SIAM J. APPL. MATH.
Vol. 75, No. 4, pp. 1445–1468

GENERALIZED CONTINUOUS TIME RANDOM WALKS, MASTER EQUATIONS, AND FRACTIONAL FOKKER–PLANCK EQUATIONS*

C. N. ANGSTMANN†, I. C. DONNELLY†, B. I. HENRY‡, T. A. M. LANGLANDS§, AND P. STRAKA†

Abstract. Continuous time random walks, which generalize random walks by adding a stochastic time between jumps, provide a useful description of stochastic transport at mesoscopic scales. The continuous time random walk model can accommodate certain features, such as trapping, which are not manifest in the standard macroscopic diffusion equation. The trapping is incorporated through a waiting time density, and a fractional diffusion equation results from a power law waiting time. A generalized continuous time random walk model with biased jumps has been used to consider transport that is also subject to an external force. Here we have derived the master equations for continuous time random walks with space- and time-dependent forcing for two cases: when the force is evaluated at the start of the waiting time and at the end of the waiting time. The differences persist in low order spatial continuum approximations; however, the two processes are shown to be governed by the same Fokker–Planck equations in the diffusion limit. Thus the fractional Fokker–Planck equation with space- and time-dependent forcing is robust to these changes in the underlying stochastic process.

Key words. continuous time random walk, fractional Fokker–Planck equation, anomalous diffusion, generalized master equation, limit theorems, fractional calculus

AMS subject classifications. 35R11, 35Q84, 60G20, 82C31

DOI. 10.1137/15M1011299

1. Introduction.

A continuous time random walk (CTRW) is a stochastic process where a particle arrives at a position, waits for a stochastic time, and stochastically jumps to a new position. The motion of the particle is governed by waiting time, and step length, probability densities [40]. Generalized CTRWs have been used as a stochastic basis for deriving fractional diffusion equations [16, 22, 36], fractional Cattenao equations [12], fractional reaction diffusion equations [53, 20, 39, 14, 52, 3, 49], fractional cable equations [21, 27, 28], fractional Fokker–Planck equations (FFPEs) [35, 46, 8, 3], and fractional chemotaxis equations [26, 15]. The evolution equation for the probability density function (PDF) of the random walking particles in a CTRW can be written as generalized master equations (GMEs) [45, 24]. If the waiting times are exponentially distributed and the step length density is Gaussian, then in the diffusion limit the evolution equation for the PDF of the random walking particles is the standard diffusion equation. The CTRW also allows for anomalous diffusion in which the mean squared displacement increases slower (subdiffusion) or faster (superdiffusion) than linearly with time. The canonical case is a fractional power of time $\langle x^2(t)\rangle \sim t^\gamma$ where $\gamma \neq 1$ [36]. Subdiffusion ($0 < \gamma < 1$) arises from CTRWs with power law waiting time densities such as Pareto or Mittag–Leffler waiting time densities. In this case, in the diffusion limit the evolution equation for the particle

*Received by the editors March 5, 2015; accepted for publication (in revised form) May 1, 2015; published electronically July 7, 2015.
http://www.siam.org/journals/siap/75-4/M101129.html
†School of Mathematics and Statistics, UNSW, Sydney NSW, 2052, Australia (c.angstman@unsw.edu.au, i.donnelly@unsw.edu.au, p.straka@unsw.edu.au).
‡Corresponding author. School of Mathematics and Statistics, UNSW, Sydney NSW, 2052, Australia (b.henry@unsw.edu.au).
§Department of Mathematics and Computing, University of Southern Queensland, Toowoomba QLD, 4350, Australia (t.langlands@usq.edu.au).

PDF is a time-fractional diffusion equation [36]. If particles undergoing a CTRW are also subject to an external force, then the diffusion limit is a Fokker–Planck equation [17, 42, 44], or, in the case of subdiffusive transport, an FFPE [35, 46, 8, 3]. The same diffusion limits can be obtained from discrete time stochastic processes [6]. The FFPE has also been shown to be consistent with a subordinated stochastic Langevin equation [50, 30, 8, 29], and a fractional Klein–Kramers equation [37].

The external force field is typically incorporated in CTRWs through a bias in the jump density [9, 46, 8]. For time-dependent forces in these studies the force affects the particle at the instant that the particle leaves the trap and jumps. However, if the external force varies in time, then the force may have been different at the time that the particle became trapped, and it may also vary during the time that the particle is trapped. This raises questions about whether the time at which the force is evaluated, relative to the time between jumps, impacts the evolution equations for the PDF, and whether or not there are any observables that could be measured, related to the time that the force is evaluated. In previous work, GMEs and Fokker–Planck equations for CTRWs with time varying external forces have been derived when the force is evaluated at the end of the waiting time, i.e., at the same instant as when the particle jumps [46, 8, 3]. A physical example where this was considered explicitly was provided by Heinsalu and coworkers [19] for the case of a dichotomously varying force field.

Here we have derived the GMEs and diffusion limit Fokker–Planck equations with time varying external forces when the force is evaluated at the start of the waiting time, and when the force is evaluated at the end of the waiting time. The GMEs are different in the two cases, but the same Fokker–Planck equations are obtained in the diffusion limit. Thus the time at which the force is evaluated, relative to the time between jumps, does not impact the diffusion limit Fokker–Planck equations. The lack of sensitivity to the diffusion limit in these two cases demonstrates an invariance in the diffusion limit Fokker–Planck equations, independent of the details of the stochastic process.

It is possible to conceive of physical examples where the force field may be evaluated at the start of the waiting time. Simple examples can be provided by considering biased CTRWs on transport networks [4, 5], where there is no diffusion limit to consider. In an example of itinerant passengers traversing an airline network, if the random walkers (travelers) are price sensitive, then the forcing could be temporal variations in ticket prices to different destinations. The itinerant travelers may choose their subsequent destination when they arrive at a new destination, sensitive to ticket prices at that time, or they may choose their subsequent destination at the moment of departure, sensitive to ticket prices at this time. In the former case the bias force is being evaluated at the start of the waiting time. Another example is that of a chemotactic cell system in which cells move at random establishing internal concentration gradients that align with an external chemotactic concentration gradient. If the cell becomes trapped and released, then upon release it will initially continue in the direction of the internal $Ca2^{+}$ gradient, corresponding to the external chemotactic gradient at the pretrapping time [11]. The effectiveness of our GMEs for modeling these and other physical systems is dependent on the effectiveness of the mathematical CTRW model in providing a mesoscopic description of the physical stochastic processes.

In section 2 we derive the GMEs for the case when the force is evaluated immediately on arrival at a new site. We refer to this as trap-time delayed forcing. The GMEs in this case are different from the GMEs that we derive when the force is evaluated immediately prior to jumping. In section 3 we consider the spatial continuum approximations of the GMEs, and in section 4 we consider the diffusion limits. The governing evolution equations are different in the low order spatial continuum approximation, but they converge to the same Fokker–Planck equations in the diffusion limit. In section 5 we have carried out numerical simulations of the GMEs in each case, and we identify differences that may be observed in experimental systems. We conclude with a summary in section 6.

2. Generalized master equations for biased CTRWs. We consider a particle undergoing nearest neighbor jumps as a CTRW on a one-dimensional lattice. Generalizing the approach in Scher and Lax [45], the flux density of particles arriving at position x_i at time t after $n+1$ steps is given by

$$q_{n+1}(x_i,t|x_0,0) = \int_0^t \Psi(x_i,t|x_{i-1},t')q_n(x_{i-1},t'|x_0,0)\,dt' + \int_0^t \Psi(x_i,t|x_{i+1},t')q_n(x_{i+1},t'|x_0,0)\,dt'. \tag{2.1}$$

Here $\Psi(x_i,t|x_j,t')$ is the transition probability density of a particle jumping from position x_j to position x_i at time t given that the particle arrived at x_j at the earlier time t'. The initial flux density for a particle that begins at position x_0 at time $t=0$ is defined as

$$q_0(x_i,t|x_0,0) = \delta_{x_i,x_0}\delta(t-0^+). \tag{2.2}$$

The total flux density of particles arriving at x_i at time t is given by summing over all possible steps:

$$\begin{aligned} q(x_i,t|x_0,0) &= \sum_{n=0}^{\infty} q_n(x_i,t|x_0,0) \\ &= \delta_{x_i,x_0}\delta(t-0^+) + \int_0^t \Psi(x_i,t|x_{i-1},t')q(x_{i-1},t'|x_0,0)\,dt' \\ &\quad + \int_0^t \Psi(x_i,t|x_{i+1},t')q(x_{i+1},t'|x_0,0)\,dt'. \end{aligned} \tag{2.3}$$

In general the effect of an external force in a CTRW model may be manifest through a change in the jump density [35, 9, 46, 8, 3], or a change in the waiting time density [15], or both. Here we suppose that the forcing is manifest through a bias in the nearest neighbor jumps. We also assume that the transition probability density is separable as

$$\Psi(x_{i+1},t|x_i,t') = p_r(x_i,t,t')\psi(t-t'), \tag{2.4}$$

$$\Psi(x_{i-1},t|x_i,t') = p_\ell(x_i,t,t')\psi(t-t'), \tag{2.5}$$

where $p_r(x_i,t,t')$ and $p_\ell(x_i,t,t')$ are the respective probabilities for jumping right from x_i to x_{i+1} and jumping left from x_i to x_{i-1} at time t given the particle arrived at x_i at the earlier time t' and $\psi(t-t')$ is the waiting time density. In Appendix A we show that this separable form of the transition probability density can be obtained from a generalized rate equation. The subsequent analysis in this article could readily be generalized to include a spatial dependence on the waiting time density, i.e., $\psi(x_i, t - t')$, but for notational convenience we have not carried this through here.

