

Feynman-Kac formula for stochastic hybrid systems

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We derive a Feynman-Kac formula for functionals of a stochastic hybrid system evolving according to a piecewise deterministic Markov process. We first derive a stochastic Liouville equation for the moment generator of the stochastic functional, given a particular realization of the underlying discrete Markov process; the latter generates transitions between different dynamical equations for the continuous process. We then analyze the stochastic Liouville equation using methods recently developed for diffusion processes in randomly switching environments. In particular, we obtain dynamical equations for the moment generating function, averaged with respect to realizations of the discrete Markov process. The resulting Feynman-Kac formula takes the form of a differential Chapman-Kolmogorov equation. We illustrate the theory by calculating the occupation time for a one-dimensional velocity jump process on the infinite or semi-infinite real line. Finally, we present an alternative derivation of the Feynman-Kac formula based on a recent path-integral formulation of stochastic hybrid systems.

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I. INTRODUCTION

An increasing number of problems in biological physics involve the coupling between a piecewise deterministic dynamical system in \mathbb{R}^d and a time-homogeneous Markov chain on some discrete space Γ [1], resulting in a type of stochastic hybrid system known as a piecewise deterministic Markov process (PDMP) [2,3]. Probably the simplest example of a PDMP is a velocity jump process where the “velocity” of some continuous process randomly switches between different values. This could be the position of a molecular motor on a filament track [4], the length of a microtubule undergoing catastrophes [5], or a bacterium displaying run and tumble [6]. Another example at the single-cell level concerns membrane voltage fluctuations in a neuron due to the stochastic opening and closing of ion channels [7–16]. The discrete states of the ion channels evolve according to a continuous-time Markov process with voltage-dependent transition rates, whereas the membrane voltage evolves according to a piecewise deterministic equation that depends on the current state of the ion channels. In the limit that the number of ion channels goes to infinity, an application of the law of large numbers recovers classical Hodgkin-Huxley-type equations. On the other hand, channel fluctuations in the finite case can lead to noise-induced neuronal spiking. Another important example is a gene regulatory network, where the continuous variable is the concentration of a protein product and the discrete variable represents the activation state of the gene [17–21]. Yet another example arises in a stochastic formulation of synaptically coupled neural networks that has a mathematical structure analogous to stochastic gene networks [22].

In many of the above examples, one finds that the transition rates between the discrete states $n \in \Gamma$ are much faster than the relaxation rates of the piecewise deterministic dynamics for $x \in \mathbb{R}^d$. In other words, there is a separation of time scales between the discrete and continuous processes, so if t/ϵ is the characteristic time scale of the Markov chain, then t is the characteristic time scale of the relaxation dynamics for some small positive parameter ϵ . In the limit $\epsilon \rightarrow 0$, one obtains

a deterministic dynamical system in which one averages the piecewise dynamics with respect to the corresponding unique stationary measure of the Markov chain (assuming it exists). An important problem is then characterizing how the underlying stochastic process approaches this deterministic limit in the case of weak noise, $0 < \epsilon \ll 1$. A rigorous mathematical approach to addressing this particular issue has recently been developed for stochastic hybrid systems using *large deviation theory* [23–25]. Such a theory provides a variational or action principle that can be used to solve first-passage time problems associated with the escape from a fixed-point attractor of the underlying deterministic system in the weak noise limit. This involves finding the most probable paths of escape, which minimize some action with respect to the set of all trajectories emanating from the fixed point. In addition, a variety of complementary techniques in applied mathematics and mathematical physics have been used to solve first-passage time problems in biological applications of stochastic hybrid systems. These include WKB approximations and matched asymptotics [10,14,15,18–21] and path integrals [26,27].

