

GENERALIZED MASTER EQUATIONS FOR RANDOM WALKS WITH TIME-DEPENDENT JUMP SIZES

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Abstract. In this work, we develop a unified generalized master equation (GME) framework that extends the theory of continuous time random walks (CTRW) to include the cases when the jump sizes may have a delayed dependence on time and are not restricted to any particular class of distributions. We compare and contrast analytical and numerical behavior of the corresponding master equations, including the instantaneous vs. delayed jump dependence on time and exponential vs. Mittag-Leffler inter-arrival times, with the latter leading to fractional evolution equation. We provide existence and uniqueness proofs for the resulting GMEs.

Key words. CTRW, GME, generalized master equations, fractional dynamics

AMS subject classifications. 45K05, 82B41

1. Introduction. The theory of continuous time random walks (CTRW) became popular in 1960s as a rather general microscopic characterization for diffusion processes. In CTRW, the number of jumps made by a walker during a time interval is a stochastic – often a homogeneous Poisson – process. This concept was first introduced by Montroll and Weiss [1], Montroll and Scher [2], and later on by Klafter and Silbey [3]. Mathematically, a CTRW is a compound renewal process, also called a renewal process with rewards, or a random walk subordinated to a renewal process, and has been treated as such in [4].

CTRW theory has found applications in many areas of science and technology. In particular, it is widely used in financial applications such as insurance risk theory and pricing financial markets [5, 6, 7, 8]. In biology, it is used to model chemotaxis [9, 10]. In geology, CTRW theory has been used in solute transport in porous and fractured media [11, 12], and in earthquake modeling [13, 14]. In physics, CTRWs are useful in modeling transport in fusion plasmas [15], electron tunneling [16], and electron transport in nanocrystalline films [17]. Multiple applications of CTRWs also include reaction-diffusion models [18]-[20], and processes involving anomalous diffusion and fractional dynamics [21, 22, 23, 24, 25, 26].

There have been several generalizations of the CTRW formalism. In [18, 20], Angstman et al. derive a generalized master equation (GME) on a lattice with non-stationary jump sizes and space dependent inter-arrival times for a single particle and for an ensemble of particles undergoing reactions while being subjected to an external force field. In [15], Milligen et al. derive a GME with jump sizes dependent on space and time and space-dependent inter-arrival times. In [27], the generalized continuous time random walk model with a inter-arrival time distribution having dependence on the preceding jump length is considered. In [28], a CTRW master equation on a lattice is derived for the delayed and instantaneous time dependence of the jump under the assumption of nearest neighbor jumps. In [29], a master equation with time-dependent jump sizes and non-homogeneous inter-arrival times was used in a one-dimensional materials coarsening model. Motivated by these earlier results, in the present work we derive GMEs for time-dependent jump sizes.

In the standard CTRW setting, both the inter-arrival times and the jump sizes are assumed to be independent and identically distributed. Moreover, the jump sizes as well as the inter-arrival times are drawn from a joint p.d.f. θ , which is referred to in the literature as the transition probability density function [9, 8]. Another typical assumption in CTRW theory is that the jump sizes are statistically independent of the inter-arrival times; the corresponding process is referred to as a decoupled (or separable)

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CTRW [18, 25, 30]. In this work, we study GMEs when the transition probability θ depends on the time of the current jump, referred to as *instantaneous dependence*, or on the time of the previous jump, referred to as *delayed dependence*. In contrast with the approach used in [28], we do not restrict the jumps to nearest neighbor sites and develop a set of higher order formulations for the systematic study of the hierarchy of CTRW models. While the derived equations are fully compatible with the results obtained in [28] in the case of nearest neighbor jumps, the new framework provides additional insight into the relationship between delayed and non-delayed models.

To fix notations, consider a random walker that starts at $X(0)$ at time $t = 0$. It stays at its position until time T_1 , when it makes a jump of size \mathcal{M}_1 . The walker then waits at $X(0) + \mathcal{M}_1$ until time $T_2 > T_1$, when it makes a new jump of size \mathcal{M}_2 . The process is then repeated. Hence, a wandering particle starts at $X(0)$ and makes a jump \mathcal{M}_n at time T_n . The times T_1, T_2, \dots are called arrival times and they describe the times at which the jump occurs. The times $\mathcal{S}_1 = T_1 - 0, \mathcal{S}_2 = T_2 - T_1, \dots$ are called inter-arrival times and they describe the time span between jumps. Hence we have that

$$T_k = \sum_{i=1}^k \mathcal{S}_i, \quad \forall k \in \mathbb{N}.$$

and the position of a walker at time t is given by

$$X_t = X_0 + \sum_{i=1}^{n_t} \mathcal{M}_i,$$

where $n_t = \max\{n : T_n \leq t\}$ is the counting process of jumps. In this context, we can think of X_t as a compound Poisson process.

We denote $w(s)$ as the probability density function of the inter-arrival times and $\mu(r)$ as the probability density function of the jump sizes. The survival function, which describes the probability that a walker arriving at a site pauses for at least time t before leaving that site, is defined by

$$\psi(t) = 1 - \int_0^t w(s) ds.$$

We will generalize the framework of CTRW by dropping the assumption of identically distributed jump sizes, i.e., we let \mathcal{M}_t be the stochastic process of jump sizes at time t with p.d.f. $\mu(r, t)$. X_t will then be the corresponding compound Poisson process. We define $p(x, t)$ to be the probability density function such that $p(x, t) dx$ gives the probability that the position of a walker lies inside the interval $(x, x + dx)$ at time t .

The general form of the transition probability of taking a jump from $X_{t_0} = x_0$ to $X_t = x$ is given by $\theta(x - x_0, t - t_0, t, t_0)$. Under the assumption that the jump sizes and the inter-arrival times are statistically independent,

$$\theta(x - x_0, t - t_0, t, t_0) = \mu(x - x_0, t, t_0) w(t - t_0, t) = \mu(r, t, t_0) w(s, t) \quad (1.1)$$

with $s = t - t_0$ and $r = x - x_0$. Table 1.1 summarizes various types of transition probability functions θ considered in this work. Master equations have been derived for the standard case in [31, 32, 9, 10]. The ‘instantaneous’ master equations have been derived in [33, 29]. In this study, we derive the ‘delayed’ master equations. Interested reader can find regularity results for this family of evolution equations in the recent works of [34, 35].

While a more general treatment is possible, in this work we focus on exponential and Mittag-Leffler inter-arrival times due to their importance in various practical applications. We show that exponential

inter-arrivals (standard CTRW model) as well as Mittag-Leffler inter-arrivals (fractional CTRW) coupled with different types of jump size distributions lead to slightly different types of GMEs.

The paper is organized as follows. In Section 2, we review the master equations derived in the case of identically distributed jump sizes and identically distributed inter-arrival times. In Section 3, we derive generalized master equations in the case of non-identically distributed jump sizes and numerically compare the instantaneous and delayed GMEs. Summary is provided in Section 4.

	$\mu(\cdot)$	$w(\cdot)$	Section
Standard Case	$\mu(x - x_0)$	$w(t - t_0)$	Section 2
Homogeneous Instantaneous Case	$\mu(x - x_0, t)$	$w(t - t_0)$	Section 3.1
Homogeneous Delayed Case	$\mu(x - x_0, t_0)$	$w(t - t_0)$	Section 3.2

Table 1.1: Different CTRW cases considered in this paper.

2. Standard CTRW framework. In this section, we assume that the jump sizes and inter-arrival times are both identically distributed, i.e., $w(s, t) = w(s)$ and $\mu(r, t) = \mu(r) \forall t \geq 0$. Hence, the transition probability of taking a jump from $X_{t_0} = x_0$ to $X_t = x$ is represented by $\theta(x - x_0, t - t_0)$. Moreover,

$$\theta(x - x_0, t - t_0) = \mu(x - x_0)w(t - t_0) = \mu(r)w(s),$$

with $s = t - t_0$ and $r = x - x_0$. Natural probabilistic reasoning, used in [2, 1], leads us to the CTRW master equation for the probability density $p(x, t) = P(X_t = x)$ of the particle, with initial configuration $p(x, 0)$, being in position x at time t

$$p(x, t) = p(x, 0)\psi(t) + \int_0^t w(t - t') \left[\int_{-\infty}^{\infty} \mu(r)p(x - r, t')dr \right] dt'. \quad (2.1)$$

Taking the Laplace and Fourier transforms of (2.1), implies the Montroll-Weiss equation [2, 1],

$$\hat{p}(k, s) = \frac{1 - \hat{w}(s)}{s} \frac{\tilde{p}(k, 0)}{1 - \hat{w}(s)\tilde{\mu}(k)}. \quad (2.2)$$

Solutions to the one-dimensional master equation (2.1) and its counterpart in Laplace-Fourier space (2.2) can be found in the literature [36, 37, 38, 39, 40, 41, 30].