The particle must jump to the left or the right at each step so that

$$p_r(x_i, t, t') + p_\ell(x_i, t, t') = 1. \tag{2.6}$$

Note that the force, manifest through the left and right bias probabilities, is always applied at the end of the waiting time, but it may be evaluated at the start, time t', or end, time t, of the waiting time. We consider both possibilities below. It is conceivable that the force could be evaluated at intermediate times, but we have not considered this further here.

2.1. Continuous time random walk trapping with nondelayed forcing. First, we review the case in which the external force field is evaluated at the same time instant that it is applied, i.e., at the instant of jumping t. We then have

$$p_r(x_i, t, t') = p_r(x_i, t), \tag{2.7}$$

$$p_\ell(x_i, t, t') = p_\ell(x_i, t), \tag{2.8}$$

and the conditional probability flux density for a particle to arrive at x_i is given by

$$\begin{aligned} q(x_i, t|x_0, 0) = \delta_{x_i,x_0}\delta(t - 0^+) + p_r(x_{i-1}, t) \int_0^t q(x_{i-1}, t'|x_0, 0)\psi(t - t')\, dt' \\ + p_\ell(x_{i+1}, t) \int_0^t q(x_{i+1}, t'|x_0, 0)\psi(t - t')\, dt'. \end{aligned} \tag{2.9}$$

The conditional probability density, $\rho(x_i, t|x_0, 0)$, that a walker, which started at x_0 at time $t = 0$, is at x_i at time t, is given by

$$\rho(x_i, t|x_0, 0) = \int_0^t \Phi(t - t')q(x_i, t'|x_0, 0)\, dt', \tag{2.10}$$

where

$$\Phi(t - t') = 1 - \int_0^{t-t'} \psi(t'')\, dt'' \tag{2.11}$$

is the survival probability of a particle not jumping before time t from x_i given it arrived at x_i at the earlier time t'.

We now seek the evolution equation for the conditional probability density for a walker starting from x_0 at time $t = 0$ to be at x_i at time t. The GMEs can be obtained by differentiating $\rho(x_i, t|x_0, 0)$ with respect to t. However, it is first necessary to take care of the singularities in the arrival fluxes at $t = 0$ [3]. We thus define

$$q(x_i, t|x_0, 0) = \delta_{x_i,x_0}\delta(t - 0^+) + q^+(x_i, t|x_0, 0). \tag{2.12}$$

In the following, for simplicity, we drop the conditional notation in ρ and q, i.e., $\rho(x_i, t) = \rho(x_i, t|x_0, 0)$ and $q(x_i, t) = q(x_i, t|x_0, 0)$. We can now differentiate (2.10) for the time evolution for the conditional probability density $\rho(x_i, t)$ to obtain

$$\begin{aligned} \frac{\partial \rho(x_i, t)}{\partial t} = p_r(x_{i-1}, t) \int_0^t \psi(t - t')q(x_{i-1}, t')\, dt' + p_\ell(x_{i+1}, t) \int_0^t \psi(t - t')q(x_{i+1}, t')\, dt' \\ - \int_0^t \psi(t - t')q(x_i, t')\, dt'. \end{aligned} \tag{2.13}$$

We can replace the integrals over the products, $\psi(t-t')q(x,t')$, with integrals over products $K(t-t')\rho(x,t')$ by defining a memory kernel $K(t-t')$ via

$$\int_0^t \psi(t-t')q(x_i,t')\,dt' = \int_0^t K(t-t')\left(\int_0^{t'} \Phi(t'-t'')q(x_i,t'')\,dt''\right)dt'$$
$$= \int_0^t K(t-t')\rho(x_i,t')\,dt'. \tag{2.14}$$

The memory kernel is equivalently defined by the Laplace transform

$$\mathcal{L}\{K(t)\} = \frac{\mathcal{L}\{\psi(t)\}}{\mathcal{L}\{\Phi(t)\}}. \tag{2.15}$$

Using (2.14) we now obtain the GMEs describing the evolution of the probability density for CTRWs with traps and nondelayed forcing:

$$\frac{\partial\rho(x_i,t)}{\partial t} = p_r(x_{i-1},t)\int_0^t K(t-t')\rho(x_{i-1},t')\,dt' + p_\ell(x_{i+1},t)\int_0^t K(t-t')\rho(x_{i+1},t')\,dt'$$
$$-\int_0^t K(t-t')\rho(x_i,t')\,dt'. \tag{2.16}$$

The GME in (2.16) is a special case of the GME for non-Markovian processes. In [23] this GME was shown to apply to CTRWs provided that the Laplace transform of the memory kernel was given by $s\mathcal{L}\{\psi(t)\}/(1-\mathcal{L}\{\psi(t)\})$. This is equivalent to the expression for the Laplace transform of the memory kernel in (2.15). A slight generalization of this result was obtained in the derivation of the space-fractional Fokker–Planck equation from a GME in [35]. The memory kernel for CTRWs was further generalized to include ageing in [1, 2].

In the special case where there is a purely time-dependent bias, the GMEs, (2.16), are equivalent to the GMEs in [46] with the identification

$$\mathcal{L}\{M(t)\} = \frac{\mathcal{L}\{\psi(t)\}}{s\mathcal{L}\{\Phi(t)\}}. \tag{2.17}$$

The equivalence of (2.16) in this article and (7) in [46], with the memory kernel in the latter equation, $M(t)$, defined by (2.17), demonstrates that the GME formalism of Sokolov and Klafter for time-dependent forces can be derived from the CTRW with a bias force applied at the end of the waiting time. If there is no bias and the kernel depends on the spatial location, then (2.16) agrees with (9) of [48].

2.2. Trap-time delayed forcing. In the trap-time delayed case the particle's jump density at a site x_i at time t is biased by the external force field evaluated at the earlier arrival time, t'. In this case

$$p_r(x_i,t,t') = p_r(x_i,t'), \tag{2.18}$$
$$p_\ell(x_i,t,t') = p_\ell(x_i,t'), \tag{2.19}$$

and the conditional probability flux density for a particle to arrive at x_i at time t is given by

$$q(x_i,t) = \delta_{x_i,x_0}\delta(t-0^+) + \int_0^t p_r(x_{i-1},t')q(x_{i-1},t')\psi(t-t')\,dt'$$
$$+\int_0^t p_\ell(x_{i+1},t')q(x_{i+1},t')\psi(t-t')\,dt'. \tag{2.20}$$

Unlike in the nondelayed forcing case, the bias probabilities cannot simply be factored out of the integrals in (2.20). However, we can follow the approach in [7] defining the directed flux densities

$$q_{r/\ell}(x_i, t) = q(x_i, t) p_{r/\ell}(x_i, t), \tag{2.21}$$

where the subscript r/ℓ denotes right or left, respectively. Substituting (2.21) into (2.20), we have equations for the left and right arrival fluxes at each site:

$$\begin{aligned} q_{r/\ell}(x_i, t) = p_{r/\ell}(x_i, t) \bigg(\delta_{x_i, x_0} \delta(t - 0^+) &+ \int_0^t p_r(x_{i-1}, t') q(x_{i-1}, t') \psi(t - t')\, dt' \\ &+ \int_0^t p_\ell(x_{i+1}, t') q(x_{i+1}, t') \psi(t - t')\, dt' \bigg). \end{aligned} \tag{2.22}$$

It also follows from the definition given in (2.21) and the conservation of probability, $p_r(x_i, t) + p_\ell(x_i, t) = 1$, that

$$q(x_i, t) = q_r(x_i, t) + q_\ell(x_i, t). \tag{2.23}$$

We now define directional conditional probability densities

$$\rho_{r/\ell}(x_i, t) = \int_0^t \Phi(t - t') q_{r/\ell}(x_i, t')\, dt', \tag{2.24}$$

where Φ is the survival function defined in (2.11). It is easy to show, using (2.10) and (2.23), that

$$\rho(x_i, t) = \rho_r(x_i, t) + \rho_\ell(x_i, t). \tag{2.25}$$

However, note that

$$\rho_{r/\ell}(x_i, t) \neq p_{r/\ell}(x_i, t) \rho(x_i, t). \tag{2.26}$$

The GMEs can be obtained by differentiating $\rho(x_i, t)$ with respect to t. Again we need to take care of the singularities in the arrival fluxes at $t = 0$. We thus define

$$q_{r/\ell}(x_i, t) = \delta_{x_i, x_0} \delta(t - 0^+) + q^+_{r/\ell}(x_i, t), \tag{2.27}$$

where

$$\begin{aligned} q^+_{r/\ell}(x_i, t) = &\int_0^t \Psi(x_i, t | x_{i-1}, t')\, q_{r/\ell}(x_{i-1}, t')\, dt' \\ &+ \int_0^t \Psi(x_i, t | x_{i+1}, t')\, q_{r/\ell}(x_{i+1}, t')\, dt' \end{aligned} \tag{2.28}$$

is right side continuous at $t = 0$.

