)$$

Thus, the waiting time PDF becomes

$$\psi(t) = \mathcal{L}^{-1} \left[\frac{1}{1 + s \frac{s-1}{s \log(s)}} \right]. \quad (2.26)$$

Its behaviour in the short and long time limits follows from Tauberian theorems [24]. For the short time limit we find

$$\psi(t) = \log \frac{1}{t}, \quad (2.27)$$

while for the long time limit the behaviour is [15]

$$\psi(t) \simeq -\frac{d}{dt} \frac{1}{\log t} = \frac{1}{t \log^2 t}. \quad (2.28)$$

The distributed order memory kernel (2.22) with power-law weight function of the form $p(\lambda) = \nu \lambda^{\nu-1}$ ($\nu > 0$) [14], is relevant in the theory of ultraslow relaxation and diffusion processes (compare also the discussion in Refs. [29, 75]). In the Laplace space it is given by

$$\hat{\gamma}(s) = \frac{\nu \gamma(\nu, -\log(s))}{s (-\log(s))^\nu}, \quad (2.29)$$

where $\gamma(\nu, x) = \int_0^x t^{\nu-1} e^{-t} dt$ is the incomplete gamma function [22]. For $s \rightarrow 0$ its behaviour is of form $\hat{\gamma}(s) \simeq \nu \Gamma(\nu) / [s (-\log(s))^\nu]$, since $\gamma(\nu, x) \simeq \Gamma(\nu)$, for large x (small s implies large $-\log(s)$). For $s \rightarrow \infty$ it behaves as $\hat{\gamma}(s) \simeq \nu / \log(s)$, where we use the relation between the incomplete gamma function and the confluent hypergeometric function [22]. For this memory kernel, the waiting time PDF is given by

$$\psi(t) = \mathcal{L}^{-1} \left[\frac{1}{1 + s \frac{\nu \gamma(\nu, -\log(s))}{s (-\log(s))^\nu}} \right], \quad (2.30)$$

so that the short time limit behaviour follows

$$\psi(t) = \frac{1}{\nu} \log \frac{1}{t}, \quad (2.31)$$

while we find [15]

$$\psi(t) \simeq -\frac{d}{dt} \frac{\Gamma(\nu+1)}{\log^\nu t} = \frac{\nu \Gamma(\nu+1)}{t \log^{\nu+1} t} \quad (2.32)$$

in the long time limit.

2.3. Truncated M-L memory kernel. In particular, we here consider the tempered kernel

$$\gamma(t) = e^{-bt} t^{\beta-1} E_{\alpha, \beta}(-\delta^\alpha t^\alpha), \quad (2.33)$$

where $E_{\alpha, \beta}(z)$ is the two parameter M-L function (8.2), $b \geq 0$, $\delta \geq 0$, and $0 < \alpha \leq \beta \leq 1$. We note that a kernel similar to the form (2.33) with $b = \delta$, $\beta = \alpha$ and $-\delta^\alpha \rightarrow \delta^\alpha$ was considered in Refs. [112, 113] in the context of tempered subdiffusion. The memory kernel in Ref. [112] approaches a non-zero constant value when t goes to infinity, thus the assumption (2.8)

is not satisfied. For that reason we use the coefficient $-\delta^\alpha$ instead δ^α in the argument of the Mittag-Leffler function in Eq. (2.33). It is easy to check that with such a substitution the kernel $\gamma(t)$ goes to zero at $t \rightarrow \infty$. As shown below, this quite general form contains a rich variety of special cases. From the Laplace transform formula (8.4) and by help of the shift rule $\mathcal{L} [f(t)e^{-at}] = \hat{F}(s + a)$, where $\mathcal{L} [f(t)] = \hat{F}(s)$, we find that

$$\hat{\gamma}(s) = \frac{(s + b)^{\alpha-\beta}}{(s + b)^\alpha + \delta^\alpha}. \tag{2.34}$$

The memory kernel (2.33) satisfies the assumption (2.8).

The mentioned special cases of the kernel (2.33) are:

(i) for $\delta = 0$ we find

$$\gamma(t) = e^{-bt} \frac{t^{\beta-1}}{\Gamma(\beta)}, \tag{2.35}$$

such that

$$\hat{\gamma}(s) = (s + b)^{-\beta}. \tag{2.36}$$

(ii) The special case with $\beta = 1$ is given by

$$\gamma(t) = e^{-bt} E_\alpha(-\delta^\alpha t^\alpha), \tag{2.37}$$

implying

$$\hat{\gamma}(s) = \frac{(s + b)^{\alpha-1}}{(s + b)^\alpha + \delta^\alpha}. \tag{2.38}$$

(iii) For $b = 0$, we have

$$\gamma(t) = t^{\beta-1} E_{\alpha,\beta}(-\delta^\alpha t^\alpha), \tag{2.39}$$

and thus

$$\hat{\gamma}(s) = \frac{s^{\alpha-\beta}}{s^\alpha + \delta^\alpha}, \tag{2.40}$$

which will be considered explicitly in the following.