In this paper, we address a different aspect of stochastic hybrid systems, namely how to derive a “Feynman-Kac” formula for functionals of a continuous variable $x(t) \in \mathbb{R}$ evolving according to a piecewise deterministic dynamics. The original Feynman-Kac formula was derived for Brownian functionals [28]. Suppose that $X(t) \in \mathbb{R}$ represents pure Brownian motion. A *Brownian functional* over a fixed time interval $[0, t]$ is formally defined as a random variable T given by

$$T = \int_0^t U[X(\tau)]d\tau, \quad (1.1)$$

where $U(x)$ is some prescribed function or distribution such that T has positive support. Two common examples are as follows [29,30]: (i) $U(X) = \delta(x - a)$ for the local time density at $x = a$, which characterizes the amount of time that a Brownian particle spends in the neighborhood of a point in space, and (ii) $U(x) = \Theta(x)$ for the occupation or residence time in \mathbb{R}^+ . Since $X(t)$, $t \geq 0$, is a Wiener process, it follows

that each realization of a Brownian path will typically yield a different value of T , which means that T will be distributed according to some probability density $P(T, t|x_0, 0)$ for $X(0) = x_0$. The statistical properties of a Brownian functional can be analyzed using path integrals and lead to the following *Feynman-Kac* formula [28]: Let $Q(s, t|x_0, 0)$ be the moment generating function (or Laplace transform of) $P(T, t|x_0, 0)$,

$$Q(s, t|x_0, t_0) = \int_0^\infty e^{-sT} P(T, t|x_0, 0) dT. \quad (1.2)$$

Then Q satisfies the modified backward Fokker-Planck equation (FPE)

$$\frac{\partial Q}{\partial t_0} = \frac{1}{2} \frac{\partial^2 Q}{\partial x_0^2} - sU(x_0)Q, \quad (1.3)$$

which is supplemented by the “final” condition $Q(s, t|x_0, t) = 1$. For a general review of Brownian functionals and their applications, see Ref. [31].

The goal of this paper is to derive the analog of Eq. (1.3) for the functional T of Eq. (1.1), with $X(t)$ the continuous component of a stochastic hybrid system rather than Brownian motion. In Sec. II we define a stochastic hybrid system and introduce our notation. In Sec. III we carry out the detailed derivation of the Feynman-Kac formula for a stochastic hybrid system. We first consider a particular realization σ of the discrete Markov process $n(t)$ and derive a stochastic Liouville equation for the moment generator Q . An analogous result was obtained in a recent study of stochastically gated Brownian functionals [32]. Following along similar lines to this previous study, we analyze the stochastic Liouville equation using methods recently developed for diffusion processes in randomly switching environments [33]. We thus obtain a Feynman-Kac formula in the form of a differential Chapman-Kolmogorov (CK) equation. We illustrate the theory in Sec. IV by considering the occupation time for a velocity jump process. Finally, in Sec. V we relate the analysis to our recent path-integral construction of stochastic hybrid systems [26,27].

II. ONE-DIMENSIONAL STOCHASTIC HYBRID SYSTEM

We begin by defining a stochastic hybrid system and, in particular, a PDMP [2,23,25]. For the sake of illustration, consider a system whose states are described by a pair $(x, n) \in \Sigma \times \{0, \dots, N_0 - 1\}$, where x is a continuous variable in $\Sigma \subset \mathbb{R}$ and n a discrete stochastic variable taking values in the finite set $\Gamma \equiv \{0, \dots, N_0 - 1\}$. (Note that one could easily extend the analysis to higher-dimensions, $x \in \mathbb{R}^d$. However, for notational simplicity, we restrict ourselves to the case $d = 1$. It is also possible to have a set of discrete variables, but one can always relabel the internal states so they are effectively indexed by a single integer.) When the internal state is n , the system evolves according to the ordinary differential equation (ODE)

$$\dot{x} = F_n(x), \quad (2.1)$$

where $F_n : \mathbb{R} \rightarrow \mathbb{R}$ is a continuous function. For fixed x , the discrete stochastic variable evolves according to a homogeneous, continuous-time Markov chain with generator $\mathbf{A}(x)$.

