Generalized master equations and fractional Fokker-Planck equations from continuous time random walks with arbitrary initial conditions

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Abstract

In the standard continuous time random walk the initial state is taken as a non-equilibrium state, in which the random walking particle has just arrived at a given site. Here we consider generalizations of the continuous time random walk to accommodate arbitrary initial states. One such generalization provides information about the initial state through the introduction of a first waiting time density that is taken to be different from subsequent waiting time densities. Another generalization provides information about the initial state through the prior history of the arrival flux density. The master equations have been derived for each of these generalizations. They are different in general but they are shown to limit to the same master equation in the case of an equilibrium initial state. Under appropriate conditions they also reduce to the master equation for the standard continuous time random walk with the non-equilibrium initial state.

The diffusion limit of the generalized master equations is also considered, with Mittag-Leffler waiting time densities, resulting in the same fractional Fokker-Planck equation for different initial conditions.

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1. Introduction

The continuous time random walk (CTRW) [1] describes the random motion of a particle that steps from one lattice site to another and waits at a given site before taking another step. The length of the step is governed by a step length probability density and the waiting time is governed by a waiting time probability density. In the standard CTRW it is assumed that

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the particle has arrived at a given position x_0 at an initial time $t = 0$ and the particle then commences its random walk, from that location. The CTRW was revisited by Tunaley [2] who considered a more general initial condition in which the probability density for the particle to be at position x at an initial time t_0 is given, along with the waiting time density for the first step, $\psi_0(t)$. In this formulation it is envisaged that the particle may have arrived at x at an earlier time and thus the waiting time density for the first step, $\psi_0(t)$, is different to the waiting time density, $\psi(t)$, in subsequent steps. The waiting time density for the first step can be related to the waiting time density for subsequent steps if it is assumed that the system is initially in an equilibrium state [3, 4]. In Section II we have derived the generalized master equation for the CTRW, with a distinct first waiting time density, and we have obtained reductions for the standard non-equilibrium initial state and for an equilibrium initial state. The equilibrium initial state that we consider is well posed for both Markovian, and non-Markovian waiting time densities, in difference to the equilibrium initial state that had been proposed earlier in this context [2, 3, 4].

The specification of a distinct first waiting time is not the only way to generalize the CTRW to include more general initial conditions. In Section III we have considered an alternate formulation of the CTRW, in which information about the initial condition is provided through the prior history of the flux density for arriving particles. We have derived the generalized master equation for this CTRW and we have obtained reductions for the standard non-equilibrium initial state and for an equilibrium initial state, recovering the master equations for the standard CTRW and the CTRW with a distinct first waiting time, respectively.

The two formulations of CTRWs and their master equations considered here; one that utilizes information about a first waiting time density, and the other that utilizes information about the prior history of the arrival flux density, provide alternate and distinct ways to treat CTRWs with general initial conditions.

In Section IV we have derived diffusion limit equations, with Mittag-Leffler waiting time densities, for the generalized master equations derived in Section II and in Section III. The fractional Fokker-Planck equations are shown to be the same in this limit, independent of the initial conditions considered, thus providing another example of CTRW models with different generalized master equations but common diffusion limits [5].

The work described here is related to the problem of ageing CTRWs [6, 7]. In ageing CTRWs it is considered that the walkers have been initiated at a time prior to the start of the observation time. Assuming that all walkers are initiated at the same time, the probability density for the first waiting time is different to the CTRW waiting time density for subsequent (or preceding jumps). The initial waiting time density was obtained for cases in which the average CTRW waiting time is finite and when the CTRW waiting time density is power law distributed [6]. In addition, a generalization of the Montroll-Weiss equation [1] for the probability density function describing the ageing CTRW was given in Fourier-Laplace space, and a long time asymptotic solution was obtained from this, along with calculations of moments.

There are two fundamental differences between ageing CTRWs and the CTRWs considered here. Firstly in the ageing CTRWs it was assumed that all particles start at the origin at an initial time $t = 0$, whereas in the CTRWs considered here the initial distribution of the particles is given as an arbitrary probability density function or an initial arrival density is given. Secondly, we have obtained explicit results for the generalized master equations and for the diffusion limit Fokker-Planck equations with the above initial conditions.

2. Master Equation for CTRWs with a Distinct First Waiting Time Density

To begin with we consider the derivation of the master equation for the CTRW with a distinct first waiting time density. The Fourier-Laplace representation of the master equation for this problem has appeared previously [2, 4]. The main reason for including a derivation of the space-time representation here is to set the notation and to enable direct comparison with the alternate formulation of CTRWs with arbitrary initial conditions, considered in the next section.