Inserting Eq. (2.34) into the expression (2.7) for the waiting time PDF we find

$$\hat{\psi}(s) = \frac{1}{1 + s \frac{(s+b)^{\alpha-\beta}}{(s+b)^\alpha + \delta^\alpha}}, \tag{2.41}$$

from which we conclude that $s\hat{\gamma}(s) = s(s + b)^{\alpha-\beta}/[(s + b)^\alpha + \delta^\alpha]$ is a Bernstein function for $0 < \alpha \leq \beta \leq 1$ (i.e., $\hat{\gamma}(s)$ is a completely monotonic function [100], in order for $\hat{\psi}(s)$ to be a completely monotonic function). For the waiting time PDF in the short time limit we then find the form

$$\psi(t) \simeq \frac{t^{-\beta}}{\Gamma(1 - \beta)}, \tag{2.42}$$

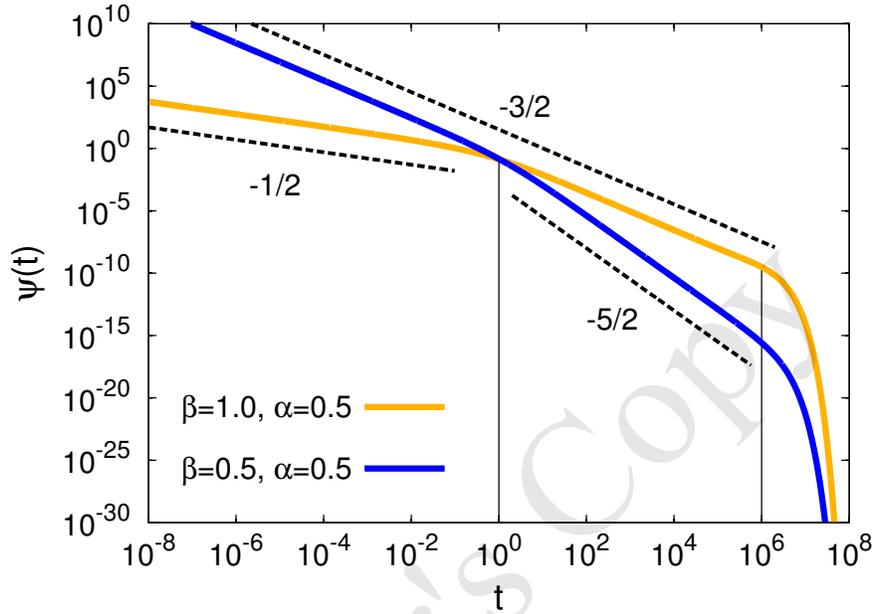


FIGURE 1. Tempered probability density function (2.43) of waiting times with $b = 1$ and $\delta = 1$. The exponents α and β are indicated in the plot. For $\beta < 1$ the initial scaling is $\simeq t^{\beta-2}$ (i.e., the exponent is $-3/2$), for $\beta = 1$ it is given by the next leading order, $\simeq t^{\beta+\alpha-2}$ (i.e., $-1/2$). The intermediate scaling is $\simeq t^{\beta-\alpha-2}$ (i.e., the exponent is $-3/2$) and $\simeq t^{\beta-2\alpha-2}$ (i.e., $-5/2$) when $\alpha = \beta$.

while the long time limit becomes

$$\psi(t) \simeq -\frac{d}{dt} e^{-bt} t^{\beta-1} E_{\alpha,\beta}(-\delta^\alpha t^\alpha), \quad (2.43)$$

where we use $\hat{\psi}(s) \simeq 1 - s\hat{\gamma}(s)$ due to assumption (2.8).

We plot the waiting time PDF (2.43) in Fig. 1.

3. Mean squared displacement

Here we provide results for the MSD for the different forms of the memory kernel $\gamma(t)$ discussed in the previous section. In terms of the Fourier transform of the PDF, the MSD of our process is obtained through the relation

$$\langle x^2(t) \rangle = \mathcal{L}^{-1} \left[-\frac{\partial^2}{\partial \kappa^2} \tilde{W}(\kappa, s) \right] \Big|_{\kappa=0}. \quad (3.1)$$

From Eq. (2.9) for the PDF, we find the general form

$$\langle x^2(t) \rangle = 2\mathcal{L}^{-1} \left[\frac{s^{-1}}{s\hat{\gamma}(s)} \right] \quad (3.2)$$

based on the memory kernel γ .

3.1. Dirac delta and power-law memory kernel. For the memory kernel (2.17), the MSD can then be expressed in terms of the two parameter M-L function,

$$\langle x^2(t) \rangle = \frac{2}{a_2} t E_{1-\alpha, 2} \left(-\frac{a_1}{a_2} t^{1-\alpha} \right). \quad (3.3)$$

For the short time this implies the normal diffusive behaviour

$$\langle x^2(t) \rangle = \frac{2}{a_2} t, \quad (3.4)$$

while in the long time limit we find the subdiffusive scaling

$$\langle x^2(t) \rangle = \frac{2}{a_1} \frac{t^\alpha}{\Gamma(1+\alpha)}. \quad (3.5)$$

As expected, the Dirac delta peak of the memory kernel dominates the short time regime of normal diffusion. Such a crossover from normal to anomalous diffusion is a generic physical behaviour for systems, in which the test particle is driven by Gaussian white noise but progressively explores a disordered environment.

3.2. Distributed order memory kernel. For the uniformly distributed order memory kernel (2.25) we employ Tauberian theorem [24] and uncover the behaviour

$$\langle x^2(t) \rangle \simeq 2 \log \frac{1}{t}, \quad (3.6)$$

in the short time limit, and we find the crossover to the ultraslow diffusive behaviour of the particle in the long time limit [12],

$$\langle x^2(t) \rangle \simeq 2 \log t. \quad (3.7)$$

An analogous result for the MSD was recently obtained from a generalized Langevin equation [93]. In Ref. [21] the same relations for the short and long time limit are obtained from a fractional Langevin equation with uniformly distributed fractional Gaussian noise.

For the distributed order memory kernel with power-law weight function (2.29) the MSD becomes

$$\langle x^2(t) \rangle = \frac{2}{\nu} \log \frac{1}{t} \quad (3.8)$$

in the short time limit, while at long times we find the behaviour [14]

$$\langle x^2(t) \rangle = \frac{2}{\Gamma(1 + \nu)} \log^\nu t. \quad (3.9)$$

The same result was obtained from a power-law distributed order fractional Langevin equation [21] and from an ultraslow CTRW with a logarithmic waiting time PDF [20, 29, 41]. Moreover, logarithmic diffusion with $\alpha = 1/2$ is found for single file (excluded volume) motion of particles on a line [62, 88], and $\alpha = 4$ is characteristic for Sinai diffusion [8, 29].