We then differentiate (2.24) to obtain

$$\frac{\partial \rho_{r/\ell}(x_i, t)}{\partial t} = q^+_{r/\ell}(x_i, t) - \delta_{x_i, x_0} \psi(t) - \int_0^t q^+_{r/\ell}(x_i, t') \psi(t - t')\, dt'. \tag{2.29}$$

Further, by substituting (2.22) into (2.29), we have

$$\begin{aligned} \frac{\partial \rho_{r/\ell}(x_i, t)}{\partial t} = &\, p_{r/\ell}(x_i, t) \left(\int_0^t \psi(t - t') q_r(x_{i-1}, t')\, dt' + \int_0^t \psi(t - t') q_\ell(x_{i+1}, t')\, dt' \right) \\ &- \int_0^t \psi(t - t') q_{r/\ell}(x_i, t')\, dt'. \end{aligned} \tag{2.30}$$

Similar to the preceding case (see (2.14)), we replace the integrals over the products $\psi(t-t')q_{r/\ell}(x,t')$ with integrals over products $K(t-t')\rho_{r/\ell}(x,t')$, arriving at the coupled sets of equations

$$\frac{\partial \rho_r(x_i,t)}{\partial t} = p_r(x_i,t)\left(\int_0^t K(t-t')\rho_r(x_{i-1},t')\,dt' + \int_0^t K(t-t')\rho_\ell(x_{i+1},t')\,dt'\right) - \int_0^t K(t-t')\rho_r(x_i,t')\,dt' \tag{2.31}$$

and

$$\frac{\partial \rho_\ell(x_i,t)}{\partial t} = p_\ell(x_i,t)\left(\int_0^t K(t-t')\rho_r(x_{i-1},t')\,dt' + \int_0^t K(t-t')\rho_\ell(x_{i+1},t')\,dt'\right) - \int_0^t K(t-t')\rho_\ell(x_i,t')\,dt'. \tag{2.32}$$

By adding and subtracting the above equations we can obtain a reformulation as a coupled system in ρ, (2.25), and

$$\varsigma(x,t) = \rho_\ell(x,t) - \rho_r(x,t). \tag{2.33}$$

This yields the GMEs describing the evolution of the probability density for CTRWs with trap-time delayed forcing:

$$\begin{aligned}\frac{\partial \rho(x_i,t)}{\partial t} &= \frac{1}{2}\int_0^t K(t-t')[\rho(x_{i-1},t') - \varsigma(x_{i-1},t')]\,dt' \\ &\quad + \frac{1}{2}\int_0^t K(t-t')[\rho(x_{i+1},t') + \varsigma(x_{i+1},t')]\,dt' \\ &\quad - \int_0^t K(t-t')\rho(x_i,t')\,dt',\end{aligned} \tag{2.34}$$

$$\begin{aligned}\frac{\partial \varsigma(x_i,t)}{\partial t} &= \frac{1}{2}(p_\ell(x_i,t) - p_r(x_i,t))\int_0^t K(t-t')[\rho(x_{i-1},t') - \varsigma(x_{i-1},t')]\,dt' \\ &\quad + \frac{1}{2}(p_\ell(x_i,t) - p_r(x_i,t))\int_0^t K(t-t')[\rho(x_{i+1},t') + \varsigma(x_{i+1},t')]\,dt' \\ &\quad - \int_0^t K(t-t')\varsigma(x_i,t')\,dt'.\end{aligned} \tag{2.35}$$

It is possible to reduce this coupled system further to a set of GMEs in the single dynamical state variable ρ. First, we note that by rearranging (2.35) and substituting in (2.34) it is easy to identify

$$\begin{aligned}&\frac{\partial \varsigma(x_i,t)}{\partial t} + \int_0^t K(t-t')\varsigma(x_i,t')dt' \\ &\quad = (p_\ell(x_i,t) - p_r(x_i,t))\left[\frac{\partial \rho(x_i,t)}{\partial t} + \int_0^t K(t-t')\rho(x_i,t')dt'\right].\end{aligned}$$

This can be written in the compact form

$$L\left[\varsigma(x_i,t)\right] = (p_\ell(x_i,t) - p_r(x_i,t))\,L\left[\rho(x_i,t)\right], \tag{2.36}$$

where $L[-]$ is the operator defined by

$$L\left[f(t)\right] = \frac{\partial f(t)}{\partial t} + \int_0^t K(t-t')f(t')dt'. \tag{2.37}$$

It is straightforward to show, using Laplace transform methods, that the operator can equivalently be defined by

$$L\left[f(t)\right] = \int_0^t \left(\chi(t-t')f(t') - f(0)\delta(t')\right)dt', \tag{2.38}$$

where the generalized function $\chi(t)$ is defined by

$$\mathcal{L}\left\{\chi(s)\right\} = \frac{1}{\mathcal{L}\left\{\Phi(s)\right\}}. \tag{2.39}$$

In the special case where $f(0) = 0$, the operator $L[-]$ can be represented as

$$L[f(t)] = \int_0^t \chi(t-t')f(t')dt', \tag{2.40}$$

and the inverse operator $L^{-1}[-]$ simplifies to

$$L^{-1}\left[f(t)\right] = \int_0^t \Phi(t-t')f(t')dt'. \tag{2.41}$$

Note that it follows from (2.37) and (2.40) that

$$\frac{\partial f(t)}{\partial t} + \int_0^t K(t-t')f(t')dt' = \int_0^t \chi(t-t')f(t')dt'. \tag{2.42}$$

In the following we assume that there is no forcing at $t = 0$, i.e., $p_\ell(x_i, 0) = p_r(x_i, 0)$ for all x_i, and hence $\varsigma(x_i, 0) = 0$ for all x_i. Formally, taking the inverse of (2.36), we have

$$\begin{aligned}
\varsigma(x_i, t) &= L^{-1}\left[(p_\ell(x_i, t') - p_r(x_i, t'))L[\rho(x_i, t')]\right] \\
&= \int_0^t \Phi(t-t')(p_\ell(x_i, t') - p_r(x_i, t')) \\
&\qquad \times \left(\int_0^{t'} \chi(t'-t'')\rho(x_i, t'')dt'' - \rho(x_i, 0)\delta(t')\right)dt' \\
&= \int_0^t \Phi(t-t')(p_\ell(x_i, t') - p_r(x_i, t'))\left(\int_0^{t'} \chi(t'-t'')\rho(x_i, t'')dt''\right)dt'.
\end{aligned}$$

By substituting the above into (2.34) we now obtain

$$\begin{aligned}\frac{\partial\rho(x_i,t)}{\partial t} &= \frac{1}{2}\int_0^t K(t-t')\left(\rho(x_{i-1},t')-2\rho(x_i,t')+\rho(x_{i+1},t')\right)dt'\\ &+\frac{1}{2}\int_0^t K(t-t')\int_0^{t'}\Phi(t'-t'')(p_\ell(x_{i-1},t'')-p_r(x_{i-1},t''))\\ &\qquad\times\int_0^{t''}\chi(t''-t''')\rho(x_{i-1},t''')dt'''dt''dt'\\ &-\frac{1}{2}\int_0^t K(t-t')\int_0^{t'}\Phi(t'-t'')(p_\ell(x_{i+1},t'')-p_r(x_{i+1},t''))\\ &\qquad\times\int_0^{t''}\chi(t''-t''')\rho(x_{i+1},t''')dt'''dt''dt' \end{aligned} \tag{2.43}$$

Equation (2.43) can be further simplified using the result

$$\int_0^t K(t-t')\int_0^{t'}\Phi(t'-t'')Y(t'')dt''dt' = \int_0^t \psi(t-t')Y(t')dt', \tag{2.44}$$

which follows from the definition of K given in (2.15). Finally, we arrive at

$$\begin{aligned}\frac{\partial\rho(x_i,t)}{\partial t} &= \frac{1}{2}\int_0^t K(t-t')\left(\rho(x_{i-1},t')-2\rho(x_i,t')+\rho(x_{i+1},t')\right)dt'\\ &+\frac{1}{2}\int_0^t \psi(t-t')(p_\ell(x_{i-1},t')-p_r(x_{i-1},t'))\int_0^{t'}\chi(t'-t'')\rho(x_{i-1},t'')dt''dt'\\ &-\frac{1}{2}\int_0^t \psi(t-t')(p_\ell(x_{i+1},t')-p_r(x_{i+1},t'))\int_0^{t'}\chi(t'-t'')\rho(x_{i+1},t'')dt''dt'. \end{aligned} \tag{2.45}$$

Equation (2.45) is the major result of this section, providing the GME for CTRWs with trap-time delay forcing.

We note that if the bias probabilities do not depend on time, then (2.45) reduces to

$$\begin{aligned}\frac{\partial\rho(x_i,t)}{\partial t} &= p_r(x_{i-1})\int_0^t K(t-t')\rho(x_{i-1},t')\,dt' + p_\ell(x_{i+1})\int_0^t K(t-t')\rho(x_{i+1},t')\,dt'\\ &-\int_0^t K(t-t')\rho(x_i,t')\,dt'. \end{aligned} \tag{2.46}$$

Equation (2.46) is equivalent to the GMEs for biased CTRWs first derived in [35].

3. Spatial continuum approximation. We now consider the spatial continuum approximations of the GMEs for both cases under the assumption that the external force, $F(x,t)$, is derivable from a scalar potential $V(x,t)$, i.e.,

$$F(x,t) = -\frac{\partial V(x,t)}{\partial x}, \tag{3.1}$$

and the bias probabilities are given by the (near thermodynamic equilibrium) Boltzmann weights [8]:

$$p_r(x_i,t) = \frac{e^{-\beta V(x_{i+1},t)}}{e^{-\beta V(x_{i+1},t)}+e^{-\beta V(x_{i-1},t)}}, \tag{3.2}$$

$$p_\ell(x_i,t) = \frac{e^{-\beta V(x_{i-1},t)}}{e^{-\beta V(x_{i+1},t)}+e^{-\beta V(x_{i-1},t)}}. \tag{3.3}$$

The spatial continuum approximation of the GMEs is then obtained by writing $x = x_i, x \pm \Delta x = x_{i\pm 1}$ and carrying out Taylor series expansions in x, retaining leading order terms up to $\mathcal{O}(\Delta x^2)$.