We consider a particle undergoing a CTRW on a one dimensional lattice. We suppose that the initial particle probability density function $\rho_0(x)$ is aribitrary and we do not know the distribution of arrival times. Following the approach suggested by [2] we compensate for the unknown arrival times by having the initial waiting time density, for the first step, different to subsequent waiting times densities. We let $q_n(x, t)$ denote the arrival flux density at position x, at time t after n steps. After one step we have

$$q_1(x, t) = \sum_{x'} \Psi_0(x, x', t)\rho_0(x) \tag{1}$$

where $\Psi_0(x, x', t)$ is the probability of a transition from x' to x at time t. In subsequent steps the arrival flux density satisfies the recursion relation

$$q_{n+1}(x, t) = \sum_{x'} \int_{0^+}^{t} \Psi(x, x', t, t')q_n(x', t')\, dt', \quad n \geq 1 \tag{2}$$

where $\Psi(x,x',t,t')$ is the probability density for transitions from x' at time t', to x at time t. In the remainder we will assume the separable transition densities,

$$\begin{aligned}\Psi_0(x,x',t) &= \lambda(x,x')\psi_0(t), \quad (3)\\ \Psi(x,x',t,t') &= \lambda(x,x')\psi(t-t'), \quad (4)\end{aligned}$$

identifying $\lambda(x,x')$ as the step length density, $\psi_0(t)$ as the waiting time density for the first step, and $\psi(t)$ as the waiting time density for subsequent steps.

We can sum over all steps, defining

$$q(x,t) = \sum_{n=1}^{\infty} q_n(x,t) \quad (5)$$

as the arrival density after any number of steps. If we sum over all steps in Eq.(2), using the result in Eq.(1), we obtain

$$q(x,t) = \sum_{x'} \lambda(x,x') \left(\psi_0(t)\rho_0(x') + \int_{0^+}^{t} \psi(t-t')q(x',t')\,dt' \right) \quad (6)$$

The probability density for a particle to be at position x at time t is then given by

$$\rho(x,t) = \int_{0^+}^{t} q(x,t')\Phi(t-t')\,dt' + \Phi_0(t)\rho_0(x), \quad (7)$$

where

$$\Phi_0(t) = 1 - \int_0^t \psi_0(t')\,dt' \quad (8)$$

is the survival probability for the first step and

$$\Phi(t-t') = 1 - \int_0^{t-t'} \psi(t'')\,dt'', \quad (9)$$

is the survival probability for subsequent steps.

We now differentiate Eq.(7) with respect to time to obtain

$$\frac{\partial \rho}{\partial t} = q(x,t) - \int_{0^+}^{t} q(x,t')\ \psi(t-t')\,dt' - \psi_0(t)\rho_0(x). \quad (10)$$

We can replace the first term on the right hand side of this equation, using Eq.(6). This results in

$$\frac{\partial \rho}{\partial t} = \sum_{x'} \lambda(x,x') \left(\psi_0(t)\rho_0(x') + \int_{0^+}^{t} \psi(t-t')q(x',t')\,dt' \right) - \psi_0(t)\rho_0(x) - \int_{0^+}^{t} q(x,t')\psi(t-t')\,dt' \quad (11)$$

The remaining dependence on $q(x,t)$ in this equation can be replaced by a dependence on $\rho(x,t)$ using Laplace transform methods. Using the notation $\hat{f}(s)$ to denote the Laplace transform of $f(t)$ with respect to time t we have the Laplace transforms of Eq.(7) and Eq.(11) given by

$$\hat{\rho}(x,s) = \hat{q}(x,s)\hat{\Phi}(s) + \hat{\Phi}_0(s)\rho_0(x), \tag{12}$$

and

$$s\hat{\rho}(x,s) - \rho_0(x) = \sum_{x'} \lambda(x,x') \left(\hat{\psi}_0(s)\rho_0(x') + \hat{\psi}(s)\hat{q}(x',s)\right) - \hat{\psi}_0(s)\rho_0(x) - \hat{\psi}(s)\hat{q}(x,s), \tag{13}$$

respectively. We can use Eq.(12) to eliminate the $\hat{q}(x,s)$ dependence in Eq.(13) and write

$$\begin{aligned} s\hat{\rho}(x,s) - \rho_0(x) = \sum_{x'} \lambda(x,x') &\left((\hat{\psi}_0(s) - \frac{\hat{\psi}(s)}{\hat{\Phi}(s)}\hat{\Phi}_0(s))\rho_0(x') + \frac{\hat{\psi}(s)}{\hat{\Phi}(s)}(\hat{\rho}(x',s)) \right) \\ &- (\hat{\psi}_0(s) - \frac{\hat{\psi}(s)}{\hat{\Phi}(s)}\hat{\Phi}_0(s))\rho_0(x) - \frac{\hat{\psi}(s)}{\hat{\Phi}(s)}(\hat{\rho}(x,s). \end{aligned} \tag{14}$$