3.3. Truncated M-L memory kernel. The MSD in the case of the truncated M-L memory kernel (2.33) is given by the three parameter M-L functions (8.3) in the form

$$\langle x^2(t) \rangle = 2t^{1-\beta} \left[E_{1,2-\beta}^{-\beta}(-bt) + \delta^\alpha t^\alpha E_{1,2+\alpha-\beta}^{\alpha-\beta}(-bt) \right]. \quad (3.10)$$

Alternatively, this MSD can be represented as

$$\begin{aligned} \langle x^2(t) \rangle &= 2 \int_0^t (t - \tau) e^{-b\tau} \left[\frac{\tau^{-\beta-1}}{\Gamma(-\beta)} + \frac{\tau^{-\beta+\alpha-1}}{\Gamma(-\beta + \alpha)} \right] d\tau \\ &= 2 {}_{RL}I_t^2 \left(e^{-bt} \left[\frac{t^{-\beta-1}}{\Gamma(-\beta)} + \frac{t^{-\beta+\alpha-1}}{\Gamma(-\beta + \alpha)} \right] \right), \end{aligned} \quad (3.11)$$

where we use the convolution theorem of the Laplace transformation and the definition of the Riemann-Liouville integral [83]

$${}_{RL}I_t^\alpha f(t) = \frac{1}{\Gamma(\alpha)} \int_0^t (t - t')^{\alpha-1} f(t') dt'. \quad (3.12)$$

Combining relations (3.10) and (3.11) we obtain the equality

$${}_{RL}I_t^2 \left(e^{-bt} \frac{t^{-\beta+\alpha-1}}{\Gamma(-\beta + \alpha)} \right) = t^{1+\alpha-\beta} E_{1,2+\alpha-\beta}^{\alpha-\beta}(-bt), \quad (3.13)$$

which can be easily shown using the series expansion of the exponential function and the three parameter M-L function (8.3).

In the short time limit we find the scaling

$$\langle x^2(t) \rangle \simeq 2 \frac{t^{1-\beta}}{\Gamma(2 - \beta)} \quad (3.14)$$

as well as the normally diffusive long time regime

$$\langle x^2(t) \rangle \simeq 2b^\beta (1 + \delta^\alpha b^{-\alpha}) t, \quad (3.15)$$

by virtue of relation (8.5). Thus, the behaviour for the truncated M-L memory kernel (2.33), for which anomalous diffusion crosses over to normal diffusion is opposite to the crossover from normal to anomalous diffusion observed in section 3.1 and the results of Refs. [12, 14, 15].

The case of the M-L memory kernel (2.39) without truncation, i.e., $b = 0$ yields the MSD

$$\langle x^2(t) \rangle = 2 \left[\frac{t^{1-\beta}}{\Gamma(2-\beta)} + \delta^\alpha \frac{t^{1+\alpha-\beta}}{\Gamma(2+\alpha-\beta)} \right], \quad (3.16)$$

from which we conclude that the particle shows accelerating subdiffusion with a crossover scaling from

$$\langle x^2(t) \rangle \simeq 2 \frac{t^{1-\beta}}{\Gamma(2-\beta)} \quad (3.17)$$

in the short time limit to the faster subdiffusive scaling

$$\langle x^2(t) \rangle \simeq 2\delta^\alpha \frac{t^{1+\alpha-\beta}}{\Gamma(2+\alpha-\beta)} \quad (3.18)$$

if $\beta > \alpha$, or to normal diffusion if $\alpha = \beta$. An analogous situation is observed for modified form distributed order diffusion equations with two fractional exponents [14, 15].

4. Multi-scaling properties

We now address the fractional order moments $\langle |x(t)|^q \rangle$ of the generalized diffusion equation (2.11). In Laplace space their definition is

$$\mathcal{L}[\langle |x(t)|^q \rangle] = \int_{-\infty}^{\infty} |x|^q \hat{W}(x, s) dx. \quad (4.1)$$

From relations (5.9) and (4.1), introducing the change of variables via $y = (s\hat{\gamma}(s))^{1/2}|x|$ we obtain

$$\mathcal{L}[\langle |x(t)|^q \rangle] = \Gamma(q+1) \frac{1}{s(s\hat{\gamma}(s))^{q/2}}. \quad (4.2)$$

Generally, fractional order moments exhibit the scaling behaviour

$$\langle |x(t)|^q \rangle = C(q)t^{\mu(q,t)}, \quad (4.3)$$

where $\mu(q, t)$ is called the multi-scaling exponent. In the simplest case we observe a self-affine behaviour for which [67]

$$\langle |x(t)|^q \rangle = C(q)t^{qH}, \quad (4.4)$$

where $H > 0$ is the Hurst exponent [67] (see also [36]). This is the case for ordinary Brownian motion with $H = 1/2$, for fractional Brownian motion ($0 < H < 1$), for Lévy flights $H = 1/\alpha$ as long as q is smaller than the stable index α , and for subdiffusive CTRW processes with scale-free, power-law waiting time PDF. According to the latter statement also dynamics governed by the fractional diffusion equation (1.2) belong to the class of

fractal or self-affine processes. Following relation (4.4) the exponent $\mu \propto q$ has a linear dependence on the fractional order q . When

$$\langle |x(t)|^q \rangle = C(q)t^{\mu(q)}, \quad (4.5)$$

where $\mu(q)$ is a given nonlinear function, we call this a multi-fractal or multi-affine process [67]. Such a multi-scaling behaviour of $\mu(q)$ was observed in different systems, e.g., the motion of freshwater and marine zooplankters [103, 101] and the anomalous diffusion of tracer particles in living cells [28]. Multi-scaling of the form (4.5) is observed in multi-fractal random walks [2] and modified CTRW models [1]. Numerical approaches to determine the multi-fractal scaling behaviour of time series were developed [53]. Ref. [89] shows that distributed order diffusion equations yield more complex forms of the q -th moment (4.3). In the context of strong anomalous diffusion and Lévy walks multi-scaling behaviour is connected to the theory of infinite invariant densities [75, 85].