The spatial continuum approximation of the GMEs, (2.16), for CTRWs with traps and nondelayed forcing, is given by

$$\begin{aligned}\frac{\partial \rho(x,t)}{\partial t} &= \frac{\Delta x^2}{2}\int_0^t K(t-t')\frac{\partial^2}{\partial x^2}\rho(x,t')\,dt' \\ &\quad -\Delta x^2 \beta \frac{\partial}{\partial x}\left(F(x,t)\int_0^t K(t-t')\rho(x,t')\,dt'\right). \end{aligned} \tag{3.4}$$

This compares with the spatial continuum approximation of the GMEs, (2.45), for CTRWs with trap-time delayed forcing:

$$\begin{aligned}\frac{\partial \rho(x,t)}{\partial t} &= \frac{\Delta x^2}{2}\int_0^t K(t-t')\frac{\partial^2}{\partial x^2}\rho(x,t')dt' \\ &\quad -\Delta x^2 \beta \frac{\partial}{\partial x}\int_0^t \psi(t-t')F(x,t')\int_0^{t'}\chi(t'-t'')\rho(x,t'')dt''dt'. \end{aligned} \tag{3.5}$$

It is straightforward to show that if $F(x,t')$ is replaced with $F(x,t)$, then (3.5) is identical to (3.4).

3.1. Exponential waiting time density. In the diffusion limit, the evolution of the PDF for CTRWs with exponential waiting time densities reduces to the standard diffusion equation. The homogeneous exponential waiting time density is given by

$$\psi(t) = \alpha e^{-\alpha t}. \tag{3.6}$$

The parameter α relates to a characteristic waiting time, and its importance can be seen when taking the diffusion limit. The expected waiting time corresponding to the exponential density is given by $\langle\tau\rangle = \frac{1}{\alpha}$, and $\langle\tau^2\rangle - \langle\tau\rangle^2 = \frac{1}{\alpha^2}$. We also have the Laplace transforms of $\mathcal{L}\{\psi(t)\} = \frac{\alpha}{s+\alpha}$ and $\mathcal{L}\{\Phi(t)\} = \frac{1-\hat{\psi}(s)}{s}$. Substituting these into (2.15) and inverting the transform gives the memory kernel

$$K(t) = \alpha\,\delta(t). \tag{3.7}$$

The spatial continuum approximation for the GMEs with exponential waiting time densities and nondelayed forcing reduces to

$$\frac{\partial \rho(x,t)}{\partial t} = \alpha\frac{\Delta x^2}{2}\frac{\partial^2}{\partial x^2}\rho(x,t) - \alpha\beta\Delta x^2\frac{\partial}{\partial x}F(x,t)\rho(x,t). \tag{3.8}$$

We now consider the spatial continuum approximation for the GMEs with exponential waiting time densities and trap-time delayed forcing. Starting with (3.5), using (3.7) for the memory kernel, and combining (2.37) and (2.38) with $F(x,0) = 0$, we first write

$$\begin{aligned}\frac{\partial \rho(x,t)}{\partial t} &= \alpha\frac{\Delta x^2}{2}\frac{\partial^2}{\partial x^2}\rho(x,t) \\ &\quad -\beta\Delta x^2\frac{\partial}{\partial x}\int_0^t \psi(t-t')F(x,t')\left(\frac{\partial \rho(x,t')}{\partial t'} + \alpha\rho(x,t')\right)dt'. \end{aligned} \tag{3.9}$$

Now using the exponential property of the waiting time density, we can write

$$\frac{\partial \rho(x,t)}{\partial t} = \alpha \frac{\Delta x^2}{2} \frac{\partial^2}{\partial x^2} \rho(x,t) - \beta \Delta x^2 \frac{\partial}{\partial x} \int_0^t F(x,t') \frac{\partial}{\partial t'} \left[\psi(t-t') \rho(x,t') \right] dt'. \tag{3.10}$$

Finally, using integration by parts, we obtain the result

$$\begin{aligned} \frac{\partial \rho(x,t)}{\partial t} &= \alpha \frac{\Delta x^2}{2} \frac{\partial^2}{\partial x^2} \rho(x,t) - \alpha \beta \Delta x^2 \frac{\partial}{\partial x} F(x,t) \rho(x,t) \\ &\quad + \beta \Delta x^2 \frac{\partial}{\partial x} \int_0^t e^{\alpha(t'-t)} \rho(x,t') \frac{\partial}{\partial t'} F(x,t') dt'. \end{aligned} \tag{3.11}$$

Equation (3.11) is the spatial continuum approximation for the GMEs for CTRWs with trap-time delayed forcing and exponential waiting times. Comparing (3.8) and (3.11) reveals an additional term in the spatial continuum approximation for trap-time delayed forcing.

3.2. Mittag–Leffler waiting time density. In the diffusion limit, the evolution of the PDF for CTRWs governed by power law waiting time densities at long times reduces to a fractional subdiffusion equation, and the variance scales sublinearly with time [36]. Here we consider the spatial continuum approximation for CTRWs, in an external space and time varying force field, with a Mittag–Leffler waiting time density [31],

$$\psi(t) = \frac{t^{\gamma} - 1}{\tau^{\gamma}} E_{\gamma,\gamma} \left[- \left(\frac{t}{\tau} \right)^{\gamma} \right] = - \frac{d}{dt} E_{\gamma,1} \left[- \left(\frac{t}{\tau} \right)^{\gamma} \right], \tag{3.12}$$

where $0 < \gamma < 1$ and

$$E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(k\alpha + \beta)} \tag{3.13}$$

is a generalized Mittag–Leffler function. The standard Mittag–Leffler function, obtained with $\beta = 1$, has been used as a phenomenological physical model for relaxation, mediating between stretched exponential relaxation at short times and power law relaxation at long times, with α as the dissipation parameter [51]. The Mittag–Leffler waiting time density has power law behavior at long times, and it also leads to algebraically tractable results at short times.

The Laplace transform of (3.12), which is readily found using equation (2.2.21) from [31], is given by

$$\mathcal{L}\left\{\psi(s)\right\} = \frac{1}{1 + (s\tau)^{\gamma}}. \tag{3.14}$$

In this case the Laplace transform of the memory kernel, (2.15), simplifies to

$$\mathcal{L}\left\{K(s)\right\} = \frac{1}{\tau^{\gamma}} s^{1-\gamma} \tag{3.15}$$

and the convolution

$$\int_0^t K(t-t') y(x,t')\, dt' = \frac{1}{\tau^{\gamma}} \; {}_0\mathcal{D}_t^{1-\gamma} y(x,t), \tag{3.16}$$

where ${}_0\mathcal{D}_t^{1-\gamma}$ is the Riemann–Liouville fractional derivative of order $1-\gamma$ [41]. The above result follows from the Laplace transform properties of fractional derivatives if we assume that the fractional integral ${}_0\mathcal{D}_t^{-\gamma} y(x,t)$ vanishes at $t=0$.

Considering the spatial continuum approximation GMEs, substituting (3.16) into (3.4) gives

$$\frac{\partial \rho(x,t)}{\partial t} = \frac{\Delta x^2}{2\tau^\gamma}\frac{\partial^2}{\partial x^2} D_t^{1-\gamma}\left[\rho(x,t)\right] - \frac{\Delta x^2}{\tau^\gamma}\beta\frac{\partial}{\partial x}F(x,t)\,{}_0\mathcal{D}_t^{1-\gamma}\left[\rho(x,t)\right]. \tag{3.17}$$

Similarly, substituting (2.42), (3.12), and (3.16) into (3.5) yields

$$\begin{aligned}\frac{\partial \rho(x,t)}{\partial t} = {} & \frac{\Delta x^2}{2\tau^\gamma}\frac{\partial^2}{\partial x^2} D_t^{1-\gamma}[\rho(x,t)] - \frac{\Delta x^2}{\tau^\gamma}\beta\frac{\partial}{\partial x}\int_0^t \left[(t-t')^{\gamma-1}E_{\gamma,\gamma}\left[-\left(\frac{t-t'}{\tau}\right)^\gamma\right]F(x,t')\right. \\ & \left.\times\left(\frac{\partial \rho(x,t')}{\partial t'} + \frac{1}{\tau^\gamma}D_{t'}^{1-\gamma}\left[\rho(x,t')\right]\right)\right] dt'.\end{aligned} \tag{3.18}$$

Using the Laplace transform properties of the Mittag–Leffler function (see, for example, [31]) it can be shown that if $F(x,t')$ is replaced by $F(x,t)$ in (3.19), then (3.19) reduces to the spatial continuum approximation for nondelayed forcing, (3.17).