We make the further assumption that the chain is irreducible for all $x \in \Sigma$, that is, for fixed x there is a nonzero probability of transitioning, possibly in more than one step, from any state to any other state of the Markov chain. This implies the existence of a unique invariant probability distribution $\rho(x)$ on Γ for fixed $x \in \Sigma$, with components $\rho_m(x)$, such that

$$\sum_{m \in \Gamma} A_{nm}(x) \rho_m(x) = 0, \quad \forall n \in \Gamma. \quad (2.2)$$

The above stochastic model defines a one-dimensional (1D) PDMP. It is also possible to consider generalizations of the continuous process, in which the ODE (2.1) is replaced by a stochastic differential equation (SDE) or even a partial differential equation (PDE). In order to allow for such possibilities, we will refer to all of these processes as examples of a stochastic hybrid system.

The generator \mathbf{A} is related to the transition matrix \mathbf{W} of the discrete Markov process according to

$$A_{nm} = W_{nm} - \delta_{nm} \sum_k W_{kn}.$$

Suppose that we decompose \mathbf{W} by writing

$$W_{nm}(x) = P_{nm}(x) \omega_m(x),$$

with $\sum_{n \neq m} P_{nm}(x) = 1$ for all x . That is, for a given x , the jumps times from state m are exponentially distributed with rate $\omega_m(x)$ and $P_{nm}(x)$ is the probability distribution that when it jumps the new state is n for $n \neq m$. The hybrid evolution of the system with respect to $x(t)$ and $n(t)$ can then be described as follows. Suppose the system starts at time zero in the state (x_0, n_0) . Call $x_0(t)$ the solution of (2.1) with $n = n_0$ such that $x_0(0) = x_0$. Let θ_1 be the random variable such that

$$\mathbb{P}(\theta_1 < t) = 1 - \exp \left\{ - \int_0^t \omega_{n_0}[x_0(t')] dt' \right\}.$$

The exponential is the probability that no jump occurs in the interval $[0, t]$ so $\mathbb{P}[\theta_1 < t]$ gives the probability that the jump does occur before time t . Then in the random time interval $s \in [0, \theta_1)$ the state of the system is $(x_0(s), n_0)$. We draw a value of θ_1 from $\mathbb{P}(\theta_1 < t)$, choose an internal state $n_1 \in \Gamma$ with probability $P_{n_1 n_0}[x_0(\theta_1)]$, and call $x_1(t)$ the solution of the following Cauchy problem on $[\theta_1, \infty)$:

$$\begin{aligned} \dot{x}_1(t) &= F_{n_1}[x_1(t)], \quad t \geq \theta_1 \\ x_1(\theta_1) &= x_0(\theta_1). \end{aligned}$$

Iterating this procedure, we construct a sequence of increasing jumping times $(\theta_k)_{k \geq 0}$ (setting $\theta_0 = 0$) and a corresponding sequence of internal states $(n_k)_{k \geq 0}$. The evolution $(x(t), n(t))$ is then defined as

$$(x(t), n(t)) = (x_k(t), n_k) \quad \text{if } \theta_k \leq t < \theta_{k+1}. \quad (2.3)$$

Given the above iterative definition of a PDMP, let $X(t)$ and $N(t)$ denote the stochastic continuous and discrete variables, respectively, at time t , $t > 0$, given the initial conditions $X(0) = x_0, N(0) = n_0$. Introduce the probability density $p_n(x, t|x_0, n_0, 0)$ with

$$\mathbb{P}\{X(t) \in (x, x + dx), N(t) = n|x_0, n_0\} = p_n(x, t|x_0, n_0, 0) dx.$$

It follows that p evolves according to the forward differential Chapman-Kolmogorov (CK) equation [1,34]

$$\frac{\partial p_n}{\partial t} = \mathbb{L} p_n, \quad (2.4)$$

with the operator \mathbb{L} (dropping the explicit dependence on initial conditions) defined according to

$$\mathbb{L} p_n(x, t) = -\frac{\partial F_n(x) p_n(x, t)}{\partial x} + \sum_{m \in \Gamma} A_{nm}(x) p_m(x, t). \quad (2.5)$$