4.1. Power-law and Dirac delta memory kernel. The q -th order moment for the memory kernel (2.17) based on the combination of Dirac delta functions and a power-law is given by the three parameter M-L function,

$$\langle |x(t)|^q \rangle = \Gamma(q+1)a_2^{-q/2}t^{q/2}E_{1-\alpha, q/2+1}^{q/2}\left(-\frac{a_1}{a_2}t^{1-\alpha}\right). \quad (4.6)$$

Thus, μ is a *time dependent* quantity and has a non-linear dependence on q (multi-scaling). For instance, for the fourth order moment, from relation (4.6), we find that

$$\langle x^4(t) \rangle = \Gamma(5)a_2^{-2}t^2E_{1-\alpha, 3}^2\left(-\frac{a_1}{a_2}t^{1-\alpha}\right), \quad (4.7)$$

from which the short time behaviour

$$\langle x^4(t) \rangle \sim \Gamma(5)a_2^{-2}\frac{t^2}{2}\left[1 - 4\frac{a_1}{a_2}\frac{t^{1-\alpha}}{\Gamma(4-\alpha)}\right] \quad (4.8)$$

follow. At long times,

$$\langle x^4(t) \rangle \simeq \Gamma(5)a_1^{-2}\frac{t^{2\alpha}}{\Gamma(1+2\alpha)}\left[1 - 2\Gamma(1+2\alpha)\frac{a_2}{a_1}\frac{t^{\alpha-1}}{\Gamma(3\alpha)}\right]. \quad (4.9)$$

Thus, the scaling crosses over from $\langle x^4(t) \rangle \simeq t^2$ at short times to $\langle x^4(t) \rangle \sim t^{2\alpha}$ at long times.

4.2. Distributed order memory kernel. For the distributed order memory kernel (2.22) we use relation (4.3). The uniformly distributed order memory kernel with $p(\lambda) = 1$ by help of Tauberian theorems then leads to the long time behaviour

$$\langle |x(t)|^q \rangle \sim \Gamma(q+1) \log^{q/2} t. \quad (4.10)$$

If we represent the q -th moment in the form (4.3), this implies $C(q) = \Gamma(q+1)$ and

$$\mu(q, t) = \frac{q}{2} \times \frac{\log(\log t)}{\log t}. \quad (4.11)$$

In the short time limit we thus have

$$\langle |x(t)|^q \rangle \sim \frac{\Gamma(q+1)}{\Gamma(1+q/2)} t^{q/2} \log^{q/2} \frac{1}{t}, \quad (4.12)$$

and thus

$$\mu(q, t) = \frac{q}{2} + \frac{q \log(\log[1/t])}{2 \log(t)}. \quad (4.13)$$

For the variable weight $p(\lambda) = \nu \lambda^{\nu-1}$ with $\nu > 0$ the long time limit yields

$$\langle |x(t)|^q \rangle \sim \Gamma(q+1) [\Gamma(1+\nu)]^{-q/2} \log^{\nu q/2} t. \quad (4.14)$$

Thus, $C(q) = \Gamma(q+1) \Gamma[(1+\nu)]^{-q/2}$ and

$$\mu(q, t) = \frac{\nu q \log(\log t)}{2 \log t}. \quad (4.15)$$

In the short time limit,

$$\langle |x(t)|^q \rangle \sim \frac{\Gamma(q+1) \nu^{-q/2}}{\Gamma(1+q/2)} t^{q/2} \log^{q/2} \frac{1}{t}. \quad (4.16)$$

Again, μ turns out to be an explicitly time dependent quantity.

4.3. Truncated M-L memory kernel. Finally, we consider the tempered two parameter M-L memory kernel (2.33), whose q -th order moment becomes

$$\langle |x(t)|^q \rangle = \Gamma(q+1) {}_{RL}I_t^{1+q/2} \left(e^{-bt} t^{-\beta q/2-1} E_{\alpha, -\beta q/2}^{-q/2}(-\delta^\alpha t^\alpha) \right), \quad (4.17)$$

where we apply the convolution theorem of the Laplace transformation and the definition of the Riemann-Liouville integral (3.12). The case (2.35) with $\delta = 0$ yields for the q -th moment

$$\begin{aligned} \langle |x(t)|^q \rangle &= \Gamma(q+1) {}_{RL}I_t^{1+q/2} \left(e^{-bt} \frac{t^{-\beta q/2-1}}{\Gamma(-\beta q/2)} \right) \\ &= \Gamma(q+1) t^{(1-\beta)q/2} E_{1, 1+(1-\beta)q/2}^{-\beta q/2}(-bt). \end{aligned} \quad (4.18)$$

For the special case with $b = 0$, i.e., without truncation, the kernel of the form (2.39) produces

$$\langle |x(t)|^q \rangle = \Gamma(q+1)t^{(1-\beta)q/2} E_{\alpha, (1-\beta)q/2+1}^{-q/2}(-\delta^\alpha t^\alpha). \quad (4.19)$$