4. Diffusion limit Fokker–Planck equations.

The diffusion limit is found by first introducing a jump length scaling parameter h and a waiting time scaling parameter τ, so that all jumps are made smaller by a factor h and all waiting times are made smaller by a factor τ, and then taking the limit $h \to 0$ and $\tau \to 0$ with a properly defined scaling relation between h and τ [43]. Without loss of generality, in the case of nearest neighbor jumps, the scaling parameter of the jump length density can be taken to be the lattice spacing Δx. We introduce a waiting time scale parameter τ by noting that if $\psi(t)$ is the waiting time density for a CTRW with waiting times $T_1, T_2, \ldots$, then

$$\psi_\tau(t) = \frac{\psi(t/\tau)}{\tau} \tag{4.1}$$

is the waiting time density for a CTRW with rescaled waiting times $\tau T_1, \tau T_2, \ldots$. It is a simple exercise to show that if $\psi(t)$ is a PDF, then $\psi_\tau(t)$ is also a PDF, and moreover,

$$\lim_{\tau\to 0}\psi_\tau(t) = \delta(t). \tag{4.2}$$

We now consider a sequence of rescaled CTRWs and take the limit $\Delta x, \tau \to 0$. It is useful to define a rescaled survival probability function

$$\Phi_\tau(t) = 1 - \int_0^t \psi_\tau(s)ds \tag{4.3}$$

and rescaled memory kernels defined by

$$\mathcal{L}\left\{K_\tau(t)\right\} = \frac{\mathcal{L}\left\{\psi_\tau(t)\right\}}{\mathcal{L}\left\{\Phi_\tau(t)\right\}} \tag{4.4}$$

and

$$\mathcal{L}\left\{\chi_\tau(t)\right\} = \frac{1}{\mathcal{L}\left\{\Phi_\tau(t)\right\}}. \tag{4.5}$$

The following result then follows from (4.4) using (4.2) and (4.5) together with the combination theorem for limits of products,

$$\lim_{\tau\to 0}\mathcal{L}\left\{K_\tau(t)\right\} = \lim_{\tau\to 0}\mathcal{L}\left\{\chi_\tau(t)\right\}. \tag{4.6}$$

In the diffusion limit, the GME for the spatial continuum approximation of rescaled CTRWs with nondelayed forcing, (3.4), can be written as

$$\begin{aligned}\frac{\partial\rho(x,t)}{\partial t} &= \lim_{\Delta x,\tau\to 0}\frac{\Delta x^2}{2}\int_0^t K_\tau(t-t')\frac{\partial^2}{\partial x^2}\rho(x,t')dt' \\ &\quad - \lim_{\Delta x,\tau\to 0}\Delta x^2\beta\frac{\partial}{\partial x}F(x,t)\int_0^t K_\tau(t-t')\rho(x,t')dt'.\end{aligned} \tag{4.7}$$

In the diffusion limit the GME for the spatial continuum approximation of rescaled CTRWs with trap-time delay forcing, (3.5), can be written as

$$\begin{aligned}\frac{\partial\rho(x,t)}{\partial t} &= \lim_{\Delta x,\tau\to 0}\frac{\Delta x^2}{2}\int_0^t K_\tau(t-t')\frac{\partial^2}{\partial x^2}\rho(x,t')dt' \\ &\quad - \lim_{\Delta x,\tau\to 0}\Delta x^2\beta\frac{\partial}{\partial x}\int_0^t \psi_\tau(t-t')F(x,t')\int_0^{t'}\chi_\tau(t'-t'')\rho(x,t'')dt''dt'.\end{aligned} \tag{4.8}$$

The first terms on the right-hand side of (4.7) and (4.8) are identical, and they reduce to a pure diffusion term in the diffusion limit.

The second terms on the right-hand side of (4.7) and (4.8) appear to be different, but it can be shown that they are equivalent in the diffusion limit. The equivalence can be established using a sequence of steps based on the dominated convergence theorem and the combination theorem for distributions. Explicitly, starting with the second term on the right-hand side of (4.8), we have

$$\begin{aligned}&\lim_{\Delta x,\tau\to 0}\Delta x^2\beta\frac{\partial}{\partial x}\int_0^t \psi_\tau(t')F(x,t-t')\left(\int_0^{t-t'}\chi_\tau(t'')\rho(x,t-t'-t'')dt''\right)dt' \\ &\quad= \lim_{\Delta x\to 0}\Delta x^2\beta\frac{\partial}{\partial x}\int_0^t \delta(t')F(x,t-t')\lim_{\tau\to 0}\left(\int_0^{t-t'}\chi_\tau(t'')\rho(x,t-t'-t'')dt''\right)dt' \\ &\quad= \lim_{\Delta x,\tau\to 0}\frac{\Delta x^2}{\beta}\frac{\partial}{\partial x}F(x,t)\int_0^t \chi_\tau(t'')\rho(x,t-t'')dt'' \\ &\quad= \lim_{\Delta x,\tau\to 0}\frac{\Delta x^2}{\beta}\frac{\partial}{\partial x}F(x,t)\int_0^t K_\tau(t'')\rho(x,t-t'')dt''.\end{aligned} \tag{4.9}$$

The final step, leading to the second term on the right-hand side of (4.7), was found by taking the Laplace transform of the convolution, then using (4.6), and then taking the inverse Laplace transform of the convolution. Thus the second terms on the right-hand sides of (4.7) and (4.8) are also equivalent in the diffusion limit.

In Appendix B we have established the equivalence between the diffusion limits of the stochastic processes defined by CTRWs with trap-time delayed forcing and nondelayed forcing using an entirely different method based on the convergence in probability of stochastic processes.

It is straightforward to show that the diffusion limit equation, (4.9), with the memory kernel corresponding to exponential waiting time densities, i.e., $K_\tau(t) =$

$\frac{1}{\tau}\delta(t)$, reduces to the standard Fokker–Planck equation

$$\frac{\partial \rho(x,t)}{\partial t} = D\frac{\partial^2}{\partial x^2}\rho(x,t) - 2\beta D\frac{\partial}{\partial x}F(x,t)\rho(x,t), \tag{4.10}$$

where

$$D = \lim_{\Delta x,\tau\to 0}\frac{\Delta x^2}{2\tau}. \tag{4.11}$$

The diffusion limit equation, (4.9), with the memory kernel corresponding to Mittag–Leffler waiting time densities, i.e., $\int_0^t K_\tau(t-t')y(x,t')\,dt' = \frac{1}{\tau^\gamma}\,{}_0\mathcal{D}_t^{1-\gamma}\,[y(x,t)]$, reduces to the subdiffusive FFPE [8]

$$\frac{\partial \rho(x,t)}{\partial t} = D_\gamma\frac{\partial^2}{\partial x^2}\,{}_0\mathcal{D}_t^{1-\gamma}\,[\rho(x,t)] - 2\beta D_\gamma\frac{\partial}{\partial x}F(x,t)\,{}_0\mathcal{D}_t^{1-\gamma}\,[\rho(x,t)]\,, \tag{4.12}$$

where

$$D_\gamma = \lim_{\Delta x,\tau\to 0}\frac{\Delta x^2}{2\tau^\gamma}. \tag{4.13}$$

Note that when $\gamma = 1$, (4.12) is identical to (4.10).

In the supplementary material we have used (4.10) and (4.12) to derive algebraic results of the first moment,

$$\langle x(t)\rangle = \int_{-\infty}^{\infty} x\rho(x,t)\,dx,$$

and the variance,

$$\sigma^2(t) = \langle(\langle x(t)\rangle - x)^2\rangle = \langle x(t)^2\rangle - \langle x(t)\rangle^2,$$

of the evolution of the probability density with a space- and time-dependent force, $F(x,t) = -x + \sin\omega t$. For the standard Fokker–Planck equation,

$$\frac{\partial \rho(x,t)}{\partial t} = D\frac{\partial^2 \rho(x,t)}{\partial x^2} + 2\beta D\rho(x,t) + 2\beta D\,(x - \sin(\omega t))\,\frac{\partial \rho(x,t)}{\partial x}, \tag{4.14}$$

we have

$$\langle x(t)\rangle = \frac{2\beta D}{\omega^2 + 4\beta^2 D^2}\left(\omega e^{-2\beta D t} + \sin(\omega t) - \omega\cos(\omega t)\right)$$

and

$$\sigma^2(t) = \frac{1}{2\beta}\left(1 - e^{-4\beta D t}\right). \tag{4.15}$$

For the FFPE,

$$\begin{aligned}\frac{\partial \rho(x,t)}{\partial t} &= D_\gamma\,{}_0\mathcal{D}_t^{1-\gamma}\frac{\partial^2 \rho(x,t)}{\partial x^2} + 2\beta D_\gamma\,{}_0\mathcal{D}_t^{1-\gamma}\rho(x,t)\\ &\quad + 2\beta D_\gamma\,(x - \sin(\omega t))\,{}_0\mathcal{D}_t^{1-\gamma}\frac{\partial \rho(x,t)}{\partial x},\end{aligned} \tag{4.16}$$

we have

$$\langle x(t)\rangle = \frac{2\beta D_\gamma}{\Gamma(\gamma)} \int_0^t t'^{\gamma-1} \sin(\omega t')\, E_\gamma\left(-2\beta D_\gamma (t-t')^\gamma\right) dt'$$

and

$$\sigma^2(t) = 2\int_0^t \left(\langle x(t')\rangle - \sin\omega t'\right)\left(2\beta D_\gamma \frac{t'^{\gamma-1}}{\Gamma(\gamma)}\left(\langle x(t')\rangle - \sin\omega t'\right) + \frac{d\langle x(t')\rangle}{dt'}\right)$$
$$\times E_\gamma\left(-4\beta D_\gamma (t-t')^\gamma\right) dt' + \frac{1}{2\beta}\left(1 - E_\gamma\left(-4\beta D_\gamma t^\gamma\right)\right). \tag{4.17}$$

In the next section we compare the diffusion limit results with numerical solutions of the associated GMEs, (3.4) and (3.5).