We now introduce the memory kernels $K(t)$ and $J(t)$ defined by the Laplace transforms

$$\hat{K}(s) = \frac{\hat{\psi}(s)}{\hat{\Phi}(s)}, \tag{15}$$

$$\hat{J}(s) = \hat{\psi}_0(s) - \frac{\hat{\psi}(s)}{\hat{\Phi}(s)}\hat{\Phi}_0(s), \tag{16}$$

and take the inverse Laplace transform of Eq.(14) to obtain

$$\begin{aligned} \frac{\partial \rho}{\partial t} = \sum_{x'} \lambda(x,x') &\left(J(t)\rho_0(x') + \int_0^t K(t-t')\rho(x',t')\,dt' \right) \\ &- J(t)\rho_0(x) - \int_0^t K(t-t')\rho(x,t')\,dt'. \end{aligned} \tag{17}$$

Note that

$$\hat{\psi}(s) = 1 - s\hat{\Phi}(s), \tag{18}$$

$$\hat{\psi}_0(s) = 1 - s\hat{\Phi}_0(s), \tag{19}$$

so that we can also write

$$\hat{J}(s) = 1 - \frac{\hat{\Phi}_0(s)}{\hat{\Phi}(s)}. \tag{20}$$

2.1. Non-equilibrium initial arrivals

In the standard CTRW it was assumed that the random walking particle arrived at x_0 at time $t = 0$. In this case $\rho_0(x) = \rho(x,0) = \delta_{x,x_0}$ and $\psi_0(t) = \psi(t)$. It further follows that in this case, $\Phi_0(t) = \Phi(t)$, hence $J(t) = 0$, and the master equation reduces to

$$\frac{\partial \rho}{\partial t} = \sum_{x'} \lambda(x,x') \int_0^t K(t-t')\rho(x',t')\,dt' - \int_0^t K(t-t')\rho(x,t')\,dt'. \tag{21}$$

2.2. Equilibrium initial arrivals

In general, a particle that is at a particular site at time $t = 0$ may have arrived at that site at an earlier time and been there for a time t_0. In equilibrium we suppose that the distribution of these times, t_0, is given by the waiting time density $\psi(t_0)$. Following the approach in Lax and Scher [3] we introduce $\psi(t|t_0)$, as the conditional density for waiting an additional time t, after time $t = 0$, given that the particle has already been there for a time t_0, before time $t = 0$. The expected waiting time density for the first step after time $t = 0$ is then given by

$$\psi_0(t) = \frac{\int_0^\infty \psi(t|t_0)\psi(t_0)\, dt_0}{\int_0^\infty \psi(t_0)\, dt_0}. \tag{22}$$

This can be re-written as

$$\psi_0(t) = \int_0^\infty \psi(t + t_0)\frac{\psi(t_0)}{\phi(t_0)}\, dt_0. \tag{23}$$

where we have used the result

$$\psi(t|t_0)\Phi(t_0) = \psi(t + t_0), \tag{24}$$

together with the normalization of the density $\psi(t)$. The approach above differs from Lax and Scher, who average over the survival probability, rather than the waiting time density, in the integrals in Eq.(22). It is a simple exercise to show that the replacement of the waiting time density with the survival probability in Eq.(22) yields the same final result for the first waiting time density in the Markovian case where waiting time density for subsequent steps is an exponential waiting time density,

$$\psi(t) = \alpha e^{-\alpha t}, \tag{25}$$

but it leads to singularities for non-Markovian, power law tailed waiting time densities. The expression in Eq.(22) is well defined for both Markovian and non-Markovian densities.