We close by the explicit calculation of the fourth order moment, using the general form (4.17). We obtain

$$\begin{aligned} \langle x^4(t) \rangle &= \Gamma(5)_{RL} I_t^3 \left(e^{-bt} t^{-2\beta-1} E_{\alpha, -2\beta}^{-2}(-\delta^\alpha t^\alpha) \right) \\ &= \Gamma(5)t^{2(1-\beta)} \left[E_{1, 3-2\beta}^{-2\beta}(-bt) + 2\delta^\alpha t^\alpha E_{1, 3-2\beta+\alpha}^{-2\beta+\alpha}(-bt) \right. \\ &\quad \left. + \delta^{2\alpha} t^{2\alpha} E_{1, 3-2\beta+2\alpha}^{-2\beta+2\alpha}(-bt) \right]. \end{aligned} \quad (4.20)$$

From here we find the behaviours in the short and long time limit,

$$\langle x^4(t) \rangle \sim \Gamma(5) \frac{t^{2(1-\beta)}}{\Gamma(1+2(1-\beta))} \quad (4.21)$$

and

$$\langle x^4(t) \rangle \sim \Gamma(5)b^{2\beta} (1 + \delta^\alpha \beta^{-\alpha})^2 \frac{t^2}{2}, \quad (4.22)$$

respectively. In the special case $b = 0$, Eq. (2.39), the fourth order moment by help of relation (4.19) becomes

$$\begin{aligned} \langle x^4(t) \rangle &= \Gamma(5)t^{2(1-\beta)} E_{\alpha, 2(1-\beta)+1}^{-2}(-\delta^\alpha t^\alpha) \\ &= \Gamma(5)t^{2(1-\beta)} \left[\frac{1}{\Gamma(1+2(1-\beta))} \right. \\ &\quad \left. + \frac{2\delta^\alpha t^\alpha}{\Gamma(1+2(1-\beta)+\alpha)} + \frac{\delta^{2\alpha} t^{2\alpha}}{\Gamma(1+2(1-\beta)+2\alpha)} \right], \end{aligned} \quad (4.23)$$

which for the short time limit has form (4.21), while the long time limit is given by

$$\langle x^4(t) \rangle \sim \Gamma(5) \frac{\delta^{2\alpha} t^{2(1+\alpha-\beta)}}{\Gamma(1+2(1+\alpha-\beta))}. \quad (4.24)$$

For $\alpha = \beta$ this implies that $\langle x^4(t) \rangle \simeq t^2$, as expected for normal Brownian motion.

5. Generalized Fokker-Planck equation, solution, and linear response

Let us now investigate the case when the diffusing test particle is confined by an external potential $V(x)$. To this end we consider the generalized

Fokker-Planck-Smoluchowski equation for $W(x, t)$ with memory kernel $\gamma(t)$,

$$\int_0^t \gamma(t-t') \frac{\partial}{\partial t'} W(x, t') dt' = \left[\frac{\partial}{\partial x} \frac{V'(x)}{m\eta_\gamma} + K_\gamma \frac{\partial^2}{\partial x^2} \right] W(x, t), \quad (5.1)$$

with the initial condition $W(x, 0) = \delta(x)$. We note that here we return to dimensional quantities, as we derive some physical relations such as the generalized Einstein-Stokes relation, for which the physical parameters are instructive. We also note that in this representation the physical dimension of the diffusion and friction coefficients K_γ and η_γ depends on the chosen form of the kernel $\gamma(t)$. For instance, for the power-law waiting time density $\psi(t) \simeq \tau^\alpha/t^{1+\alpha}$, the generalized diffusion coefficient $K_\alpha = \sigma^2/(2\tau^\alpha)$ has the physical dimension $\text{cm}^2/\text{sec}^\alpha$, and the dimension of $\eta_\gamma = \text{sec}^{\alpha-2}$. We also note that from comparison of the stationary solution of the Fokker-Planck-Smoluchowski equation—i.e., by setting $\partial W(x, t)/\partial t = 0$ —we immediately obtain the generalized Einstein-Stokes relation

$$K_\gamma = \frac{k_B T}{m\eta_\gamma}. \quad (5.2)$$

For the choice $\gamma(t) = \delta(t)$ the generalized Fokker-Planck-Smoluchowski equation (5.1) reduces to the Fokker-Planck-Smoluchowski equation. Furthermore, for the power-law form $\gamma(t) = t^{-\alpha}/\Gamma(1-\alpha)$ it turns to the Fokker-Planck-Smoluchowski equation [43, 72, 73, 76, 77]

$${}_C D_t^\alpha W(x, t) = \left[\frac{\partial}{\partial x} \frac{V'(x)}{m\eta_\alpha} + K_\alpha \frac{\partial^2}{\partial x^2} \right] W(x, t). \quad (5.3)$$

For the distributed order memory kernel (2.22), the generalized Fokker-Planck-Smoluchowski equation (5.1) becomes the distributed order Fokker-Planck-Smoluchowski equation [15]

$$\int_0^1 \tau^{\lambda-1} p(\lambda) \frac{\partial^\lambda}{\partial t^\lambda} W(x, t) d\lambda = \left[\frac{\partial}{\partial x} \frac{V'(x)}{m\eta_1} + K_1 \frac{\partial^2}{\partial x^2} \right] W(x, t). \quad (5.4)$$

Consider a constant restoring force switched on at $t = 0$,

$$F(x) = -\frac{dV(x)}{dx} = F\Theta(t), \quad (5.5)$$

i.e., $V(x) = -Fx$, where $\Theta(t)$ is the Heaviside step function. Laplace and Fourier transforming Eq. (5.1) for this constant force, we find

$$\tilde{W}(\kappa, s) = \frac{\hat{\gamma}(s)}{s\hat{\gamma}(s) + i\frac{F}{m\eta_\gamma}\kappa + K_\gamma\kappa^2}. \quad (5.6)$$