We are not aware of standard methods that can be used to obtain analytical solutions to general FFPEs of the form (4.12). However, some progress has been made on related nonlinear fractional partial differential equations using variational iteration methods [18], Adomian decomposition methods [13], and homotopy perturbation methods [38].

5. Numerical comparisons. In this section we carry out numerical integrations of the coupled GMEs for CTRWs with traps and nondelayed forcing, (2.16), and with trap-time delayed forcing, (2.45). The numerical integrations have been carried out for both exponential waiting time densities and Mittag–Leffler densities, given by

$$\psi(t) = \frac{1}{\tau} e^{-\frac{t}{\tau}} \tag{5.1}$$

and

$$\psi(t) = \frac{t^{-\frac{1}{2}}}{\tau^{\frac{1}{2}}} E_{\frac{1}{2},\frac{1}{2}}\left[-\left(\frac{t}{\tau}\right)^{\frac{1}{2}}\right], \tag{5.2}$$

respectively.

The GMEs were solved using an implicit time stepping method similar to [25] and, in the case of Mittag–Leffler waiting time densities, the fractional derivatives were approximated using the $L1$ scheme [41]. Dirichlet boundary conditions were employed with the PDF set to zero at each end of the spatial domain.

The external force field was taken to vary in both space and time as

$$F(x,t) = -x + \epsilon \sin(5\pi t). \tag{5.3}$$

In the case $\epsilon = 0$, where the external force does not vary in time, the results from the numerical simulations for the first moment and the variance are indistinguishable for the nondelayed forcing and the trap-time delayed forcing, in agreement with the algebraic analysis. The further discussion below is based on the case $\epsilon = 1$, i.e., the external force varies periodically in time.

The numerical solutions are characterized by parameters $\beta, \tau, \Delta x, \Delta t$. The local accuracy of the $L1$ approximation to the fractional derivative is $O(\Delta t^{1+\gamma})$, and the global error in the numerical method is $O(\Delta t^\gamma)$ [25]. Convergence of the numerical solution to the exact solution of the GME is obtained in the limit $\Delta t \to 0$. Convergence of the numerical solution to the diffusion limit of the GME requires numerical convergence, the limit $\Delta t \to 0$, in addition to convergence to the diffusion limit, $\Delta x \to 0$, $\tau \to 0$, and $D = \Delta x^2/2\tau^\gamma$ finite.

In Figure 1 we show plots of the variance as a function of time obtained from the numerical solutions of the GMEs for both nondelayed forcing and trap-time delayed forcing, with exponential waiting time densities and parameters $\beta = 10$ and (a) $\Delta x = 0.05, \tau = 2.5 \times 10^{-3}, \Delta t = 1.0 \times 10^{-4}$; and (b) $\Delta x = 0.025, \tau = 6.25 \times 10^{-4}, \Delta t = 1.0 \times 10^{-4}$. These parameter values correspond to the same $D = \frac{\Delta x^2}{2\tau} = 0.5$. We have also plotted the variance based on the diffusion limit Fokker–Planck equation using the same $D = 0.5$ and $\beta = 10$.

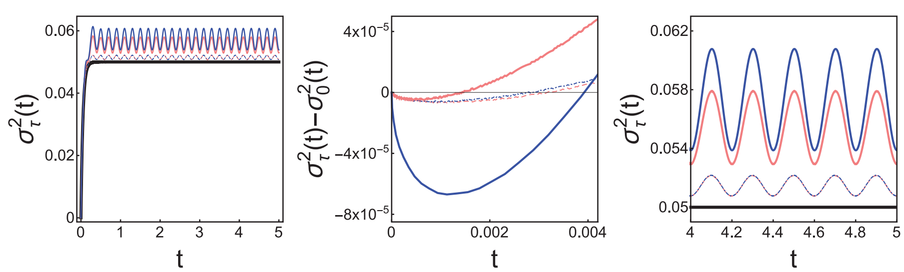

FIG. 1. *Plots of the variance, $\sigma_\tau^2(t)$, of the numerical solutions of the GMEs, with exponential waiting times for trap-time delayed forcing,* (2.45) *(blue/dark gray lines) and nondelayed forcing,* (2.16) *(red/light gray lines). The external force is given by $F(x, t) = -x + \epsilon \sin(5\pi t)$. Also shown is variance of the solution, $\sigma_0^2(t)$, obtained algebraically in the diffusive limit,* (4.15) *(thick black lines). Plots of σ^2 for different values of the characteristic waiting time, τ, show the approach to the diffusion limit as τ is decreased. Dashed lines denote $\tau = 6.25 \times 10^{-4}$, and solid lines denote $\tau = 0.025$.*

There are four features to observe in these plots: (i) There are differences between the numerical solutions of the GME at nonzero τ between the nondelayed forcing and trap-time delayed forcing. (ii) The solutions to the GMEs approach the diffusion limit in both forcing cases as τ is decreased for fixed D and β. (iii) The variance from the GMEs is less than the variance in the diffusion limit at very short times but is greater than the variance in the diffusion limit at longer times. (iv) Oscillations with a characteristic period of $T \approx 0.2$ are present in the variance of the GMEs; however, the oscillations are not present in the diffusion limit. The oscillations are in phase in both the nondelayed and trap-time delayed cases.

In Figure 2 we show plots of the variance as a function of time obtained from the numerical solutions of the GMEs for both the nondelayed forcing case and the trap-time delayed forcing case, with Mittag–Leffler waiting time densities and parameters $\gamma = \frac{1}{2}, \beta = 10$, and (a) $\Delta x = 0.1, \tau = 0.1, \Delta t = 1.0 \times 10^{-5}$; and (b) $\Delta x = 0.05, \tau = 6.25 \times 10^{-3}, \Delta t = 1.0 \times 10^{-4}$. These parameter values have the same $D = \frac{\Delta x^2}{2\tau^\gamma} \approx 0.0158$. We have also plotted the variance based on the diffusion limit FFPE using the same D, β, γ.

Similar to the exponential case, the following features can be observed: (i) There are differences between the numerical solutions of the GME at $\tau > 0$ between the two forcing cases. (ii) The numerical solutions to the GMEs approach the diffusion limit in both forcing cases as τ is decreased for fixed D and β. (iii) The variance from the GMEs is less than the variance in the diffusion limit at very short times but is greater than the variance in the diffusion limit at longer times. (iv) The numerical solutions of

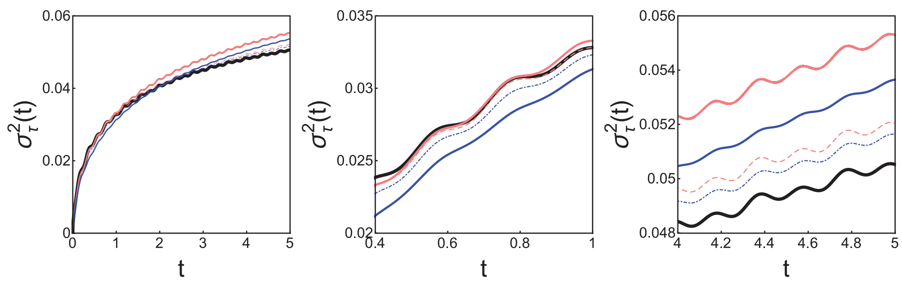

FIG. 2. *Plots of the variance, $\sigma_\tau^2(t)$, of the numerical solutions of the GMEs, with Mittag–Leffler waiting times and $\gamma = 0.5$, for trap-time delayed forcing,* (2.45) *(blue/dark gray lines), and nondelayed forcing,* (2.16) *(red/light gray lines). The external force is given by $F(x,t) = -x + \epsilon \sin(5\pi t)$. Also shown is variance of the solution, $\sigma_0^2(t)$, obtained algebraically in the diffusive limit,* (4.17) *(thick black lines). Plots of σ^2 for different values of the characteristic waiting time, τ, show the approach to the diffusion limit as τ is decreased. Dashed lines denote $\tau = 6.25 \times 10^{-3}$, and solid lines denote $\tau = 0.1$.*

the GMEs show oscillations with a characteristic period of $T = 0.2$. Oscillations with the same period are also present in the diffusion limit variance, but these oscillations are not in phase with the nondelayed and trap-timed delayed results.

6. Conclusion. We have analyzed the behavior of two cases of space- and time-dependent forcing on a particle whose underlying stochastic process is a continuous time random walk (CTRW). In both cases the force is applied immediately prior to jumping and it is manifest in a biased nearest neighbor jump. In the first case the time-dependent force is evaluated at the time immediately prior to jumping, while in the second case the force is evaluated at the beginning of the waiting time. We have derived the generalized master equations (GMEs) governing an ensemble of particles for both cases of forcing. The equations are different for the two cases, and the difference persists in a spatial continuum approximation. In both cases the GMEs converge to the same equation in the diffusion limit: a Fokker–Planck equation for biased CTRWs with an exponential waiting time density, and a fractional Fokker–Planck equation (FFPE) for biased CTRWs with a Mittag–Leffler waiting time density.

We have carried out numerical simulations that confirm agreement in the diffusion limit but show observable differences away from this limit.