2.1. Exponential inter-arrival times. Let $w(t) = \lambda \exp(-\lambda t)$, $\forall t > 0$. Then we write (2.1) as,

$$e^{\lambda t}p(x, t) = p(x, 0) + \lambda \int_0^t \int_{\mathbb{R}} e^{\lambda \tau} \mu(r)p(x - r, \tau)drd\tau \quad (2.3)$$

Differentiating (2.3), we obtain

$$\frac{d}{dt}[e^{\lambda t}p(x, t)] = \lambda \int_{\mathbb{R}} \mu(r)e^{\lambda t}p(x - r, t)dr. \quad (2.4)$$

Hence

$$\frac{\partial}{\partial t}p(x, t) = \lambda \int_{\mathbb{R}} \mu(r)[p(x - r, t) - p(x, t)]dr. \quad (2.5)$$

We have derived the continuous time random walk master equation (2.5) for exponentially distributed inter-arrival times. By differentiating (2.4), we have that

$$\lambda^2 p(x, t) + 2\lambda \frac{\partial}{\partial t} p(x, t) + \frac{\partial^2}{\partial t^2} p(x, t) = \int_{\mathbb{R}} \mu(r) \left[\lambda^2 p(x-r, t) + \lambda \frac{\partial}{\partial t} p(x-r, t) \right] dr. \quad (2.6)$$

Letting $\bar{p}(x, t) = \lambda^2 p(x, t) + \lambda \frac{\partial}{\partial t} p(x, t)$, we have that (2.6) implies

$$\frac{\partial}{\partial t} \bar{p}(x, t) = \lambda \int_{\mathbb{R}} [\bar{p}(x-r, t) - \bar{p}(x, t)] \mu(r) dr. \quad (2.7)$$

Hence under the assumption of identically distributed jump sizes, we have that $p(x, t)$ satisfies both (2.5) and (2.7).

Let us describe a known solution to (2.2) found in [25]. Taking the Laplace and Fourier transform of (2.4), we derive

$$u \hat{p}(k, u) - \bar{p}(k, 0) = \lambda \tilde{\mu}(k) \hat{p}(k, u) - \lambda \hat{p}(k, u). \quad (2.8)$$

Let $p(x, 0) = \delta(x)$ and choose a kernel $\mu(r)$ with Taylor approximation in Fourier space given by

$$\tilde{\mu}(k) \sim 1 - \sigma^2 k^2 + \mathcal{O}(k^4),$$

such as the Gaussian kernel with mean 0 and variance σ^2 . Then we can solve for $\hat{p}(k, u)$ in (2.8), up to order $\mathcal{O}(uk^2)$

$$\hat{p}(k, u) = \frac{1}{u + \sigma^2 \lambda k^2}. \quad (2.9)$$

After taking the inverse Laplace and inverse Fourier transform of (2.9), we derive the well-known Gaussian propagator

$$p(x, t) = \frac{1}{\sqrt{4\pi\lambda\sigma^2 t}} \exp\left(-\frac{x^2}{4\lambda\sigma^2 t}\right) \quad (2.10)$$

which satisfies the standard diffusion equation

$$\frac{\partial}{\partial t} p(x, t) = \sigma^2 \lambda \frac{\partial^2}{\partial x^2} p(x, t). \quad (2.11)$$

We will show in later sections that the instantaneous and delayed master equations also reduce to a standard diffusion equation under some assumptions on the initial condition $p(x, 0)$ and the jump size distribution $\mu(r, t)$.

2.2. Mittag-Leffler inter-arrival times. We begin with a succinct summary of definitions in fractional calculus. We define the Riemann-Liouville fractional derivative as

$$D_x^\beta f(x) = \frac{d}{dx} (I^{1-\beta}(f)[x]), \quad \beta \in (0, 1).$$

and the Caputo fractional derivative as

$$\partial_x^\beta f(x) = I^{1-\beta}(f') [x], \quad \beta \in (0, 1)$$

where the fractional operator

$$I^\beta(f)[x] = \begin{cases} \frac{1}{\Gamma(\beta)} \int_0^x \frac{f(t)}{(x-t)^{1-\beta}} dt, & \text{if } \beta \in (0, 1] \\ f(t), & \text{if } \beta = 0 \end{cases}$$

is referred to as the Riemann-Liouville fractional integral of order $\beta \in [0, 1]$. The Caputo and Riemann-Liouville fractional derivatives are related by

$$\partial_x^\beta f(x) = D_x^\beta f(x) - \frac{f(0)}{x^\beta \Gamma(1-\beta)}, \quad (2.12)$$

where $\Gamma(\cdot)$ denotes the gamma function. We now let $w(t) = -\frac{d}{dt}E_\beta(-t^\beta)$ for $\beta \in (0, 1)$ where $E_\beta(\cdot)$ denotes the Mittag-Leffler function defined by

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

The interested reader may find more information on the Mittag-Leffler function in [42]. Following the steps in [31], we have that (2.1) reduces to

$$\partial_t^\beta p(x, t) = \int_{\mathbb{R}} [p(x-r, t) - p(x, t)] \mu(r) dr. \quad (2.13)$$

3. Generalized CTRW framework: homogeneous case. In this section, we assume that the jump sizes are not identically distributed, i.e., $\mu(r, t)$; but the inter-arrival times are, i.e., $w(s, t) = w(s) \forall t \geq 0$.

3.1. Instantaneous dependence. In the case of instantaneous dependence, the transition probability of taking a jump from $X_{t_0} = x_0$ to $X_t = x$ is represented by $\theta(x - x_0, t - t_0, t)$. In particular,

$$\theta(x - x_0, t - t_0, t) = \mu(x - x_0, t) w(t - t_0) = \mu(r, t) w(s), \quad (3.1)$$

with $s = t - t_0$ and $r = x - x_0$. In [29] it was shown that the following result holds.

LEMMA 3.1. *In CTRW with transition probability $\theta(r, s, t) = \mu(r, t) w(s)$, the probability distribution function $p(x, t)$ satisfies the master equation*

$$p(x, t) = \psi(t) p(x, 0) + \int_0^t \int_{\mathbb{R}} w(t-s) \mu(r, s) p(x-r, s) dr ds, \quad (3.2)$$

for all $x \in \mathbb{R}$ and $t > 0$, where $p(x, 0)$ is the initial condition.

3.1.1. Exponential inter-arrival times. The following result holds for the case of exponential inter-arrival times and instantaneous dependence of jump sizes, in direct analogy with equation (2.5) derived for the identically distributed jump size case. Note that it is not possible to derive an analogue of equation (2.6) for this case.

LEMMA 3.2. *Let the inter-arrival times in Lemma 3.1 be exponentially distributed according to $w(t) = \lambda e^{-\lambda t}$. Then the probability density $p(x, t)$ satisfies*

$$\frac{\partial}{\partial t} p(x, t) = \lambda \int_{\mathbb{R}} \mu(r, t) [p(x-r, t) - p(x, t)] dr. \quad (3.3)$$

Proof. The proof of this result is given in Lemma 2 in [29]. \square

Clearly, using a time-independent Gaussian jump size distribution with mean 0 and variance σ^2 and initial condition $p(x, 0) = \delta(x)$, leads to $p(x, t)$ of the form (2.10) which satisfies the diffusion equation (2.11) as seen in Section 2.1. Therefore under these assumptions, we have that (3.3) behaves as the standard diffusion equation.