For a particular form of the memory kernel one can then find closed forms of the PDF W by applying inverse Fourier-Laplace transform techniques

to relation (5.6). The inverse Fourier transform can indeed be obtained for general γ ,

$$\hat{W}(x, s) = \hat{P}(x, s) \exp \left[-\frac{F}{2m\eta_\gamma K_\gamma} x \right], \quad (5.7)$$

where

$$\hat{P}(x, s) = \frac{\hat{\gamma}(s)}{2K_\gamma} \frac{\exp \left[-\sqrt{\frac{s\hat{\gamma}(s)}{K_\gamma} + \left(\frac{F}{2m\eta_\gamma K_\gamma} \right)^2} \times |x| \right]}{\sqrt{\frac{s\hat{\gamma}(s)}{K_\gamma} + \left(\frac{F}{2m\eta_\gamma K_\gamma} \right)^2}}. \quad (5.8)$$

In the force free case ($F = 0$) this PDF becomes

$$\hat{W}(x, s) = \frac{1}{2s} \sqrt{\frac{s\hat{\gamma}(s)}{K_\gamma}} e^{-\sqrt{\frac{s\hat{\gamma}(s)}{K_\gamma}} |x|} = -\frac{1}{2} \frac{\partial}{\partial |x|} \frac{1}{s} \exp \left(-\sqrt{\frac{s\hat{\gamma}(s)}{K_\gamma}} \times |x| \right). \quad (5.9)$$

From the PDF we calculate the moments $\langle x^n(t) \rangle$ of the process by using the differentiation trick

$$\langle x^n(t) \rangle = \mathcal{L}^{-1} \left[i^n \frac{\partial^n}{\partial \kappa^n} \tilde{W}(\kappa, s) \right] \Big|_{\kappa=0}. \quad (5.10)$$

For the first moment, the mean particle displacement, we obtain

$$\langle x(t) \rangle_F = \frac{F}{m\eta_\gamma} \mathcal{L}^{-1} \left[\frac{s^{-1}}{s\hat{\gamma}(s)} \right], \quad (5.11)$$

and the second moment is given by

$$\langle x^2(t) \rangle_F = 2K_\gamma \mathcal{L}^{-1} \left[\frac{s^{-1}}{s\hat{\gamma}(s)} \right] + 2 \left(\frac{F}{m\eta_\gamma} \right)^2 \mathcal{L}^{-1} \left[\frac{s^{-1}}{s^2\hat{\gamma}^2(s)} \right]. \quad (5.12)$$

In the force free case ($F = 0$), the second moment reduces to Eq. (3.2). From relations (5.11) and (3.2) we thus obtain the linear response relation (second Einstein relation)

$$\langle x(t) \rangle_F = \frac{F}{2k_B T} \langle x^2(t) \rangle_0 \quad (5.13)$$

for any general form of the memory kernel $\gamma(t)$. This general property follows from the form (5.1) of the generalized Fokker-Planck-Smoluchowski equation with its additive drift term and the generalized Einstein-Stokes relation (5.2).

6. Relaxation of modes

By help of the separation ansatz $W(x, t) = X(x)T(t)$ the generalized Fokker-Planck-Smoluchowski equation (5.1) leads to the two equations

$$\int_0^t \gamma(t - \tau) \frac{d}{d\tau} T(\tau) d\tau = -\lambda T(t), \tag{6.1}$$

$$\left[\frac{\partial}{\partial x} \frac{V'(x)}{m\eta_\gamma} + K_\gamma \frac{\partial^2}{\partial x^2} \right] X(x) = -\lambda X(x), \tag{6.2}$$

where λ is a separation constant. Therefore, the solution of Eq. (5.1) is given as the sum $W(x, t) = \sum_n X_n(x)T_n(t)$, where $X_n(x)T_n(t)$ is the eigenfunction corresponding to the eigenvalue λ_n .

From Laplace transform of the temporal eigen-equation (6.1) we obtain the relaxation law

$$T_n(t) = T_n(0) \mathcal{L}^{-1} \left[\frac{\hat{\gamma}(s)}{s\hat{\gamma}(s) + \lambda_n} \right]. \tag{6.3}$$

We note that in the long time limit $t \rightarrow \infty$, corresponding to $\lim_{s \rightarrow 0} s\hat{\gamma}(s) = 0$, Eq. (6.3) has the asymptotic behaviour

$$T_n(t) \sim T_n(0) \mathcal{L}^{-1} \left[\frac{\hat{\gamma}(s)}{\lambda_n} \left(1 - \frac{s\hat{\gamma}(s)}{\lambda_n} \right) \right] \sim \frac{T_n(0)}{\lambda_n} \gamma(t)|_{t \rightarrow \infty}. \tag{6.4}$$

The choice of a Dirac delta memory kernel reduces the general relaxation law (6.3) to the exponential form

$$T_n(t) = T_n(0) e^{-\lambda_n t}. \tag{6.5}$$

For a power-law memory kernel we obtain the known M-L relaxation with power-law asymptote [72],

$$T_n(t) = T_n(0) E_\alpha(-\lambda_n t^\alpha) \sim \frac{T_n(0)}{\lambda_n} \frac{t^{-\alpha}}{\Gamma(1 - \alpha)}, \tag{6.6}$$

where $E_\alpha(z)$ is the one parameter M-L function (8.1). Here we note that for $0 < \alpha < 1$, $E_\alpha(-t^\alpha)$ is a completely monotonic function [32]. For the distributed order memory kernel with $p(\lambda) = 1$ we find the logarithmic decay

$$T_n(t) \sim \frac{T_n(0)}{\lambda_n \tau} \frac{1}{\log t/\tau} \tag{6.7}$$

and for $p(\lambda) = \nu \lambda^{\nu-1}$ the behaviour is [15]

$$T_n(t) \sim \frac{T_n(0)}{\lambda_n \tau} \frac{\Gamma(\nu + 1)}{\log^\nu t/\tau}. \tag{6.8}$$