The first term on the right-hand side represents the probability flow associated with the piecewise deterministic dynamics for a given n , whereas the second term represents jumps in the discrete state n . Now define the averaged function $\bar{F} : \mathbb{R} \rightarrow \mathbb{R}$ by

$$\bar{F}(x) = \sum_{n \in \Gamma} \rho_n(x) F_n(x).$$

Intuitively speaking, one would expect the stochastic hybrid system (2.1) to reduce to the deterministic dynamical system

$$\begin{aligned} \dot{x}(t) &= \bar{F}[x(t)] \\ x(0) &= x_0 \end{aligned} \quad (2.6)$$

in the fast switching limit $\omega_n \rightarrow \infty$. For the Markov chain then undergoes many jumps over a small time interval Δt during which $\Delta x \approx 0$, and thus the relative frequency of each discrete state n is approximately $\rho_n(x)$. This can be made precise in terms of a law of large numbers for stochastic hybrid systems proven in Refs. [24,25].

In the following we will take either $\Sigma = \mathbb{R}$ or $\Sigma = \mathbb{R}^+ = [0, \infty)$. In the latter case we will impose the no-flux boundary condition $J(0, t) = 0$ with

$$J(x, t) = \sum_{n=0}^{N_0-1} F_n(x) p_n(x, t), \quad x \in \Sigma. \quad (2.7)$$

Note, however, that from a PDE perspective, the CK equation is an N_0 th-order quasilinear equation on Σ . In general, well-posed boundary conditions for a quasilinear PDE have to be determined using the theory of characteristics. In particular, for certain choices of the functions $F_n(x)$ it is necessary to supplement the no-flux boundary condition at $x = 0$ by auxiliary boundary conditions. For example, suppose that the functions $F_n(x)$ do not change sign within the interval Σ . In particular, there exists an integer m , $1 \leq m \leq N_0 - 1$, such that for all $0 < x$ we have $F_n(x) < 0$ for $0 \leq n \leq m - 1$ and $F_n(x) > 0$ for $m \leq n \leq N_0 - 1$. Assume that $F_n(0) = 0$ for $0 \leq n \leq m - 1$ and $F_n(L) = 0$ for $m \leq n \leq N_0 - 1$. In that case, the no-flux boundary condition can only be satisfied if $p_n(0, t) = 0$ for all $m \leq n \leq N_0 - 1$. This issue does not arise for the velocity jump process considered in Sec. IV.

III. DERIVATION OF FEYNMAN-KAC FORMULA

Let $\sigma(t, t_0) = \{n(\tau) \in \Gamma, t_0 < \tau \leq t | n(t_0) = n_0\}$ denote a particular realization of the discrete Markov process in the interval $[t_0, t]$. For a given realization σ , Eq. (2.1) reduces to a deterministic, nonautonomous ODE. Suppose that the initial state of the continuous variable, $x(t_0) = y$, is randomly

generated from a density $p_0(y)$. Let

$$P(x, t) = \int_{\Sigma} \mathbb{P}[x(t) = x | x(t_0) = y] p_0(y) dy$$

denote the probability density of the state at time t for fixed σ . The probability density evolves according to the stochastic Liouville equation

$$\frac{\partial}{\partial t} P(x, t) = \left[-\frac{\partial}{\partial x} F_{n(t)}(x) \right] P(x, t), \quad (3.1)$$

with $P(x, t_0) = p_0(x)$. Note that the density $P(x, t)$ is a random field with respect to realizations of σ . [For notational simplicity we drop the explicit dependence on σ from $P(x, t)$.] One could numerically estimate $P(x, t)$ for a given σ by running multiple trials with initial conditions generated by p_0 —the important point being that each trial has the same fixed realization σ . The corresponding solution $p_n(x, t)$ of the CK equation (2.4) would then be recovered by setting $p_0(x) = \delta(x - x_0)$ and averaging over different realizations of the discrete process, that is,

$$p_n(x, t) = \mathbb{E}_{\sigma} [P(x, t) 1_{n(t)=n}], \quad (3.2)$$

where the subscript σ denotes expectation with respect to σ .