Before stating the existence and uniqueness result, we first need to define the space of the solution $C(D; C^1([0, \tau]))$ in the following manner. $C(D; C^1([0, \tau])) = \{f \in D \times [0, \tau] \mid \|f\|_{C(D; C^1([0, \tau]))} < \infty\}$ with

$$\|f\|_{C(D;C^1([0,\tau]))} = \max_{x \in D, t \in [0,\tau]} |f(x,t)| + \max_{x \in D, t \in [0,\tau]} \left| \frac{\partial}{\partial t} f(x,t) \right|.$$

THEOREM 3.3. *Assume $\mu(r,t) \in C(D \times [0,\tau])$ where $D \subset \mathbb{R}$ is the compact support of $\mu(r,t)$. Then for any $p(x,0) \in C(D)$, there exists a unique solution $p(x,t) \in C(D;C^1([0,\tau]))$ to (3.3).*

Proof. Consider the integral form of the equation (3.3),

$$e^{\lambda t} p(x,t) = p(x,0) + \lambda \int_0^t \int_{\mathbb{R}} e^{\lambda s} p(x-r,s) \mu(r,s) dr ds. \quad (3.4)$$

If we let $f(x,t) = e^{\lambda t} p(x,t)$ and $g(x,t) = p(x,t)$, we can write (3.4) as

$$f(x,t) = \lambda \int_0^t \int_{\mathbb{R}} \mu(r,s) f(x-r,s) dr ds + g(x,0) = g(x,0) + \lambda \int_0^t \int_{\mathbb{R}} \mu(x-r,s) f(r,s) dr ds. \quad (3.5)$$

Since $p(x,0) \in C(D)$, $g(x,0) \in C(D)$. Since μ is continuous on a compact domain, then

$$|\mu(r,t)| < M < \infty, \quad \forall r, t.$$

We now proceed by Picard iteration, i.e.,

$$\begin{aligned} f_0(x,t) &= g(x,0) \\ f_1(x,t) &= g(x,0) + \lambda \int_0^t \int_{\mathbb{R}} \mu(x-r,s) g(r,0) dr ds \\ f_1(x,t) &= g(x,0) + \lambda \int_0^t \int_{\mathbb{R}} K_1(x,r,s) g(r,0) dr ds, \end{aligned}$$

where $K_1(x,r,s) = \mu(x-r,s)$. Using induction, we have

$$f_n(x,t) = g(x,0) + \lambda \sum_{j=1}^n \lambda^{j-1} \int_0^t \int_{\mathbb{R}} K_j(x,r,s) g(r,0) dr ds, \quad (3.6)$$

where K_j is defined recursively as

$$K_{j+1}(x,r,s) = \int_0^s \int_{\mathbb{R}} \mu(x-r_1,s) K_j(r_1,r,s_1) dr_1 ds_1.$$

$K_j(x,0,s)$ can be thought as the j -fold convolution of the jump sizes. Since $K_{j+1}(x,r,s) \leq M \frac{s^j}{j!}$,

$$\sum_{j=1}^{\infty} \lambda^{j-1} K_j(x,r,s) = \sum_{j=0}^{\infty} \lambda^j K_{j+1}(x,r,s) \leq M \sum_{j=0}^{\infty} \frac{(\lambda s)^j}{j!} = M e^{\lambda s} < \infty.$$

So the series converges uniformly by the Weierstrass M-test. This implies that the sequence f_n converges. Then $f(x,t) = \lim_{n \rightarrow \infty} f_n(x,t)$ takes the form

$$f(x,t) = g(x,0) + \lambda \int_0^t \int_{\mathbb{R}} R(x,r,s) g(r,0) dr ds, \quad (3.7)$$

where

$$R(x,r,s) = \sum_{j=1}^{\infty} \lambda^{j-1} K_j(x,r,s)$$

is called the resolvent kernel of μ . $f(x, t)$ satisfies (3.5), since

$$\begin{aligned} f(x, t) &= \lim_{n \rightarrow \infty} f_n(x, t) \\ &= g(x, 0) + \lambda \int_0^t \int_{\mathbb{R}} \mu(x-r, s) \lim_{n \rightarrow \infty} f_{n-1}(r, s) dr ds \\ &= g(x, 0) + \lambda \int_0^t \int_{\mathbb{R}} \mu(x-r, s) f(r, s) dr ds, \end{aligned}$$

which proves existence. Let us now write (3.5) in operator form

$$(I - L)[f](x, t) = g(x, 0),$$

where the mapping $L : C(D \times [0, \tau]) \rightarrow C(D \times [0, \tau])$ is defined by

$$L[f](x, t) = \lambda \int_0^t \int_{\mathbb{R}} \mu(x-r, s) f(r, s) dr ds.$$

To prove uniqueness of the solution $f(x, t)$, it is enough to show that the homogeneous equation

$$(I - L)[f](x, t) = 0$$

is satisfied only by the trivial solution. This follows from the Banach fixed-point theorem, hence $I - L$ is invertible and there exists a unique solution $f(x, t) \in C(D \times [0, \tau])$ satisfying (3.5). Since g and f are defined in terms of p , we have that for a given $p(x, 0) \in C(D)$, there exists a unique solution $p(x, t) \in C(D \times [0, \tau])$ satisfying (3.5). Due to (3.7), we have that $p(x, t) \in C(D; C^1([0, \tau]))$. \square

REMARK 3.1. *The solution of (3.7) can be written as*

$$p(x, t) = e^{-\lambda t} p(x, 0) + \lambda e^{-\lambda t} \int_0^t \int_{\mathbb{R}} R(x, r, s) p(r, 0) dr ds. \quad (3.8)$$

Note that (3.8) matches results found in the literature [24, 43, 30] for time independent jump sizes and exponentially distributed inter-arrival times.

3.1.2. Mittag-Leffler inter-arrival times. The following result holds for the case of Mittag-Leffler inter-arrival times and instantaneous dependence of jump sizes. It is the direct analogue of (2.13) derived in the identically distributed jump size case.

LEMMA 3.4. *Let the inter-arrival times in Lemma 3.1 be distributed according to $w(t) = -\frac{d}{dt} E_\beta(-t^\beta)$ for $\beta \in (0, 1)$. Then probability density $p(x, t)$ satisfies*

$$\partial_t^\beta p(x, t) = \int_{\mathbb{R}} \mu(r, t) [p(x-r, t) - p(x, t)] dr. \quad (3.9)$$

Proof. The proof follows the same steps as in Lemma 2 of [29]. \square

The following Section contains the main results of this paper. Namely, it provides derivations of the generalized master equations and corresponding existence-uniqueness proofs for the case of delayed dependence of the jump sizes.

3.2. Delayed dependence. In the case of delayed dependence, the transition probability of taking a jump from $X_{t_0} = x_0$ to $X_t = x$ is represented by $\theta(x - x_0, t - t_0, t_0)$. In particular,

$$\theta(x - x_0, t - t_0, t_0) = \mu(x - x_0, t_0) w(t - t_0) = \mu(r, t_0) w(s), \quad (3.10)$$

with $s = t - t_0$ and $r = x - x_0$.

3.2.1. Exponential inter-arrival times. As in the previous case of instantaneous dependence, we first consider exponentially distributed inter-arrival times. We obtain the following analogue of (2.7) derived for the identically distributed jump sizes case. Note that in contrast with the instantaneous case, there is no analogue of equation (2.5) in this case.

THEOREM 3.5. *Consider CTRW with transition probability $\theta(r, s, t_0) = \mu(r, t_0)w(s)$ and $w(s) = \lambda e^{-\lambda s}$. The probability density function $p(x, t)$, with initial configuration $p(x, 0)$, satisfies the following generalized master equation*

$$\frac{\partial}{\partial t} \bar{p}(x, t) = \lambda \int_{\mathbb{R}} [\bar{p}(x - r, t) - \bar{p}(x, t)] \mu(r, t) dr, \quad (3.11)$$

where

$$\bar{p}(x, t) = p(x, t) + \frac{1}{\lambda} \frac{\partial}{\partial t} p(x, t), \quad (3.12)$$

Proof. Following the steps as in the proof of Lemma 3.1, we have the Volterra integral equation for the probability density function $Q(x, t)$ representing walkers arriving in the interval $(x, x + dx)$ at time t after any number of steps

$$Q(x, t) = \delta_x \delta(t) + \int_0^t \int_{\mathbb{R}} \mu(r, \tau) w(t - \tau) Q(x - r, \tau) dr d\tau. \quad (3.13)$$