3. Master Equation for CTRWs with a Prior History of the Arrival Flux Density

Rather then prescribe an initial waiting time density, distinct to subsequent waiting time densities we can instead suppose that the process could have started at any time in the past and the arrival density at position x and time t after n steps is represented by the unknown arrival density $q_n(x, t)$. In this case we have the recursion relation

$$q_{n+1}(x, t) = \sum_{x'} \int_{-\infty}^{t} \Psi(x, t, x', t')q_n(x', t')\, dt'. \tag{26}$$

The arrival density after any number of steps is now represented by a doubly infinite sum

$$q(x,t) = \sum_{n=-\infty}^{+\infty} q_{n+1}(x,t), \tag{27}$$

and then, using Eq.(26), we have the recursion relation

$$\begin{aligned} q(x,t) &= \sum_{x'} \int_{-\infty}^{t} \Psi(x,t,x',t') q(x',t')\, dt' && (28) \\ &= \sum_{x'} \int_{-\infty}^{t} \lambda(x,x')\psi(t-t') q(x',t')\, dt' && (29) \end{aligned}$$

where we have assumed that $\Psi(x,t,x',t') = \lambda(x,x')\psi(t-t')$.

The probability density for the particle to be at position x at time t is now given by

$$\rho(x,t) = \int_{-\infty}^{t} \Phi(t-t') q(x,t')\, dt'. \tag{30}$$

It is convenient to define

$$\rho_0(x,t) = \int_{-\infty}^{0} \Phi(t-t') q(x,t')\, dt' \tag{31}$$

and then

$$\rho(x,t) = \rho_0(x,t) + \int_{0}^{t} \Phi(t-t') q(x,t')\, dt'. \tag{32}$$

We note that the waiting time density is the negative of the derivative of the survival probability, i.e.,

$$\psi(t) = -\frac{d\Phi(t)}{dt}. \tag{33}$$

Using this result it is straightforward to differentiate Eq.(32), and Eq.(31) with respect to time to obtain

$$\frac{\partial \rho}{\partial t} = -j_0(x,t) + q(x,t) - \int_{0}^{t} \psi(t-t') q(x,t')\, dt', \tag{34}$$

where

$$j_0(x,t) = \int_{-\infty}^{0} \psi(t-t') q(x,t')\, dt'. \tag{35}$$

Using Eq.(35) we can re-write Eq.(29) as

$$q(x,t) = \sum_{x'} \lambda(x,x') j_0(x',t) + \sum_{x'} \int_{0}^{t} \lambda(x,x')\psi(t-t') q(x',t')\, dt', \tag{36}$$

and then substitute this result into the second term of Eq.(34) to obtain

$$\frac{\partial \rho}{\partial t} = \sum_{x'} \lambda(x,x') j_0(x',t) - j_0(x,t) + \sum_{x'} \int_{0}^{t} \lambda(x,x')\psi(t-t') q(x',t')\, dt' - \int_{0}^{t} \psi(t-t') q(x,t')\, dt'. \tag{37}$$

The dependence on $q(x,t)$ in Eq.(37) after time $t=0$ can be eliminated using Laplace transform methods. Using the hat notation adopted earlier and also denoting the Laplace transform of $f(t)$ with respect to t by $\mathcal{L}\left[f(t)|t,s\right]$, where s is the Laplace transform variable, we have

$$\hat{\Phi}(s)\hat{q}(x,s) = \rho(x,s) - \rho_0(x,s), \tag{38}$$

and

$$\mathcal{L}\left[\int_0^t \psi(t-t')q(x,t')\,dt'|t,s\right] = \hat{\psi}(s)\hat{q}(x,s). \tag{39}$$

We now define the memory kernel $K(t)$ through the Laplace transform,

$$\hat{K}(s) = \frac{\hat{\psi}(s)}{\hat{\Phi}(s)} \tag{40}$$

and combine this with the results of Eqs.(38), (39), (40) to arrive at

$$\mathcal{L}\left[\int_0^t \psi(t-t')q(x,t')\,dt'|t,s\right] = \hat{K}(s)(\hat{\rho}(x,s) - \hat{\rho}_0(x,s)). \tag{41}$$

Finally we invert the Laplace transform in Eq.(41) and substitute this into Eq.(37) to arrive at

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= \sum_{x'}\lambda(x,x')j_0(x',t) + \sum_{x'}\lambda(x,x')\int_0^t K(t-t')(\rho(x',t') - \rho_0(x',t'))\,dt' \\ &\quad - j_0(x,t) - \int_0^t K(t-t')(\rho(x,t') - \rho_0(x,t'))\,dt'.\end{aligned} \tag{42}$$