Appendix A. A decoupled CTRW transition probability density for space- and time-dependent forcing. In this paper we have considered CTRWs with a biased jump density to model the effects of a time-dependent force. The transition probability density, $\Psi(x,t|x',t')$, for jumping from site x' to site x at time t, given arrival at site x' at time t', in this case is given by the product of a space- and time-dependent jump density and a waiting time density dependent on the residence time $t - t'$. Explicitly,

$$\Psi(x,t|x',t') = \lambda(x,t|x',t')\psi(x',t-t'). \tag{A.1}$$

In this appendix we show how this form of the transition probability density can be obtained from a generalized rate equation. We begin by assuming that in any small interval in time, $[t, t + \Delta t)$, a particle that arrived at position x' at time t' and had not yet jumped until time t has a probability of jumping to an adjacent lattice site x given by

$$\mathbb{P}(x,[t,t+\Delta t)|x',t') = \omega(x,t|x',t')\Delta t + o(\Delta t). \tag{A.2}$$

This defines $\omega(x,t|x',t')$ as the time- and space-dependent rate of change of this probability per unit time. In general this rate may change, depending on space- and time-dependent forcing.

The probability that the particle does not jump in any arbitrarily small time interval between t' and t, but then does jump at time t, can be written as

$$\begin{aligned}\lim_{\Delta t\to 0}\Psi(x,t|x',t')\Delta t &= \lim_{\Delta t\to 0}\mathbb{P}(x,[t,t+\Delta t)|x',t') \\ &\quad\times\prod_{i=1}^{\frac{t-t'}{\Delta t}}\prod_{x''}(1-\mathbb{P}(x'',[t'+(i-1)\Delta t,t'+i\Delta t)|x',t')) \\ &= \lim_{\Delta t\to 0}\omega(x,t|x',t')\Delta t\prod_{i=1}^{\frac{t-t'}{\Delta t}}\prod_{x''}(1-\omega(x'',t'+(i-1)\Delta t|x',t')\Delta t)\,. \end{aligned}\tag{A.3}$$

This can be simplified as follows:

$$\begin{aligned}&\lim_{\Delta t\to 0}\Psi(x,t|x',t')\Delta t \\ &\quad= \lim_{\Delta t\to 0}\omega(x,t|x',t')\Delta t\exp\left(\sum_{x''}\sum_{i=1}^{\frac{t-t'}{\Delta t}}\log(1-\omega(x'',t'+(i-1)\Delta t|x',t')\Delta t)\right) \\ &\quad\approx \lim_{\Delta t\to 0}\omega(x,t|x',t')\Delta t\exp\left(\sum_{x''}\sum_{i=1}^{\frac{t-t'}{\Delta t}}-\omega(x'',t'+(i-1)\Delta t|x',t')\Delta t\right) \\ &\quad= \lim_{\Delta t\to 0}\Delta t\,\omega(x,t|x',t')\exp\left(-\sum_{x''}\int_{t'}^{t}\omega(x'',t''|x',t')\,dt''\right). \end{aligned}\tag{A.4}$$

Thus we obtain the CTRW transition probability density for space- and time-dependent forcing as

$$\Psi(x,t|x',t') = \omega(x,t|x',t')e^{-\sum\limits_{x''}\int_{t'}^{t}\omega(x'',t''|x',t')\,dt''}. \tag{A.5}$$

We can now identify

$$\lambda(x,t|x',t') = \frac{\omega(x,t|x',t')}{\sum\limits_{x''}\omega(x'',t|x',t')} \tag{A.6}$$

and

$$\psi(t|x',t') = \sum_{x''}\omega(x'',t|x',t')e^{-\sum\limits_{x''}\int_{t'}^{t}\omega(x'',t''|x',t')\,dt''} \tag{A.7}$$

to be the jump probability density and the waiting time density, respectively. Note that ψ is not dependent on the arrival site, x, but only on the departure site, x'.

Note that in general both the jump density and the waiting time density are affected by the space- and time-dependent force, through the dependence in $\omega(x,t|x',t')$. However, if

$$\omega(x,t|x',t') = \alpha(x,t|x',t')\beta(t-t'), \tag{A.8}$$

and if the total rate of transitions to the left and right is not affected by the time dependence in the external force, then

$$\sum_{x''} \alpha(x'',t|x',t') = \alpha_0(x'). \tag{A.9}$$

Substituting (A.8) and (A.9) into (A.6) we obtain

$$\lambda(x,t|x',t') = \frac{\alpha(x,t|x',t')}{\alpha_0(x')}, \tag{A.10}$$

and substituting into (A.7) we obtain

$$\psi(t|x',t') = \alpha_0(x')\beta(t-t')e^{-\alpha_0(x')\int_0^{t-t'}\beta(s)\,ds}. \tag{A.11}$$

Thus, in this case, the jump density $\lambda(x,t|x',t')$ is affected by the time dependence in the force, but the waiting time density $\psi(x',t-t')$ is a function of the residence time $t-t'$ and is unaffected by the time dependence in the force.

As a particular example consider a Pareto waiting time density with a purely time-dependent force. With nearest neighbor jumps denoted by $+$ and $-$, the rates are given by

$$\omega_\pm(t|t') = \begin{cases} 0, & t-t' < t_0, \\ \frac{\alpha_\pm(t)}{t-t'}, & t-t' > t_0. \end{cases} \tag{A.12}$$

If we further assume that the sum, $\alpha_0 = \alpha_+(t) + \alpha_-(t)$, is independent of time, then

$$\omega_+(t|t') + \omega_-(t|t') = \begin{cases} 0, & t-t' < t_0, \\ \frac{\alpha_0}{t-t'}, & t-t' > t_0. \end{cases} \tag{A.13}$$

Substituting these rates into (A.6) and (A.7), we obtain a jump density that is only dependent on t,

$$\lambda_\pm(t|t') = \begin{cases} 0, & t-t' < t_0, \\ \frac{\alpha_\pm(t)}{\alpha_0}, & t-t' > t_0, \end{cases} \tag{A.14}$$

and a waiting time density that is only dependent on $t-t'$,

$$\psi(t|t') = \begin{cases} 0, & t-t' < t_0, \\ \frac{\alpha_0}{t-t'}\exp\left(-\alpha_0\int_{t_0}^{t-t'}\frac{\alpha_0}{s}\,ds\right), & t-t' > t_0. \end{cases} \tag{A.15}$$

This waiting time density simplifies to

$$\psi(t|t') = \begin{cases} 0, & t-t' < t_0, \\ \frac{\alpha_0 t_0^{\alpha_0}}{(t-t')^{\alpha_0+1}}, & t-t' > t_0. \end{cases} \tag{A.16}$$

Appendix B. The space-time diffusion limit approach to forced CTRWs. In this appendix we establish the equality of the CTRW scaling limits in both trap-time delayed and nondelayed forcing cases, on the level of stochastic processes. This extends the above results, since the probability laws for the *trajectories* of the two limit processes are shown to be equal—not just the probability laws for their position at a fixed time t. We remind the reader that knowledge of the probability densities $\rho(x,t)$ for every $t > 0$ only implies the knowledge of the joint densities $\rho(x_1,\dots,x_n;t_1,\dots,t_n)$ at multiple times if the process is Markovian. The CTRW, however, is only semi-Markovian [34], and thus special arguments are needed to show the equality of two such multitime distributions [33, 10]. Below, we show that for both trap-time delayed and nondelayed forcing, in the scaling limit the random trajectories follow the same probability law.

A CTRW trajectory is uniquely determined by its sequence of jump times and the positions at these times. We denote the time of the kth jump as $\tilde{T}_k$ and the position immediately after the kth jump as $\tilde{X}_k$. Then at time $t \in [\tilde{T}_k, \tilde{T}_{k+1})$ the position of the CTRW is $\tilde{X}_k$. The discrete trajectory $k \mapsto (\tilde{X}_k, \tilde{T}_k)$ admits an interpretation as a Markov chain in $\mathbb{R}^{d+1}$, due to the renewal of the trajectory at each jump time. An external force field can be introduced through a jump bias in the transition kernel for the Markov chain. In the case where the bias is evaluated at the time of jumping, the nondelayed forcing case, the transition kernel for the Markov chain is

$$\begin{aligned}\Psi(x,t|x',t') = p_r(x',t)\psi(t-t')\delta(x-x'-\Delta x)\\ + p_\ell(x',t)\psi(t-t')\delta(x-x'+\Delta x).\end{aligned} \tag{B.1}$$

In the case where the bias is evaluated at the time of the previous jump, the trap-time delayed case, the transition kernel is

$$\begin{aligned}\Psi(x,t|x',t') = p_r(x',t')\psi(t-t')\delta(x-x'-\Delta x)\\ + p_\ell(x',t')\psi(t-t')\delta(x-x'+\Delta x).\end{aligned} \tag{B.2}$$

Here, the probabilities to jump right/left from site x at time t are given by

$$2p_r(x,t) = 1 + F(x,t)\Delta x + \mathcal{O}(\Delta x^3), \tag{B.3}$$

$$2p_\ell(x,t) = 1 - F(x,t)\Delta x + \mathcal{O}(\Delta x^3), \tag{B.4}$$

where $F(x,t)$ is a space- and time-dependent external force.

We now show that if the external force $F(x,t)$ is fixed, the scaling limits of the Markov chain trajectories are identical in both the nondelayed case and the trap-time delayed case. We first turn $(\tilde{X}_k, \tilde{T}_k)$ into a continuous time Markov chain by defining the stochastic process

$$r \mapsto (X_r, T_r) := (\tilde{X}_{N(r/\epsilon)}, \tilde{T}_{N(r/\epsilon)}),$$

where $N(r)$ is a standard Poisson process, with unit increments at exponentially distributed times with mean 1. Note that r is an auxiliary time, which is distinct from the physical time t, and ϵ is a scale parameter for the auxiliary time. The law of the process $r \mapsto (X_r, T_r)$ is uniquely determined by its *infinitesimal generator*, defined as

$$\mathcal{L}f(x,t) = \lim_{h\to 0} \frac{1}{h}\langle f(X_h,T_h) - f(x,t)\rangle. \tag{B.5}$$

Here, f is any function such that the above limit exists, and the ensemble average $\langle\cdot\rangle$ is taken over all trajectories of the process $r \mapsto (X_r, T_r)$ which start at (x, t).