The probability density function of being at x at time t given that the walker starts at the origin $P(x, t|0)dx$ can now be computed as the product of the probability of arriving in this interval at some time $\tau < t$, multiplied by the probability that no transition occurs in the remaining time $t - \tau$. Thus

$$\begin{aligned} P(x, t|0) &= \int_0^t \psi(t - \tau) Q(x, \tau) d\tau \\ &= \psi(t) \delta_x + \int_0^t w(t - \tau) \int_0^\tau \int_{\mathbb{R}} \mu(r, s) \psi(\tau - s) Q(x - r, s) dr ds d\tau \end{aligned} \quad (3.14)$$

Taking the Laplace transform of $P(x, t|0) = \int_0^t \psi(t - \tau) Q(x, \tau) d\tau$ and rearranging terms,

$$\hat{Q}(x, u) = u \hat{P}(x, u|0) + \lambda \hat{P}(x, u|0) = u \hat{P}(x, u|0) - P(x, 0|0) + \lambda \hat{P}(x, u|0) + \delta_x. \quad (3.15)$$

Hence taking the inverse Laplace transform of (3.15) provides us with such expression,

$$Q(x, t) = \frac{\partial}{\partial t} P(x, t|0) + \lambda P(x, t|0) + \delta(t) \delta_x. \quad (3.16)$$

Substituting (3.16) into (3.14), we have that $P(x, t|0)$ satisfies the following renewal equation

$$\begin{aligned} P(x, t|0) &= \psi(t) \delta_x + \\ &+ \int_0^t w(t - \tau) \int_0^\tau \int_{\mathbb{R}} \mu(r, s) \frac{w(\tau - s)}{\lambda} \left(\frac{\partial}{\partial s} P(x - r, s|0) + \lambda P(x - r, s|0) + \delta(s) \delta_{x-r} \right) dr ds d\tau. \end{aligned} \quad (3.17)$$

If instead $P(x, 0|x_0) = \delta_{x-x_0}$, then (3.17) changes to

$$\begin{aligned} P(x, t|x_0) &= \psi(t) \delta_{x-x_0} + \\ &+ \int_0^t w(t - \tau) \int_0^\tau \int_{\mathbb{R}} \mu(r, s) \frac{w(\tau - s)}{\lambda} \left(\frac{\partial}{\partial s} P(x - r, s|x_0) + \lambda P(x - r, s|x_0) + \delta(s) \delta_{x-r-x_0} \right) dr ds d\tau. \end{aligned} \quad (3.18)$$

Since the initial state of the walker is given by $p(x, 0)$, then

$$p(x, t) = \int_{\mathbb{R}} P(x, t|x_0)p(x_0, 0)dx_0.$$

Hence $p(x, t)$ satisfies the following master equation

$$p(x, t) = \psi(t)p(x, 0) + \int_0^t \int_{\mathbb{R}} w(t-\tau) \int_0^\tau \mu(r, s) \frac{w(\tau-s)}{\lambda} \left(\frac{\partial}{\partial s} p(x-r, s) + \lambda p(x-r, s) + \delta(s)p(x-r, 0) \right) ds dr d\tau, \quad (3.19)$$

as follows from (3.18). Taking the Laplace transform of (3.19) and manipulating the terms, we arrive at

$$\begin{aligned} \hat{\Phi}(u)(u\hat{p}(x, u) - p(x, 0)) + \hat{p}(x, u) &= \\ = \int_{\mathbb{R}} \mathcal{L}_t \left[\int_0^t \mu(r, s) \frac{w(t-s)}{\lambda} \left(\frac{\partial}{\partial s} p(x-r, s) + \lambda p(x-r, s) + \delta(s)p(x-r, 0) \right) ds \right] (u) dr, \end{aligned} \quad (3.20)$$

where

$$\hat{\Phi}(u) = \frac{1 - \hat{w}(u)}{u\hat{w}(u)}.$$

We have that

$$w(t) = \lambda e^{-\lambda t} \implies \hat{w}(u) = \frac{\lambda}{u + \lambda} \implies \hat{\Phi}(u) = \frac{1}{\lambda} \implies \Phi(t) = \frac{1}{\lambda} \delta(t).$$

Thus taking the inverse Laplace transform of (3.20),

$$\frac{\partial}{\partial t} p(x, t) + \lambda p(x, t) = \int_{\mathbb{R}} \int_0^t \mu(r, s) w(t-s) \left(\frac{\partial}{\partial s} p(x-r, s) + \lambda p(x-r, s) + \delta(t)p(x-r, 0) \right) ds dr. \quad (3.21)$$

Substituting $w(s) = \lambda e^{-\lambda s}$ into (3.21),

$$\frac{d}{dt} [e^{\lambda t} p(x, t)] = \lambda \int_{\mathbb{R}} \int_0^t \mu(r, s) \frac{d}{ds} [e^{\lambda s} p(x-r, s)] ds dr + \lambda \int_{\mathbb{R}} \mu(r, 0) F(x-r) dr. \quad (3.22)$$

Taking the derivative of (3.22) with respect to t ,

$$\frac{d^2}{dt^2} [e^{\lambda t} p(x, t)] = \lambda \int_{\mathbb{R}} \mu(r, t) \frac{d}{dt} [e^{\lambda t} p(x-r, t)] dr. \quad (3.23)$$

Finally, we have that (3.23) is equivalent to

$$\lambda^2 p(x, t) + 2\lambda \frac{\partial}{\partial t} p(x, t) + \frac{\partial^2}{\partial t^2} p(x, t) = \int_{\mathbb{R}} [\lambda^2 p(x-r, t) + \lambda \frac{\partial}{\partial t} p(x-r, t)] \mu(r, t) dr. \quad (3.24)$$

Letting $\bar{p}(x, t) = p(x, t) + \frac{1}{\lambda} \frac{\partial}{\partial t} p(x, t)$, we see that $\bar{p}(x, t)$ satisfies (3.11). \square

In summary, we have that $p(x, t)$ satisfies (3.24) and (3.11) which are the analogues of (2.6) and (2.7), respectively, for the identically distributed jump size case. However, there is no analogue of equation (2.5) for $p(x, t)$ in this case.

REMARK 3.2. *The system (3.11)-(3.12) can be solved using the following two-step procedure. First, $\bar{p}(x, t)$ can be resolved from equation (3.11). Next, the following expression can be used to find $p(x, t)$ from (3.12)*

$$p(x, t) = e^{-\lambda t} p(x, 0) + \lambda \int_0^t \bar{p}(x, s) e^{\lambda(s-t)} ds. \quad (3.25)$$

REMARK 3.3. We can notice that under certain assumptions, we have that system (3.11)-(3.12) behave as the standard diffusion (2.11). Indeed, let $p(x, 0) = \delta(x)$ and choose the kernel $\mu(r, t) = \mu(r)$ with Taylor approximation in Fourier space given by $\mu(k) \sim 1 - \sigma^2 k^2 + \mathcal{O}(k^4)$, as is the case for the Gaussian kernel, for instance. Taking the Laplace and Fourier transform of (3.11), we derive an expression similar to (2.9):

$$\hat{\tilde{p}}(k, u) = \frac{\tilde{p}(k, 0)}{u + \sigma^2 \lambda k^2}. \quad (3.26)$$

In Fourier-Laplace space, (3.26) becomes

$$\hat{\tilde{p}}(k, u) = \left(\frac{\lambda + u}{\lambda} \right) \hat{p}(k, u) - \frac{1}{\lambda}. \quad (3.27)$$

Let $\bar{p}(x, 0) = \delta(x) + \sigma^2 \delta''(x)$. Plugging (3.27) in (3.26), we derive the following expression for $\hat{p}(k, u)$:

$$\frac{\lambda + u}{\lambda} \hat{p}(k, u) = \frac{1 - \sigma^2 k^2}{u + \lambda \sigma^2 k^2} + \frac{1}{\lambda} + \mathcal{O}(uk^2) \quad (3.28)$$

Now (3.28) can be simplified to

$$\hat{p}(k, u) = \frac{1}{u + \lambda \sigma^2 k^2}. \quad (3.29)$$

After taking the inverse Laplace and Fourier transforms of (3.29), $p(x, t)$ is of the form (2.10) and satisfies the diffusion equation (2.11).