The arbitrary initial condition is expressed in the relation for $j_0(x,t)$, or $\rho_0(x,t)$, which involve the arrival density $q(x,t)$ prior to the time $t=0$. As an alternative if we knew the probability density $i(x,-t)$ for the particle to be at x, given that it arrived there at time $t<0$ then we could readily obtain

$$q(x,t) = \frac{i(x,-t)}{\Phi(-t)}. \tag{43}$$

3.1. Non-equilibrium initial arrivals

In the formulation of the model in this section, the standard CTRW initial condition, that the random walking particle arrived at x_0 at time $t=0$, is given by

$$q(x,t) = \delta(t)\delta_{x,x_0} \quad t \leq 0. \tag{44}$$

If we substitute this into Eq.(31) and Eq.(35) we obtain

$$\rho_0(x,t) = \Phi(t)\delta_{x,x_0}, \tag{45}$$

$$j_0(x,t) = \psi(t)\delta_{x,x_0}. \tag{46}$$

Taking the Laplace transforms of Eq.(45) and Eq.(46) and using the definition of $\hat{K}(s)$ in Eq.(15) it follows that $\hat{j}_0(x,s) = \hat{K}\hat{\rho}_0(x,s)$ and thus

$$j_0(x,t) = \int_0^t K(t-t')\rho_0(x,t')\,dt'. \tag{47}$$

Substituting, Eq.(47) into Eq.(42) we arrive at the standard generalized master equation, Eq.(21).

3.2. Equilibrium initial arrivals

In equilibrium we assume that

$$i(x,-t) = \rho_0^\star(x)\psi(-t), \quad t \leq 0 \tag{48}$$

and thus

$$q(x,t) = \rho_0^\star(x)\frac{\psi(-t)}{\Phi(-t)}, \quad t \leq 0. \tag{49}$$

If we substitute the equilibrium arrival density into Eq.(35), and Eq.(31), then after a simple change of variables in the integrals, we arrive at the results

$$j_0(x,t) = \rho_0^\star(x)\int_0^\infty \psi(t+t_0)\frac{\psi(t_0)}{\Phi(t_0)}\,dt_0, \tag{50}$$

and

$$\rho_0(x,t) = \rho_0^\star(x)\int_0^\infty \Phi(t+t_0)\frac{\psi(t_0)}{\Phi(t_0)}\,dt_0. \tag{51}$$

Using the expression for the first waiting time density, Eq.(23), in the above we can now write

$$\begin{aligned} j_0(x,t) &= \rho_0^\star(x)\psi_0(t), && (52)\\ \rho_0(x,t) &= \rho_0^\star(x)\Phi_0(t), && (53) \end{aligned}$$

where $\Phi_0(t)$ is the survival probability for the first waiting time density.

Finally, substituting the results for $j_0(x,t)$ and $\rho_0(x,t)$ into the generalized master equation, Eq.(42), we arrive at

$$\begin{aligned} \frac{\partial \rho}{\partial t} = &\sum_{x'}\lambda(x,x')\rho_0^\star(x')\psi_0(t) + \sum_{x'}\lambda(x,x')\int_0^t K(t-t')(\rho(x',t') - \rho_0^\star(x')\Phi_0(t'))\,dt' \\ &- \rho_0^\star(x)\psi_0(t) - \int_0^t K(t-t')(\rho(x,t') - \rho_0^\star(x)\Phi_0(t'))\,dt'. \end{aligned} \tag{54}$$

The generalized master equation for equilibrium arrivals derived in this framework can be shown to be identical to the generalized master equation obtained for distinct first waiting time densities in section 2, Eq.(34). To establish this equivalence we consider the Laplace transform of Eq.(54),

$$\begin{aligned} s\hat{\rho}(x,s) - \rho(x,0) = &\sum_{x'} \lambda(x,x')\rho_0^\star(x')\hat{\psi}_0(s) - \rho_0^\star(x)\hat{\psi}_0(s) \\ &+ \sum_{x'} \lambda(x,x')(\hat{K}(s)\hat{\rho}(x',s) - \hat{K}(s)\hat{\Phi}_0(s)\rho_0^\star(x')) \\ &- (\hat{K}(s)\hat{\rho}(x,s) - \hat{K}(s)\Phi_0(s)\rho_0^\star(x)) \end{aligned} \tag{55}$$

and then re-arrange terms to write

$$\begin{aligned} s\hat{\rho}(x,s) - \rho(x,0) = &\sum_{x'} \lambda(x,x')(\hat{\psi}_0(s) - \hat{K}(s)\hat{\Phi}_0(s))\rho_0^\star(x') - (\hat{\psi}_0(s) - \hat{K}(s)\hat{\Phi}_0(s))\rho_0^\star(x) \\ &+ \sum_{x'} \lambda(x,x')\hat{K}(s)\hat{\rho}(x',s) - \hat{K}(s)\hat{\rho}(x,s). \end{aligned} \tag{56}$$

Using Eq.(15) and Eq.(16), we can now write this as

$$\begin{aligned} s\hat{\rho}(x,s) - \rho(x,0) = &\sum_{x'} \lambda(x,x')\hat{J}(s)\rho_0^\star(x') - \hat{J}(s)\rho_0^\star(x) \\ &+ \sum_{x'} \lambda(x,x')\hat{K}(s)\hat{\rho}(x',s) - \hat{K}(s)\hat{\rho}(x,s), \end{aligned} \tag{57}$$

and taking the inverse Laplace transform we arrive at Eq.(17).