Following our recent analysis of stochastically gated Brownian functionals [32], let $X_{\sigma}(t)$ denote a sample trajectory of the continuous process for a given realization σ and introduce the analog of the Brownian functional (1.1),

$$\mathcal{T}(t, t_0) = \int_{t_0}^t U[X_{\sigma}(t')] dt'. \quad (3.3)$$

(For ease of notation, we suppress the explicit dependence of \mathcal{T} on σ .) The process $X_{\sigma}(t)$ is not time homogeneous so the lower limit cannot always be set to zero. Let $P(\mathcal{T}, t, t_0)$ be the corresponding probability density for \mathcal{T} . Since $\mathcal{T} \geq 0$, we can introduce the analog of the moment generating function (1.2):

$$Q(s, t, t_0) = \int_0^{\infty} e^{-s\mathcal{T}} P(\mathcal{T}, t, t_0) d\mathcal{T}. \quad (3.4)$$

We will proceed by first deriving a Feynman-Kac formula for Q and fixed σ , which takes the form of a stochastic Liouville equation. We will then obtain the corresponding Feynman-Kac formula averaged with respect to different realizations σ , which takes the form of a differential CK equation.

A. Stochastic Liouville equation for fixed σ

The first step is to introduce a path-integral representation of the sample paths $X_{\sigma}(t)$, that is, the solution trajectories of the Liouville equation (3.1) generated by the distribution of initial conditions p_0 . First, discretize time by dividing the given interval $[t_0, t]$ into N equal subintervals of size Δt such that $t - t_0 = N\Delta t$ and set $x_j = X_{\sigma}(j\Delta t)$, $n_j = n(j\Delta t)$ for $j = 0, \dots, N$. The probability density for x_0, x_1, \dots, x_N , given a particular realization of the stochastic discrete variables n_j , $j = 0, \dots, N - 1$, is

$$\begin{aligned} P_{\sigma}(x_0, x_1, \dots, x_N) &\equiv \int_{\Sigma} P(x_0, x_1, \dots, x_N | n_0, \dots, n_{N-1}) \\ &= p_0(x_0) \prod_{j=1}^{N-1} \delta[x_{j+1} - x_j - F_{n_j}(x_j) \Delta t]. \end{aligned}$$

We define corresponding discretized versions of the functional \mathcal{T} and moment generating functional Q according to $\mathcal{T} = \sum_{j=0}^N U(X_j)\Delta t$, and

$$\begin{aligned} Q(s,t,t_0) &= \int_0^\infty e^{-sT} \int_{\Sigma^{N+1}} \delta\left[\mathcal{T} - \sum_{j=0}^N U(X_j)\Delta t\right] \\ &\quad \times P_\sigma(x_0,x_1,\dots,x_N) \left[\prod_{j=0}^N dx_j\right] dT \\ &= \int_{\Sigma^{N+1}} \exp\left[-s \sum_{j=0}^N U(X_j)\Delta t\right] \\ &\quad \times P_\sigma(x_0,x_1,\dots,x_N) \left[\prod_{j=0}^N dx_j\right], \end{aligned} \quad (3.5)$$

where Σ^{N+1} denotes the $N + 1$ -dimensional product space $\Sigma \times \Sigma \times \dots \times \Sigma \subset \mathbb{R}^{N+1}$. Now taking the continuum limit $\Delta t \rightarrow 0, N \rightarrow \infty$ such that $N\Delta t = t - t_0$ yields the formal path-integral representation of the moment generating function Q :