REMARK 3.4. Notice that to get to the diffusion behavior for $p(x, t)$ in the argument above, we needed to fix $\bar{p}(x, 0) = \delta(x) + \sigma^2 \delta''(x)$. If instead we let $\bar{p}(x, 0) = \delta(x)$, then (3.26) simplifies to

$$\hat{\tilde{p}}(k, u) = \frac{1}{u + \sigma^2 \lambda k^2} \quad (3.30)$$

and $\bar{p}(x, t)$ takes the form (2.10) after taking the inverse Laplace and Fourier transforms. Hence we obtain diffusion in $\bar{p}(x, t)$, while by means of (3.25), we can see that $p(x, t)$ satisfies

$$p(x, t) = e^{-\frac{1}{\lambda}t} p(x, 0) + \frac{1}{\lambda} e^{-\frac{1}{\lambda}t} \int_0^t \frac{1}{\sqrt{4\pi\sigma^2\lambda s}} \exp\left(-\frac{x^2}{4\sigma^2\lambda s} + \frac{s}{\lambda}\right) ds. \quad (3.31)$$

THEOREM 3.6. Assume $\mu(r, t) \in C(D \times [0, \tau])$ where $D \subset \mathbb{R}$ is the compact support of $\mu(r, t)$. Then for any $p(x, 0) \in C(D)$, there exists a unique solution $p(x, t) \in C(D; C^2([0, \tau]))$ to (3.24).

Proof. Proof is similar to the argument in Theorem 3.3. The additional regularity of the solution comes from (3.25). \square

3.2.2. Mittag-Leffler inter-arrival times. The following result relating Caputo and Riemann-Liouville fractional derivatives is useful.

LEMMA 3.7. Let D_t^β denote the Riemann-Liouville fractional derivative and ∂_t^β denote the Caputo fractional derivative with $\beta \in (0, 1)$. Then

$$\begin{aligned} D_t^\beta \left(\partial_t^{1-\beta} p(x, t) \right) &= \frac{\partial}{\partial t} p(x, t), \\ D_t^\beta \left(\frac{p(x, 0)}{\Gamma(\beta)} t^{\beta-1} \right) &= 0, \text{ and} \\ D_t^\beta \left(\frac{\partial}{\partial t} p(x, t) \right) &= \frac{\partial}{\partial t} \partial_t^\beta p(x, t). \end{aligned}$$

Proof. We start by proving the first relation

$$\begin{aligned} D_t^\beta \left(\partial_t^{1-\beta} p(x, t) \right) &= \frac{\partial}{\partial t} I^{1-\beta} I^\beta \left(\frac{\partial}{\partial t} p(x, t) \right) \\ &= \frac{\partial}{\partial t} I \left(\frac{\partial}{\partial t} p(x, t) \right) \\ &= \frac{\partial}{\partial t} p(x, t), \end{aligned}$$

where $I(\cdot)$ denotes the Riemann-Liouville fractional integral of order 1. The second relation is standard and can be found in any book on fractional calculus e.g. [42], and the third relation follows immediately from the definition of the Caputo and Riemann-Liouville fractional derivatives. \square

In the following theorem, we use Lemma 3.7 to derive the corresponding generalized master equation for Mittag-Leffler inter-arrival times.

THEOREM 3.8. *Consider CTRW with transition probability $\theta(r, s, t_0) = \mu(r, t_0)w(s)$ and $w(s) = -\frac{d}{ds}E_\beta(-s^\beta)$ with $\beta \in (0, 1)$. The probability density function $p(x, t)$, with initial configuration $p(x, 0)$, satisfies the following generalized master equation*

$$D_t^\beta \bar{p}(x, t) = \int_{\mathbb{R}} [\bar{p}(x-r, t) - \bar{p}(x, t)] \mu(r, t) dr, \quad (3.32)$$

where $\bar{p}(x, t) = \frac{\partial}{\partial t} p(x, t) + \partial_t^{1-\beta} p(x, t) + p(x, 0)\Phi_\beta(t)$ and $\Phi_\beta(t) = \frac{t^{\beta-1}}{\Gamma(\beta)}$.

Proof. We have that

$$w(t) = -\frac{d}{dt} E_\beta(-t^\beta) \implies \psi(t) = E_\beta(-t^\beta).$$

Then

$$\hat{w}(u) = \frac{1}{u^\beta + 1}, \quad \hat{\psi}(u) = \frac{1}{u + u^{1-\beta}}, \quad \text{and} \quad \hat{\Phi}_\beta(u) = u^{-\beta}.$$

Following similar steps as in the proof of Theorem 3.5, we take the Laplace transform of $P(x, t|0) = \int_0^t \psi(t-\tau)Q(x, \tau)d\tau$ and rearrange terms,

$$\hat{Q}(x, u) = (u\hat{P}(x, u|0) - P(x, 0|0)) + (u^{1-\beta}\hat{P}(x, u|0) - u^{-\beta}P(x, 0|0)) + \delta_x + u^{-\beta}\delta_x. \quad (3.33)$$

Taking the inverse Laplace transform of (3.33),

$$Q(x, t) = \frac{\partial}{\partial t} P(x, t|0) + \partial_t^{1-\beta} P(x, t|0) + \delta_x \delta(t) + \delta_x \Phi_\beta(t). \quad (3.34)$$

Now using this form of $Q(x, t)$ in the relation (3.14) together with $\psi(s) = E_\beta(-s^\beta)$, we have that $P(x, t|0)$ satisfies the following renewal equation

$$\begin{aligned} P(x, t|0) &= \psi(t)\delta_x + \int_0^t w(t-\tau) \int_{\mathbb{R}} \mu(r, s) E_\beta(-(\tau-s)^\beta) \cdot \\ &\cdot \left(\frac{\partial}{\partial s} P(x-r, s|0) + \partial_s^{1-\beta} P(x-r, s|0) + \delta(s)\delta_{x-r} + \delta_{x-r}\Phi_\beta(s) \right) dr ds d\tau. \end{aligned} \quad (3.35)$$

If instead $P(x, 0|x_0) = \delta_{x-x_0}$, then (3.35) becomes

$$\begin{aligned} P(x, t|x_0) &= \psi(t)\delta_{x-x_0} + \int_0^t w(t-\tau) \int_{\mathbb{R}} \mu(r, s) E_\beta(-(\tau-s)^\beta) \cdot \\ &\cdot \left(\frac{\partial}{\partial s} P(x-r, s|x_0) + \partial_s^{1-\beta} P(x-r, s|x_0) + \delta(s)\delta_{x-r-x_0} + \delta_{x-r-x_0}\Phi_\beta(s) \right) dr ds d\tau. \end{aligned} \quad (3.36)$$

Finally, for $p(x, t) = \int_{\mathbb{R}} P(x, t|x_0)p(x_0, 0)dx_0$, we get the following generalized master equation

$$p(x, t) = \psi(t)p(x, 0) + \int_0^t \int_{\mathbb{R}} w(t - \tau) \int_0^\tau \mu(r, s) E_\beta(-(\tau - s)^\beta) \cdot \left(\frac{\partial}{\partial s} p(x - r, s) + \partial_s^{1-\beta} p(x - r, s) + \delta(s)p(x - r, 0) + p(x - r, 0)\Phi_\beta(s) \right) ds dr d\tau. \quad (3.37)$$

Taking the Laplace transform of (3.37) and manipulating the resulting expression,

$$\begin{aligned} & \left[u(u^\beta \hat{p}(x, u) - u^{\beta-1} p(x, 0)) - \partial_t^\beta p(x, 0) \right] + 2(u\hat{p}(x, u) - p(x, 0)) + \\ & + (u^{1-\beta} \hat{p}(x, u) - u^{-\beta} p(x, 0)) + p(x, 0) + p(x, 0)u^{-\beta} = \\ & = \int_{\mathbb{R}} \mathcal{L}_t \left[\mu(r, t) \left(\frac{\partial}{\partial t} p(x - r, t) + \partial_t^{1-\beta} p(x - r, t) + \delta(t)p(x - r, 0) + p(x - r, 0)\Phi_\beta(t) \right) \right] (u) dr. \end{aligned} \quad (3.38)$$

Finally, taking the inverse Laplace transform of (3.38),

$$\begin{aligned} & \left[\frac{\partial}{\partial t} \partial_t^\beta p(x, t) + \frac{\partial}{\partial t} p(x, t) \right] + \left[\frac{\partial}{\partial t} p(x, t) + \partial_t^{1-\beta} p(x, t) + \delta(t)p(x, 0) + p(x, 0)\Phi_\beta(t) \right] = \\ & \int_{\mathbb{R}} \mu(r, t) \left[\frac{\partial}{\partial t} p(x - r, t) + \partial_t^{1-\beta} p(x - r, t) + \delta(t)p(x - r, 0) + p(x - r, 0)\Phi_\beta(t) \right] dr. \end{aligned} \quad (3.39)$$