4. Diffusion Limits

In this section we have considered the diffusion limit of the generalized master equations, Eq.(17), and Eq.(54), for CTRWs with arbitrary initial arrivals. Formally this limit is taken by introducing a jump length scaling parameter h and a waiting time scale parameter τ and then considering the limit $h \to 0$ and $\tau \to 0$. Following the approach in [5] we will consider nearest neighbour jumps on a one-dimensional lattice, with the lattice spacing Δx taken as the jump scale parameter. In the case of nearest neighbour jumps the step length density is given by

$$\lambda_{x,x'} = p_r(x')\delta_{x',x-\Delta x} + p_\ell(x')\delta_{x',x+\Delta x}, \tag{58}$$

where $p_r(x)$ is the probability of jumping from x one lattice spacing to the right and $p_\ell(x)$ is the probability of jumping from x one lattice spacing to the left. Note that

$$p_r(x) + p_\ell(x) = 1. \tag{59}$$

The time scale τ is introduced by replacing the densities with scaled densities. The scaled waiting time density $\psi_\tau(t)$ is related to the standard waiting time density $\psi(t)$ by

$$\psi_\tau(t) = \frac{1}{\tau}\psi(\frac{t}{\tau}). \tag{60}$$

From this scaled density we can then obtain the scaled survival probability

$$\Phi_\tau(t) = 1 - \int_0^t \psi_\tau(t')\, dt', \tag{61}$$

the scaled first waiting time density

$$\psi_{0,\tau}(t) = \int_0^\infty \psi_\tau(t+t_0)\frac{\psi_\tau(t_0)}{\phi_\tau(t_0)}\, dt_0, \tag{62}$$

and the scaled first survival probability

$$\Phi_{0,\tau}(t) = 1 - \int_0^t \psi_{0,\tau}(t')\, dt'. \tag{63}$$

The scaled functions $K_\tau(t)$ and $J_\tau(t)$ are then defined through the Laplace transform relations in Eq.(15) and Eq.(16) with the densities and replaced by scaled densities.

Using the step density in Eq.(58), with time scaled waiting time densities, Eq.(17) becomes

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= J_\tau(t)\left(p_r(x-\Delta x)\rho_0(x-\Delta x) + p_\ell(x+\Delta x)\rho_0(x+\Delta x) - \rho_0(x)\right)\\ &+ \int_0^t K_\tau(t-t')\left(p_r(x-\Delta x)\rho(x-\Delta x,t) + p_\ell(x+\Delta x)\rho(x+\Delta x,t) - \rho(x,t)\right).\end{aligned} \tag{64}$$

We now expand the spatial functions as Taylor series, and use the identity in Eq.(59) to obtain

$$\begin{aligned}\frac{\partial\rho}{\partial t} &= J_\tau(t)\left(\frac{\Delta x^2}{2}\frac{\partial^2\rho_0}{\partial x^2} - \Delta x^2\frac{\partial}{\partial x}\left((\frac{p_r(x)-p_\ell(x)}{\Delta x})\rho_0(x)\right)\right)\\ &+ \int_0^t K_\tau(t-t')\left(\frac{\Delta x^2}{2}\frac{\partial^2\rho}{\partial x^2} - \Delta x^2\frac{\partial}{\partial x}\left((\frac{p_r(x)-p_\ell(x)}{\Delta x})\rho(x,t)\right)\right) + O(\Delta x^3)\end{aligned} \tag{65}$$