Since we have different processes (X_r, T_r) for different scaling parameters ϵ, we reflect this in our notation as $(X_r^\epsilon, T_r^\epsilon)$ and write $\mathcal{L}^\epsilon$ for the corresponding generator. A spatial scale Δx and a time scale τ also enter the analysis through Ψ. Letting simultaneously $\epsilon \to 0$, $\Delta x \to 0$, $\tau \to 0$ in a way which we specify below, we show that $\lim_{\epsilon\to 0} \mathcal{L}^\epsilon f(x,t) = \mathcal{L} f(x,t)$ exists for every smooth f with bounded support and that this limit is the same in both forcing cases.

The limiting operator $\mathcal{L}$ is itself the generator of a Markov process (X_r, T_r). This shows that the scaling limits of the space-time trajectories have the same law, namely that of the process (X_r, T_r) generated by $\mathcal{L}$. From the equality of the space-time trajectories, one then infers the equality of the limiting CTRW trajectories using a continuous mapping approach as in [47]: On one hand, the sequence of the probability laws of the trajectories $(X_r^\epsilon, T_r^\epsilon)$ converges as $\epsilon \to 0$ to the probability law of (X_r, T_r). On the other hand, the mapping Υ from trajectories of $(X_r^\epsilon, T_r^\epsilon)$ to trajectories of the CTRW is continuous (in a topological sense). Hence by the continuous mapping theorem, the sequence of probability laws of CTRW trajectories converges as $\epsilon \to 0$. The (unique) limit is given by Υ applied to the trajectories of (X_r, T_r).

To show the equality of the limit $\mathcal{L}$ in both the nondelayed and trap-time delayed cases, we begin by calculating the infinitesimal generator of the continuous time Markov chain $r \mapsto (X_r^\epsilon, T_r^\epsilon)$. It is

$$\mathcal{L}^\epsilon f(x', t') = \frac{1}{\epsilon} \int_0^{t'} \int_{-\infty}^{\infty} [f(x,t) - f(x',t')] \Psi(x, t | x', t') \, dx \, dt. \tag{B.6}$$

The proof follows by conditioning on the number of jumps N in the time interval $[0, h)$ and noting that $\mathbb{P}(N = 0) = 1 - h/\epsilon + \mathcal{O}(h^2)$, $\mathbb{P}(N = 1) = h/\epsilon + \mathcal{O}(h^2)$, $\mathbb{P}(N = k) = \mathcal{O}(h^2)$, $k \geq 2$. Now let Ψ be as in the nondelayed case, (B.1). We assume Pareto waiting times with tail parameter $\gamma \in (0, 1)$ and scale τ, that is,

$$\Phi(t) = (1 + \tau^{-1/\gamma} t)^{-\gamma}, \quad \psi(t) = \gamma \tau^{-1/\gamma} (1 + \tau^{-1/\gamma} t)^{-1-\gamma}.$$

For later use, we note that the following asymptotics hold as $\tau \to 0$, with $a > 0$ held fixed:

$$\begin{aligned} \tau^{-1} \int_a^\infty \psi(t) f(t) \, dt &= \gamma \tau^{-1-1/\gamma} \int_a^\infty (1 + \tau^{-1/\gamma} t)^{-1-\gamma} f(t) dt \\ &= \gamma \tau^{-1-1/\gamma} \int_a^\infty (\tau^{1/\gamma})^{1+\gamma} (\tau^{1/\gamma} + t)^{-1-\gamma} f(t) dt \\ &\to \gamma \int_a^\infty f(t) t^{-1-\gamma} \, dt \end{aligned} \tag{B.7}$$

and

$$\tau^{-1} \int_0^a t \psi(t) \, dt = \gamma \tau^{-1-1/\gamma} \int_0^a t (1 + \tau^{-1/\gamma} t)^{-1-\gamma} \, dt \tag{B.8}$$

$$\begin{aligned} &\leq \gamma \tau^{-1-1/\gamma} \int_0^a t (0 + \tau^{-1/\gamma} t)^{-1-\gamma} \, dt \\ &= \gamma \int_0^a t^{-\gamma} \, dt = \mathcal{O}(a^{1-\gamma}). \end{aligned} \tag{B.9}$$

We then calculate

$$\begin{aligned}\mathcal{L}^\epsilon f(x,t) &= \frac{1}{2\epsilon}\frac{1}{\epsilon}\int_0^t\int_{-\infty}^{\infty}\psi(u-t)[(1+\Delta x F(x,u))\delta(y-x-\Delta x)\\ &\quad +(1-\Delta x F(x,u))\delta(y-x+\Delta x)](f(y,u)-f(x,t))\,dy\,du\\ &= \frac{1}{2\epsilon}\int_0^t \psi(u-t)[(1+\Delta x F(x,u))(f(x+\Delta x,u)-f(x,t))\\ &\quad +(1-\Delta x F(x,u))(f(x-\Delta x,u)-f(x,t))]\,du\\ &= \frac{1}{2\epsilon}\int_t^\infty \psi(u-t)[f(x+\Delta x,u)-2f(x,t)+f(x-\Delta x,u)\\ &\quad +\Delta x F(x,u)(f(x+\Delta x,u)-f(x-\Delta x,u))]\,du\\ &= \frac{1}{2\epsilon}\int_0^\infty \psi(v)[f(x+\Delta x,t+v)-2f(x,t+v)+f(x-\Delta x,t+v)\\ &\quad +2f(x,t+v)-2f(x,t)\\ &\quad +\Delta x F(x,t+v)(f(x+\Delta x,t+v)-f(x-\Delta x,t+v))]dv.\end{aligned}$$

We fix some $a>0$ and split the integral on the domain $[0,\infty)$ into the local part $[0,a)$ and the nonlocal part $[a,\infty)$. Using that $\psi(t)\to\delta(t)$ as $\tau\to 0$ and (B.9), the local part equals

$$\begin{aligned}&\frac{1}{2\epsilon}\int_0^a \psi(v)\left\{\Delta x^2\left[\frac{\partial^2}{\partial x^2}f(x,t+v)+2F(x,t+v)\frac{\partial}{\partial x}f(x,t+v)+\mathcal{O}(a^3)\right]\right.\\ &\left.\quad +\,2\frac{\partial}{\partial t}f(x,t)v+\mathcal{O}(a^2)\right\}dv\\ &= \frac{\Delta x^2}{2\epsilon}\int_0^a \psi(v)\left[\frac{\partial^2}{\partial x^2}f(x,t+v)+2F(x,t+v)\frac{\partial}{\partial x}f(x,t+v)+\mathcal{O}(a^3)\right]dv\\ &\quad +\frac{1}{\epsilon}\int_0^a\psi(v)\left\{v\frac{\partial}{\partial t}f(x,t)+\mathcal{O}(a^2)\right\}dv\\ &\to \frac{1}{2}\frac{\partial^2}{\partial x^2}f(x,t)+2F(x,t)\frac{\partial}{\partial x}f(x,t)+\mathcal{O}(a^3)+\mathcal{O}(a^{1-\gamma}),\end{aligned} \tag{B.10}$$

where we assumed that $\Delta x^2/\epsilon\to 1$.

Using (B.7) and

$$\begin{aligned}f(x+\Delta x,t)-2f(x,t)+f(x-\Delta x,t)&=\mathcal{O}(\Delta x),\\ \Delta x F(x,t+v)(f(x+\Delta x,t+v)-f(x-\Delta x,t+v))]&=\mathcal{O}(\Delta x^2)\end{aligned} \tag{B.11}$$

uniformly in (x,t), we see that the nonlocal part has the scaling limit

$$\begin{aligned}\int_a^\infty [f(x,t+v)-f(x,t)]v^{-1-\gamma}\,dv &= \int_0^\infty [f(x,t+v)-f(x,t)]v^{-1-\gamma}\,dv+\mathcal{O}(a^{1-\gamma})\\ &= \Gamma(1-\gamma)\frac{\partial^\gamma}{\partial(-t)^\gamma}f(x,t)+\mathcal{O}(a^{1-\gamma}),\end{aligned} \tag{B.12}$$

where we have assumed $\tau/\epsilon\to 1$. (The last equality is also called the "generator form" of the negative γ-fractional derivative [32, (3.31)]. We assume that the test function f vanishes as $\|(x,t)\|\to\infty$, and it can be shown that generator form, Riemann–Liouville form, and Caputo form are all equivalent.) Since our choice of a was arbitrary and the scaling limits hold uniformly for all (x, t), we see that

$$\mathcal{L}f(x,t) = \frac{1}{2}\frac{\partial^2}{\partial x^2}f(x,t) + 2F(x,t)\frac{\partial}{\partial x}f(x,t) + \Gamma(1-\gamma)\frac{\partial^\gamma}{\partial(-t)^\gamma}f(x,t). \tag{B.13}$$

One then repeats the same calculation, arriving at the same result with the trap-time delayed forcing. The FFPE is then obtained from this infinitesimal generator by following the sequence of steps in [8].

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