Since $t > 0$, (3.39) simplifies to

$$\begin{aligned} & \left[\frac{\partial}{\partial t} \partial_t^\beta p(x, t) + \frac{\partial}{\partial t} p(x, t) \right] + \left[\frac{\partial}{\partial t} p(x, t) + \partial_t^{1-\beta} p(x, t) + p(x, 0)\Phi_\beta(t) \right] = \\ & \int_{\mathbb{R}} \mu(r, t) \left[\frac{\partial}{\partial t} p(x - r, t) + \partial_t^{1-\beta} p(x - r, t) + p(x - r, 0)\Phi_\beta(t) \right] dr. \end{aligned}$$

Letting $\bar{p}(x, t) = \frac{\partial}{\partial t} p(x, t) + \partial_t^{1-\beta} p(x, t) + p(x, 0)\Phi_\beta(t)$ and applying Lemma 3.7, we see that $\bar{p}(x, t)$ satisfies (3.32), which is the analogue of (2.13) for the identically distributed jump size case. Note that (3.32) involves a Riemann-Liouville fractional derivative instead of the Caputo derivative, as seen in (2.13). \square

REMARK 3.5. *Since the relation between the Caputo and Riemann-Liouville fractional derivatives (2.12) involves evaluating $p(x, t)$ at time $t = 0$. This brings limitations on the initial distribution of $p(x, t)$; in particular, a Dirac delta function as an initial distribution of the walkers for the delayed master equation is prohibited.*

In the next section, we use a Gaussian initial distribution – to circumvent the issue raised by Remark 3.5 – to numerically compare the evolutions between the instantaneous and delayed GMEs.

3.3. Numerical comparison of instantaneous and delayed dependence. In this Section, we compare numerical solutions of the master equations described in the literature and those derived in this work. To do this, we need to specify the kernel $\mu(r, t)$ and set-up an initial condition $p(x, 0)$. We consider three types of kernels: the Gaussian kernel

$$\mu_1(r, t; a) = \frac{1}{\sqrt{2\pi\sigma^2(t)}} \exp\left(-\frac{(r - at)^2}{2\sigma^2(t)}\right) \quad (3.40)$$

where $\sigma(t) = \frac{1}{\sqrt{t+1}}$, the Laplacian kernel

$$\mu_2(r; a) = \frac{a}{2} \exp(-a|r|) \quad (3.41)$$

and the Cauchy kernel

$$\mu_3(r; a) = \frac{1}{\pi(a + r^2)}. \quad (3.42)$$

Note that $\mu_1(r, 0; 0)$ is the standard normal distribution with mean 0 and variance 1, $\mu(r, t, 0)$ is the same distribution with shrinking variance, and $\mu(r, t, a)$ allows the kernel to move left or right over time. We also consider two different initial conditions for $p(x, 0)$, the Dirac delta distribution and the standard Gaussian distribution. In our numerical implementation, we use uniform discretization for the time interval $(0, 50)$ with mesh size $\tau = 0.1$. The infinite support of the distributions $p(x, t)$ and $\mu(r, t)$ is approximated by the interval $(-20, 20)$ and mesh size 0.4, which was sufficient for capturing the critical features of the distributions. The approximated support is taken to be larger for the figures using a jump size distribution with time-dependent mean. We use explicit Euler scheme with trapezoidal rule for integration to solve the resulting differential equations. Finally, the delayed equations are of higher order (second order for the delayed case with exponential inter-arrival times) and they require a second initial condition. The second initial condition is picked by carrying out one step of the Euler scheme for the corresponding instantaneous generalized master equations.

We start by assuming that inter-arrival times are exponential with rate $\lambda = 1$, for simplicity. First, in Figure 3.1, we compare the numerical solution of the equation (3.3), representing instantaneous case with time-independent Gaussian jump distribution $\mu_1(r, 0; 0)$ and a Dirac delta initial condition, against the exact solution of the diffusion equation (2.10). We observe a reasonably good agreement between the graphs throughout the evolution, which improves over time. This is to be expected due to the asymptotic nature of the equation (2.10) as a diffusion limit for (3.3), as described in [25]. The use of the Dirac delta as an initial condition in Figure 3.1 is not prohibited because the GME (3.3) doesn't apply any fractional derivatives.

Next we compare the numerical solutions of the GMEs for the instantaneous case (3.3) and the delayed case (3.11). In Figure 3.2, we show that the evolutions of (3.3) and (3.11) with time-independent kernel $\mu_1(r, 0; 0)$ and a Gaussian initial condition are identical. This is due to the fact that (3.11) represents the differentiated form of (3.3) when $\mu(r, t)$ is independent of time.

In Figure 3.3, we compare the evolution of (3.3) against (3.11) with time-dependent kernel $\mu_1(r, t; 0)$ and a Gaussian initial condition. In this case, the evolutions of (3.3) and (3.11) are not the same because $\mu(r, t)$ depends in time, and the equation (3.3) is no longer the differentiated form of (3.11). In fact, one may observe that for this choice of the kernel the solution of (3.11) evolves visibly faster than that of (3.3). Finally in Figure 3.4, we compare the evolution of (3.3) against (3.11) with kernel $\mu_1(r, t; 0.05)$ and a Gaussian initial condition. Once again, the evolutions are not identical since the traveling kernel depends on time. Same as before, we see a slowing down effect of (3.3) comparing to (3.11).

We proceed by replacing exponentially distributed inter-arrival times by Mittag-Leffler inter-arrival times, and comparing solutions for the corresponding GMEs from the instantaneous case (3.9) and the delayed case (3.32).

Here are some details on the discretization of the Caputo fractional derivative and the Riemann-Liouville fractional derivative adopted in this work. We implement an L^1 approximation scheme for the Caputo derivative described in [44]:

$$\partial_t^\alpha g(t_{k+1}) \approx \frac{1}{\Gamma(2-\alpha)} \sum_{l=0}^{l=k} \frac{g(t_{l+1}) - g(t_l)}{\tau^\alpha} a_{k-l} \quad (3.43)$$

with $a_{k-l} = (k+1-l)^{1-\alpha} - (k-l)^{1-\alpha}$, $t_k = k\tau$, and $t_0 = 0$ where τ denotes the size of the time discretization. Since the Caputo fractional derivative is related to the Riemann-Liouville fractional derivative by

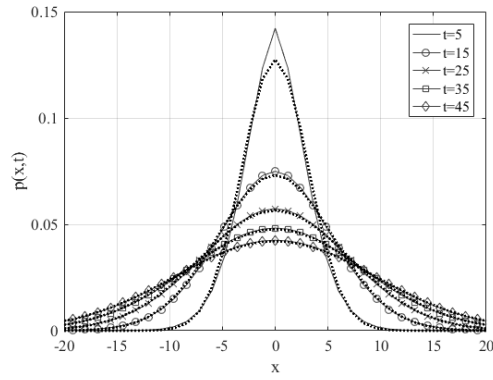


Fig. 3.1: Comparison of the numerical solution of (3.3) with jump kernel $\mu_1(r, 0; 0)$ and a Dirac delta initial condition (marked lines) against the exact solution (2.10) of the diffusion equation (dots).

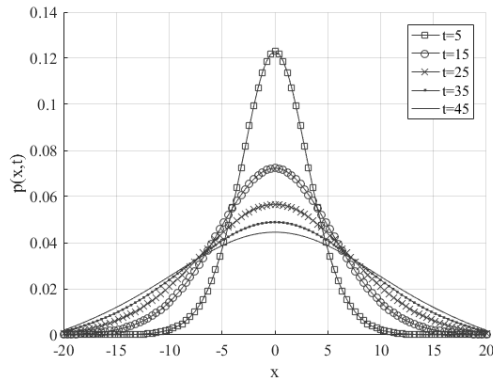


Fig. 3.2: The evolution of (3.3) and (3.11) with jump kernel $\mu_1(r, 0; 0)$ and a Gaussian initial condition. The graphs are in perfect agreement.