Finally we introduce the force function

$$F(x) = \lim_{\Delta x\to 0}\frac{1}{\beta}\frac{p_r(x)-p_\ell(x)}{\Delta x} \tag{66}$$

and the Fokker-Planck equation is obtained in the limit,

$$\begin{aligned}\frac{\partial\rho(x,t)}{\partial t} &= \lim_{\tau\to 0,\Delta x\to 0} J_\tau(t)\left(\frac{\Delta x^2}{2}\frac{d^2\rho_0(x)}{dx^2} - \beta\Delta x^2\frac{d}{dx}\left(F(x)\rho_0(x)\right)\right)\\ &+ \lim_{\tau\to 0,\Delta x\to 0}\int_0^t K_\tau(t-t')\left(\frac{\Delta x^2}{2}\frac{\partial^2\rho(x,t')}{\partial x^2} - \beta\Delta x^2\frac{\partial}{\partial x}\left(F(x)\rho(x,t')\right)\right) dt'.\end{aligned} \tag{67}$$

The diffusion limit of Eq.(54), is obtained in a similar fashion. After replacing the densities with scaled densities and taking Taylor series expansions in the spatial variable we arrive at the intermediate result

$$\begin{aligned}\frac{\partial\rho(x,t)}{\partial t} &= \lim_{\tau\to 0,\Delta x\to 0}\left(\frac{\Delta x^2}{2}\frac{\partial^2 j_0(x,t)}{\partial x^2} - \beta\Delta x^2\frac{\partial}{\partial x}\left(F(x)j_0(x,t)\right)\right)\\ &+ \lim_{\tau\to 0,\Delta x\to 0}\int_0^t K_\tau(t-t')\left(\frac{\Delta x^2}{2}\frac{\partial^2(\rho(x,t')-\rho_0(x,t'))}{\partial x^2}\, dt' - \beta\Delta x^2\frac{\partial}{\partial x}\left(F(x)(\rho(x,t')-\rho_0(x,t'))\right)\right) dt'.\end{aligned} \tag{68}$$

In the diffusion limit we further have

$$\begin{aligned}
\lim_{\tau\to 0} j_0(x,t) &= \lim_{\tau\to 0}\int_{-\infty}^{0} \psi_\tau(t-t')q(x,t')\,dt' \\
&= \int_{-\infty}^{0} \delta(t-t')q(x,t')\,dt' \\
&= q(x,t) \qquad (69)
\end{aligned}$$

and thus

$$\begin{aligned}
\frac{\partial\rho(x,t)}{\partial t} = \lim_{\tau\to 0,\Delta x\to 0}\int_0^t K_\tau(t-t')\Bigg(&\frac{\Delta x^2}{2}\frac{\partial^2(\rho(x,t')-\rho_0(x,t'))}{\partial x^2} \\
&-\beta\Delta x^2\frac{\partial}{\partial x}\left(F(x)(\rho(x,t')-\rho_0(x,t'))\right)\Bigg)\,dt'. \qquad (70)
\end{aligned}$$

In the case of equilibrium initial conditions, Eq.(52) and Eq.(53), it is straightforward to show that

$$\lim_{\tau\to 0,\Delta x\to 0}\Delta x^2\int_0^t K(t-t')\rho_0(x,t')\,dt' = -\lim_{\tau\to 0,\Delta x\to 0}\Delta x^2 J(t)\rho_0(x), \qquad (71)$$

so that the Fokker-Plank equations, Eq.(67) and Eq.(68) agree in this limit, as expected.

To proceed beyond the general Fokker-Planck equations in Eq.(67) and Eq.(68) we need to consider particular cases of the waiting time density.

4.1. Exponential waiting time density

The scaled exponential waiting time density is given by

$$\psi_\tau = \frac{1}{\tau}e^{-\frac{t}{\tau}}. \qquad (72)$$

It follows from Eq.(62) that the scaled first waiting time density $\psi_{0,\tau}(t) = \psi_\tau(t)$; thus $\Phi_{0,\tau}(t) = \Phi_\tau(t)$, and then from Eq.(16), we have $J_\tau(t) = 0$. It then follows from Eq.(71) that the terms depending on $\rho_0(x)$ and $\rho_0(x,t)$ vanish in Eq.(67) and Eq.(68), respectively. It is then a simple matter to evaluate

$$K_\tau(t) = \frac{1}{\tau}\delta(t) \qquad (73)$$

and then take the limits in Eq.(67), or Eq.((67), and arrive at the standard Fokker-Planck equation,

$$\frac{\partial\rho}{\partial t} = D\frac{\partial^2\rho}{\partial x^2} - 2D\beta\frac{\partial}{\partial x}\left(F(x)\rho(x,t)\right), \qquad (74)$$

where

$$D = \lim_{\tau\to 0,\Delta x\to 0}\frac{\Delta x^2}{2\tau}. \qquad (75)$$

4.2. Mittag-Leffler waiting time density

The scaled Mittag-Leffler waiting time density is given by [8]