Finally, the truncated M-L memory kernel (2.33) yields a power-law relaxation with exponential cutoff,

$$T_n(t) \sim \frac{T_n(0)}{\lambda_n} \delta^{-\alpha} e^{-bt} \frac{t^{\beta-\alpha-1}}{\Gamma(\beta-\alpha)}. \quad (6.9)$$

7. Harmonic external potential

The solution of the spatial eigen-equation (6.2) for the physically important case of an external harmonic potential $V(x) = \frac{1}{2}m\omega^2 x^2$, where ω is a frequency, is given in terms of Hermite polynomials $H_n(z)$ [22]

$$X_n(x) = C_n H_n \left(\sqrt{\frac{m\omega^2}{2k_B T}} x \right) \exp \left(-\frac{m\omega^2}{2k_B T} x^2 \right), \quad (7.1)$$

where the eigenvalue spectrum (of the corresponding Sturm-Liouville problem) is given by $\lambda_n = n \frac{\omega^2}{\eta_\gamma}$ for $n = 0, 1, 2, \dots$, and C_n is the normalization constant. From the normalization condition $\int_{-\infty}^{\infty} X_n^2(x) dx = 1$ we obtain the solution in the following form (compare Refs. [72, 76, 77] for the case of a power-law kernel)

$$W(x, t) = \sqrt{\frac{m\omega^2}{2\pi k_B T}} \sum_n \frac{1}{2^n n!} H_n \left(\sqrt{\frac{m\omega^2}{2k_B T}} x \right) \exp \left(-\frac{m\omega^2}{2k_B T} x^2 \right) \times \mathcal{L}^{-1} \left[\frac{\hat{\gamma}(s)}{s\hat{\gamma}(s) + n \frac{\omega^2}{\eta_\gamma}} \right]. \quad (7.2)$$

The term $n = 0$ provides the Gaussian stationary solution

$$W(x, t) = \sqrt{\frac{m\omega^2}{2\pi k_B T}} \exp \left(-\frac{m\omega^2}{2k_B T} x^2 \right). \quad (7.3)$$

It is instructive to derive the first and second moments of the generalized diffusion process in the presence of the harmonic potential $V(x)$. The first moment follows the integro-differential equation

$$\int_0^t \gamma(t-t') \frac{\partial}{\partial t'} \langle x(t') \rangle dt' + \frac{\omega^2}{\eta_\gamma} \langle x(t) \rangle = 0, \quad (7.4)$$

from which by Laplace transform we find the relaxation law for the initial condition $x_0 = \int_{-\infty}^{\infty} x W_0(x) dx$,

$$\langle x(t) \rangle = x_0 \mathcal{L}^{-1} \left[\frac{\hat{\gamma}(s)}{s\hat{\gamma}(s) + \frac{\omega^2}{\eta_\gamma}} \right]. \quad (7.5)$$

Thus for a Dirac delta memory kernel the mean follows the exponential relaxation

$$\langle x(t) \rangle = x_0 e^{-\omega^2 t / \eta_\gamma}, \quad (7.6)$$

as it should. In the case of a power-law memory kernel the M-L relaxation pattern [72, 76, 77]

$$\langle x(t) \rangle = x_0 E_\alpha \left(-\frac{\omega^2}{\eta_\gamma} t^\alpha \right) \quad (7.7)$$

emerges, which in the long time limit assumes the power-law scaling

$$\langle x(t) \rangle \sim \frac{x_0 \eta_\gamma}{\omega^2 \Gamma(1 - \alpha)} \times t^{-\alpha}. \quad (7.8)$$

Starting with a general form $\gamma(t)$ of the memory kernel the asymptotic behaviour of the mean follows in the form

$$\langle x(t) \rangle = x_0 \frac{\eta_\gamma}{\omega^2} \gamma(t) |_{t \rightarrow \infty}, \quad (7.9)$$

since $\lim_{s \rightarrow 0} s \hat{\gamma}(s) = 0$.

The dynamics of the second moment is governed by the integro-differential equation

$$\int_0^t \gamma(t-t') \frac{\partial}{\partial t'} \langle x^2(t') \rangle dt' + 2 \frac{\omega^2}{\eta_\gamma} \langle x^2(t) \rangle = 2K_\gamma. \quad (7.10)$$

Laplace transformation produces

$$\langle x^2(t) \rangle = x_0^2 \mathcal{L}^{-1} \left[\frac{\hat{\gamma}(s)}{s \hat{\gamma}(s) + 2 \frac{\omega^2}{\eta_\gamma}} \right] + \mathcal{L}^{-1} \left[\frac{2K_\gamma}{s \hat{\gamma}(s) + 2 \frac{\omega^2}{\eta_\gamma}} \right], \quad (7.11)$$

which can be rewritten as

$$\langle x^2(t) \rangle = x_{\text{th}}^2 + (x_0^2 - x_{\text{th}}^2) \mathcal{L}^{-1} \left[\frac{\hat{\gamma}(s)}{s \hat{\gamma}(s) + 2 \frac{\omega^2}{\eta_\gamma}} \right], \quad (7.12)$$

where $x_0 = x(0)$ is the initial value of the position, and

$$x_{\text{th}}^2 = \frac{k_B T}{m \omega^2} \quad (7.13)$$

is the stationary (thermal) value, which is reached in the long time limit since $\mathcal{L}^{-1} [\hat{\gamma}(s) / [s \hat{\gamma}(s) + 2\omega^2/\eta_\gamma]] \sim \eta_\gamma / [2\omega^2] \gamma(t) |_{t \rightarrow \infty} \rightarrow 0$. For the Dirac delta memory kernel the second moment approaches the thermal value exponentially,

$$\langle x^2(t) \rangle = x_{\text{th}}^2 + (x_0^2 - x_{\text{th}}^2) \exp \left(-2 \frac{\omega^2}{\eta_\gamma} t \right), \quad (7.14)$$

while for the power-law memory kernel we find the power-law relaxation

$$\begin{aligned}\langle x^2(t) \rangle &= x_{\text{th}}^2 + (x_0^2 - x_{\text{th}}^2) E_\alpha \left(-2 \frac{\omega^2}{\eta_\gamma} t^\alpha \right) \\ &\sim x_{\text{th}}^2 + (x_0^2 - x_{\text{th}}^2) \frac{\eta_\gamma}{2\omega^2} \frac{t^{-\alpha}}{\Gamma(1-\alpha)}.\end{aligned}\quad (7.15)$$