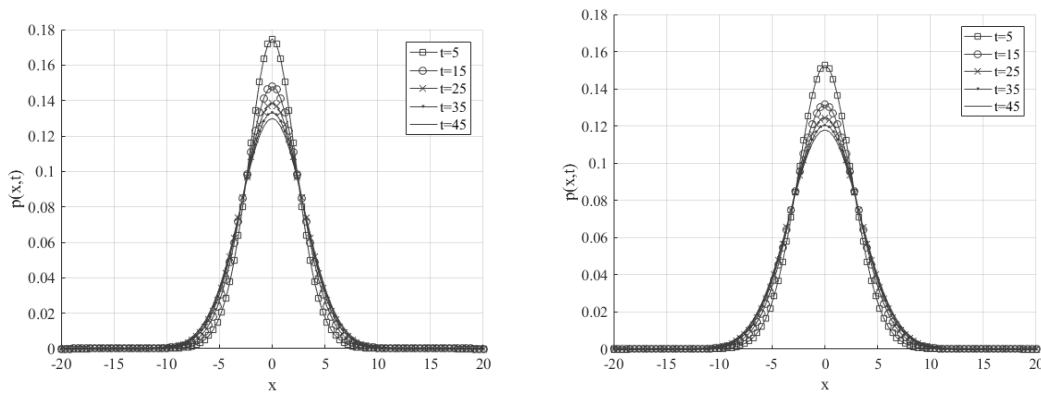


Fig. 3.3: Comparison of the evolution of (3.3)(left) against (3.11)(right) with jump kernel $\mu_1(r, t; 0)$ and starting from the same Gaussian distribution.

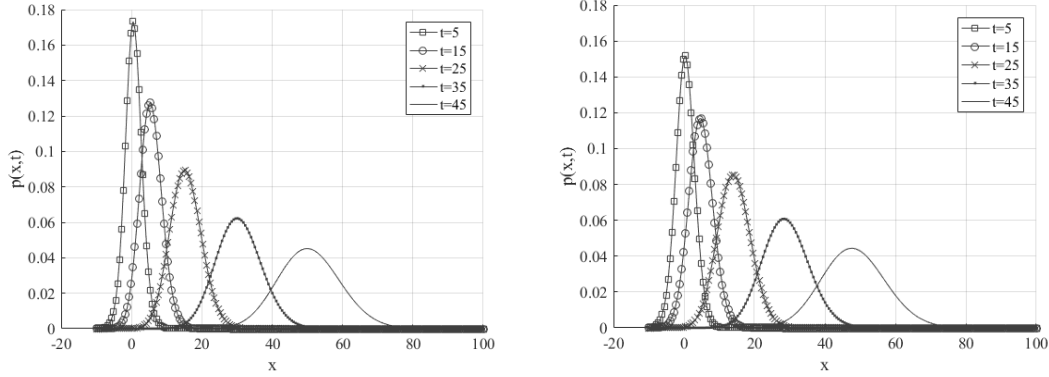


Fig. 3.4: Comparison of the evolution of (3.3)(left) against (3.11)(right) with jump kernel $\mu_1(r, t; 0.05)$ and starting from the same Gaussian distribution.

(2.12), then (3.43) can also be used to numerically approximate the Riemann-Liouville fractional derivative, i.e.,

$$D_t^\alpha g(t_{k+1}) \approx \frac{g(t_0)}{t_{k+1}^\alpha \Gamma(1-\alpha)} + \frac{1}{\Gamma(2-\alpha)} \sum_{l=0}^{l=k} \frac{g(t_{l+1}) - g(t_l)}{\tau^\alpha} a_{k-l}. \quad (3.44)$$

Using these discretizations, in Figure 3.5, we compare the evolution of (3.9) against (3.32) using time-independent kernels $\mu_1(r, 0; 0)$, $\mu_2(r; 0.7)$, and $\mu_3(r; 0.3)$ with a Gaussian initial condition. Unlike the exponential case, the evolutions should not be identical since (3.9) does not represent the differentiated form of (3.32) even with $\mu(r, t)$ being independent of time. Similarly to the case of exponential inter-arrival times, we observe that the delayed equation (3.32) is evolving faster than the instantaneous case given by (3.9).

In Figure 3.6, we compare the evolution of (3.9) against (3.32) with time-dependent kernel $\mu_1(r, t; 0)$ and a Gaussian initial condition. Note that in the time window chosen for this numerical experiment, the numerical solution of (3.32) keeps on diffusing, while the evolution of (3.9) undergoes transition from diffusive regime to aggregation, resulting in the growth of the peak at $x = 0$. Finally in Figure 3.7, we compare the evolution of (3.9) against (3.32) with kernel $\mu_1(r, t; 0.05)$ and a Gaussian initial condition. One may observe that while the delayed equation still gives a faster evolution, the forms of the resulting solution curves in both cases are significantly different. It stresses the fact that the difference between the delayed and instantaneous CTRWs is magnified by the memory effect created by the “fat-tailed” inter-arrival time distributions.

4. Summary. CTRW theory has been developed and successfully utilized in a variety of contexts. The main workhorse of this theory is the master equation formalism allowing to describe the evolution of probability distributions associated with random walk dynamics. In this work we were motivated by the desire to systematically treat different scenarios arising in this framework.

Table 4.1 summarizes the results of this work by providing an overview of different master equations derived from a variety of jump size and inter-arrival time distributions. When the distributions are identically distributed, we arrive at the standard integro-differential equation for the exponential case (2.5), as derived in [9, 10], and fractional integro-differential equation for the Mittag-Leffler case (2.13), as seen in [31, 32]. The focus of this study was on the case when the jump sizes are not identically distributed, which comes in two forms: *instantaneous*, referred to as $\mu(r, t)$ in the Table, and *delayed*,