$$\psi_\tau(t) = \frac{t^{\gamma-1}}{\tau^\gamma} E_{\gamma,\gamma}\left[-(\frac{t}{\tau})\right] \tag{76}$$

where

$$E_{\alpha,\beta}[z] = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k\alpha+\beta)} \tag{77}$$

is the generalized Mittag-Leffler function. The corresponding memory kernel $K_\tau(t)$ satisfies the convolution property (see for example, [5])

$$\int_0^t K_\tau(t-t')y(x,t')\,dt' = \frac{1}{\tau^\gamma}\,{}_0\mathcal{D}_t^{1-\gamma} y(x,t) \tag{78}$$

where

$${}_0\mathcal{D}_t^{1-\gamma} y(x,t) = \frac{1}{\Gamma(\gamma)}\frac{d}{dt}\int_0^t \frac{y(x,t')}{(t-t')^{1-\gamma}}\,dt' \tag{79}$$

is the Riemann-Liouville fractional derivative [9] and it is assumed that the fractional integral ${}_0\mathcal{D}_t^{-\gamma} y(x,t)$ vanishes at $t=0$.

After substituting the memory kernel into Eq.(70), and taking the limits we arrive at

$$\frac{\partial\rho(x,t)}{\partial t} = {}_0\mathcal{D}_t^{1-\gamma}\left(D_\gamma \frac{\partial^2(\rho(x,t)-\bar{\rho}_0(x,t))}{\partial x^2} - 2\beta D_\gamma \frac{\partial}{\partial x}\left(F(x)(\rho(x,t)-\bar{\rho}_0(x,t))\right)\right) \tag{80}$$

where

$$D_\gamma = \lim_{\tau\to 0,\Delta x\to 0} \frac{\Delta x^2}{2\tau^\gamma}, \tag{81}$$

and

$$\bar{\rho}_0(x,t) = \lim_{\tau\to 0,\Delta x\to 0} \rho_0^*(x)\int_0^\infty \frac{\Phi_\tau\left(t+t_0\right)\psi_\tau\left(t_0\right)}{\Phi_\tau\left(t_0\right)}dt_0. \tag{82}$$

The expression for $\bar{\rho}_0(x,t)$ can be shown to be equal to zero by first re-writing

$$\bar{\rho}_0(x,t) = \lim_{\tau\to 0,\Delta x\to 0} \rho_0^*(x)\int_0^\infty \frac{\Phi\left(\frac{t+t_0}{\tau}\right)\frac{1}{\tau}\psi\left(\frac{t_0}{\tau}\right)}{\Phi_\tau\left(\frac{t_0}{\tau}\right)}dt_0, \tag{83}$$

and then using the change of variables $t_0 = t'\tau$,

$$\bar{\rho}_0(x,t) = \lim_{\tau\to 0,\Delta x\to 0} \rho_0^*(x)\int_0^\infty \frac{\Phi\left(\frac{t}{\tau}+t'\right)\psi\left(t'\right)}{\Phi\left(t'\right)}dt' = 0. \tag{84}$$

Hence we recover the fractional Fokker-Planck equation first derived from CTRWs with the non-equlibrium initial condition $q(x,0) = \delta_{x,x_0}$ [10],

$$\frac{\partial\rho(x,t)}{\partial t} = {}_0\mathcal{D}_t^{1-\gamma}\left(D_\gamma \frac{\partial^2\rho(x,t)}{\partial x^2} - 2\beta D_\gamma \frac{\partial}{\partial x}\left(F(x)\rho(x,t)\right)\right). \tag{85}$$

Note that if $\gamma = 1$, the fractional Fokker-Planck equation reduces to the standard Fokker-Planck equation, Eq.(74).

The generalized master equations and fractional Fokker-Planck equations from continuous time random walks with arbitrary initial conditions obtained here can be extended to include space- and time- dependent forces, following the approach in [11, 12].

4.3. Conclusion

Continuous time random walks provide a useful framework for modelling particle motions in complex media. Different variants of the CTRWs can be obtained, including different representations of time dependent forcing [5], and in the cases considered here, different initial states. The generalized master equations for the time evolution of the probability density governing the position of particles in the different variants of the CTRWs are in general different. However the details of the variants, relating to the timing of the forcing, and the initial conditions, do not carry over in the diffusion limit to the Fokker-Planck equations. The standard Fokker-Planck equation for Markovian processes and the fractional Fokker-Planck equation for non-Markovian processes are robust in this sense making them applicable across a broad range of modelling applications.

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