In the case of the distributed order memory kernel (2.22) with constant $p(\lambda) = 1$ we have

$$\langle x^2(t) \rangle \sim x_{\text{th}}^2 + (x_0^2 - x_{\text{th}}^2) \frac{\eta_\gamma}{2\omega^2 \tau} \frac{1}{\log(t/\tau)}.\quad (7.16)$$

When the distribution is of power-law form, $p(\lambda) = \nu \lambda^{\nu-1}$ the second moment assumes the form

$$\langle x^2(t) \rangle \sim x_{\text{th}}^2 + (x_0^2 - x_{\text{th}}^2) \frac{\eta_\gamma}{2\omega^2 \tau} \frac{\Gamma(\nu+1)}{\log^\nu(t/\tau)}.\quad (7.17)$$

Finally, for the truncated M-L memory kernel (2.33) the thermal value is reached in the following way

$$\langle x^2(t) \rangle \sim x_{\text{th}}^2 + (x_0^2 - x_{\text{th}}^2) \frac{\eta_\gamma}{2\omega^2} \delta^{-\alpha} e^{-bt} \frac{t^{\beta-\alpha-1}}{\Gamma(\beta-\alpha)}.\quad (7.18)$$

8. Appendix: Mittag-Leffler functions

The one parameter M-L function is defined by [22]

$$E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}.\quad (8.1)$$

The two parameter M-L function reads [22]

$$E_{\alpha,\beta}(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + \beta)},\quad (8.2)$$

such that $E_{\alpha,1}(z) = E_\alpha(z)$. The three parameter M-L function, also called Prabhakar function [84] is given by

$$E_{\alpha,\beta}^\delta(z) = \sum_{n=0}^{\infty} \frac{(\delta)_n}{\Gamma(\alpha n + \beta)} \frac{z^n}{n!},\quad (8.3)$$

its Laplace transform is [84]

$$\mathcal{L} \left[t^{\beta-1} E_{\alpha,\beta}^\delta(\pm at^\alpha) \right] (s) = \frac{s^{\alpha\delta-\beta}}{(s^\alpha \mp a)^\delta}, \quad \Re(s) > |a|^{1/\alpha},\quad (8.4)$$

and the convergence in complex plane of series in this function is studied in details in [82]. The three parameter M-L function has been applied to

various anomalous diffusion and relaxation processes [11, 89, 91, 93, 94, 110, 111, 112]. Note that $E_{\alpha,\beta}^1(z) = E_{\alpha,\beta}(z)$. For large values of the variable z the following expansion holds [91, 93, 95]

$$E_{\alpha,\beta}^\delta(-z) = \frac{z^{-\delta}}{\Gamma(\delta)} \sum_{n=0}^{\infty} \frac{\Gamma(\delta+n)}{\Gamma(\beta-\alpha(\delta+n))} \frac{(-z)^{-n}}{n!}, \quad |z| > 1. \quad (8.5)$$

In particular, this reduces to the known expansion of the two parameter M-L function [22]

$$E_{\alpha,\beta}(-z) = - \sum_{n=1}^{\infty} \frac{(-z)^{-n}}{\Gamma(\beta-\alpha n)}, \quad |z| > 1. \quad (8.6)$$

The multinomial or multivariate M-L function was introduced by Luchko and Gorenflo [64],

$$\begin{aligned} & E_{(a_1, a_2, \dots, a_N), b}(z_1, z_2, \dots, z_N) \\ &= \sum_{j=1}^{\infty} \sum_{k_1 \geq 0, k_2 \geq 0, \dots, k_N \geq 0}^{k_1 + k_2 + \dots + k_N = j} \binom{j}{k_1 k_2 \dots k_N} \frac{\prod_{i=1}^N (z_i)^{k_i}}{\Gamma(b + \sum_{i=1}^N a_i k_i)}, \end{aligned} \quad (8.7)$$

where

$$\binom{j}{k_1 k_2 \dots k_N} = \frac{j!}{k_1! k_2! \dots k_N!}, \quad (8.8)$$

are the multinomial coefficients. Note that for $N = 1$ we recover the two-parameter M-L function (8.2).

9. Conclusion

We studied a generalized diffusion equation with a general memory kernel with the sole restriction that its Laplace transform is a completely monotonic function. This allows us to consider a wide variety of examples, namely, a combination of a Dirac delta and power-law function, distributed order kernels, and a tempered Mittag-Leffler kernel. Exact results for the associated waiting time PDFs are obtained and we show that for the underlying generalized Fokker-Planck-Smoluchowski equation the linear response relation is satisfied. Moreover, we derive the first and second moments in a confining harmonic potential as well as the general form of the PDF. Finally, we investigate the mode relaxation and the multi-scaling properties from the fractional order moments. In particular, we demonstrate that the multi-scale exponent may also become explicitly time dependent. Our model will be useful in the quantitative description of the anomalous diffusion behaviour in complex systems, including ultraslow and strongly anomalous dynamics.

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