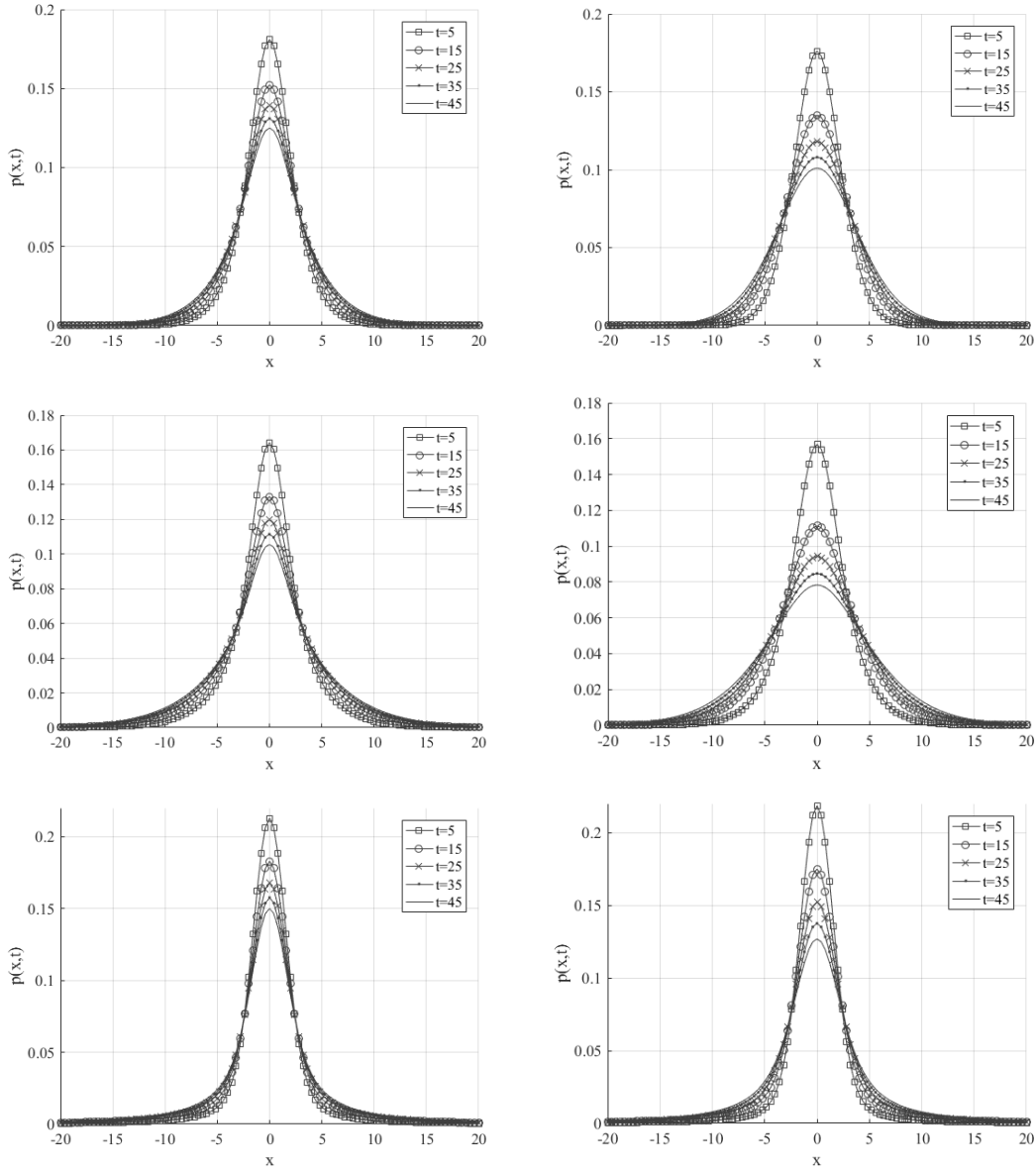


Fig. 3.5: Comparison of the evolution of (3.9)(left column) against (3.32)(right column) using different jump kernels and starting from the same Gaussian distribution. Top row: Gaussian kernel $\mu_1(r; 0; 0)$. Middle row: Laplacian kernel $\mu_2(r; 0.7)$. Bottom row: Cauchy kernel $\mu_3(r; 0.3)$.

referred to as $\mu(r, t_0)$ in the Table. For the *instantaneous* case, the master equation (3.3) was already derived in [29] for exponential inter-arrival times, while the proof in [33] for the Mittag-Leffler inter-arrival times can be generalized to yield (3.9).

The main contribution of this work is the derivation of the master equations for the *delayed* case with exponential (3.11) and Mittag-Leffler (3.32) inter-arrival times distributions. Unlike previous scenarios, CTRWs with delayed jump size dependence in both of these cases obey master equations of a different type. Namely, these walks are described by a higher order master equation, which can be re-written in terms of an auxiliary probability function, to take on a form resembling the standard first order master

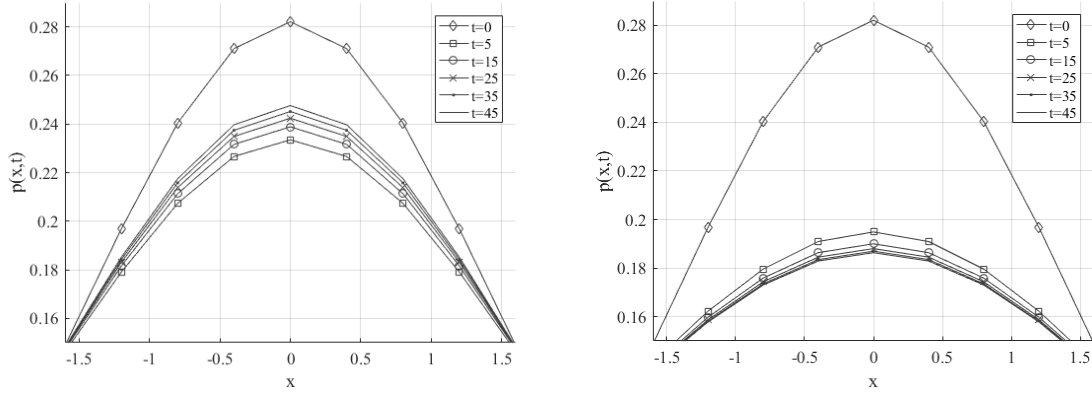


Fig. 3.6: Comparison of the evolution of (3.9)(left) against (3.32)(right) with jump kernel $\mu_1(r, t; 0)$, starting from the same Gaussian distribution. The solution of (3.32) keeps diffusing, while the solution of (3.9) undergoes a reversal in its trend (it goes down initially then starts growing). Both figures have been magnified around the peak to be able to illustrate this behavior, and only that portion of the graph is shown.

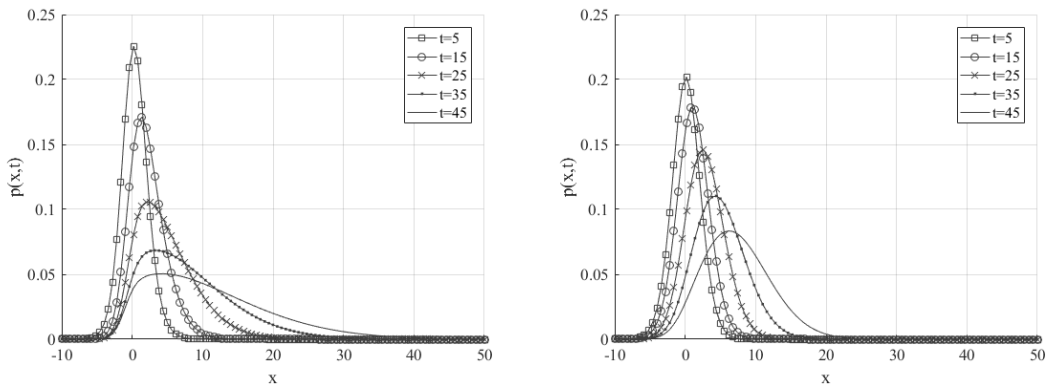


Fig. 3.7: Comparison of the evolution of (3.9)(left) against (3.32)(right) with kernel $\mu_1(r, t; 0.05)$, starting from the same Gaussian distribution.

equation (2.5) and (2.13), respectively. One may notice that there are similarities between (3.32) in the delayed case and (3.9) in the instantaneous case, however, the Riemann-Liouville fractional derivative needs to be replaced with the Caputo fractional derivative. The delayed master equation with exponential inter-arrival times, for the special case of nearest neighbor jumps, reduces to the generalized master equation for trap time delayed forcing derived in [28].

We have observed numerical differences between the CTRWs with exponential and Mittag-Leffler inter-arrival times. For the exponentially distributed inter-arrival times, if the jump sizes are time independent, both dynamics are equivalent; they only differ in the case of time dependent jump sizes. The solution of the delayed GME tends to evolve faster than the instantaneous one. In the Mittag-Leffler scenario, the delayed case evolution is significantly different than in the instantaneous case. Even with time independent jump sizes, the dynamics are not equivalent. Moreover, the forms of the solution curves deviate significantly between the delayed and instantaneous GMEs in the case of time dependent jump

sizes.

Jump sizes	Inter-arrival times	Equation
Homogeneous Poisson case, arrival rate λ		
$\mu(r)$	$\frac{\partial}{\partial t}p(x, t) = \lambda \int_{\mathbb{R}} \mu(r)[p(x-r, t) - p(x, t)]dr$	(2.5)
$\mu(r, t)$	$\frac{\partial}{\partial t}p(x, t) = \lambda \int_{\mathbb{R}} \mu(r, t)[p(x-r, t) - p(x, t)]dr$	(3.3)
$\mu(r, t_0)$	$\begin{cases} \bar{p}(x, t) = p(x, t) + \frac{1}{\lambda} \frac{\partial}{\partial t}p(x, t) \\ \frac{\partial}{\partial t}\bar{p}(x, t) = \lambda \int_{\mathbb{R}} \mu(r, t)[\bar{p}(x-r, t) - \bar{p}(x, t)]dr \end{cases}$	(3.11)
Fractional case, $w(s) = -\frac{d}{ds}E_{\beta}(-s^{\beta})$		
$\mu(r)$	$\partial_t^{\beta}p(x, t) = \int_{\mathbb{R}} \mu(r)[p(x-r, t) - p(x, t)]dr$	(2.13)
$\mu(r, t)$	$\partial_t^{\beta}p(x, t) = \int_{\mathbb{R}} \mu(r, t)[p(x-r, t) - p(x, t)]dr$	(3.9)
$\mu(r, t_0)$	$\begin{cases} \bar{p}(x, t) = \frac{\partial}{\partial t}p(x, t) + \partial_t^{1-\beta}p(x, t) + p(x, 0)\Phi_{\beta}(t) \\ D_t^{\beta}\bar{p}(x, t) = \int_{\mathbb{R}} \mu(r, t)[\bar{p}(x-r, t) - \bar{p}(x, t)]dr \end{cases}$	(3.32)

Table 4.1: Summary of generalized master equations.

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