$$\begin{aligned} Q(s,t,t_0) &= \int_\Sigma \left[\int_{x(t_0)=x_0}^{x(t)=x} \exp\left(-s \int_{t_0}^t U[x(\tau)]d\tau\right) \right. \\ &\quad \left. \times \mathcal{P}_\sigma[x] \mathcal{D}[x] \right] p_0(x_0) dx_0, \end{aligned} \quad (3.6)$$

where

$$\begin{aligned} &\int_{x(t_0)=x_0}^{x(t)=x} \mathcal{P}_\sigma[x] \mathcal{D}[x] \\ &= \lim_{\Delta t \rightarrow 0, N \rightarrow \infty} \int_{\Sigma^N} P_\sigma(x_0,x_1,\dots,x_N) \prod_{j=1}^{N-1} dx_j. \end{aligned}$$

The next step is to introduce the propagator G according to

$$Q(s,t,t_0) = \int_{\Sigma^2} G(s,x,t|x_0,t_0) p_0(x_0) dx_0, \quad (3.7)$$

with

$$\begin{aligned} G(s,x,t|x_0,t_0) &= \left[\int_{x(t_0)=x_0}^{x(t)=x} \exp\left(-s \int_{t_0}^t U[x(\tau)]d\tau\right) \mathcal{P}_\sigma[x] \mathcal{D}[x] \right] \\ &\equiv \left\langle \exp\left(-s \int_{t_0}^t U[x(\tau)]d\tau\right) \right\rangle_{x(t_0)=x_0}, \end{aligned} \quad (3.8)$$

where $\langle \dots \rangle$ denotes averaging over realizations of $X_\sigma(t)$. Note that G satisfies the initial condition $G(x,t_0|x_0,t_0) = \delta(x - x_0)$. We can now proceed along analogous lines to the derivation of the Feynman-Kac formula for Brownian motion. That is,

$$\begin{aligned} G(s,x,t + \Delta t|x_0,t_0) &= \left\langle \exp\left(-s \int_{t_0}^{t+\Delta t} U[x(\tau)]d\tau\right) \right\rangle_{x(t_0)=x_0}^{x(t+\Delta t)=x} \end{aligned}$$

$$\begin{aligned} &\approx \left\langle \exp\left(-s \int_{t_0}^t U[x(\tau)]d\tau\right) \right\rangle_{x(t_0)=x_0}^{x(t)=x-\Delta x} e^{-sU(x)\Delta t} \\ &= e^{-sU(x)\Delta t} G(s,x - \Delta x,t|x_0,t_0). \end{aligned}$$

We have split the time interval $[t_0, t + \Delta t]$ into two parts $[t_0, t]$ and $[t, t + \Delta t]$ and introduced the intermediate state $x(t) = x - \Delta x$ with Δx determined by $\Delta x = F_{n(t)}(x - \Delta x)\Delta t$. Expressing Δx in terms of Δt and Taylor expanding with respect to Δt yields the following PDE in the limit $\Delta t \rightarrow 0$:

$$\frac{\partial G}{\partial t} = -\frac{\partial F_{n(t)}(x)G}{\partial x} - sU(x)G. \quad (3.9)$$

In contrast to the standard Feynman-Kac formula (1.3) for Brownian motion, Eq. (3.9) is in the form of a stochastic PDE (SPDE) due to the dependence of F on the discrete state $n(t)$. More precisely, Eq. (3.9) is a piecewise deterministic PDE.

Having solved for G , the moment generating function is obtained from Eq. (3.7). From the definition of Q , see Eq. (3.4), we can then determine the k th moment of the functional (3.3) averaged with respect to the continuous process $X_\sigma(t)$:

$$\begin{aligned} \langle \mathcal{T}^k \rangle &\equiv \int_0^\infty \mathcal{T}^k P(\mathcal{T}, t, t - \tau) d\mathcal{T} \\ &= (-1)^k \frac{d^k}{ds^k} Q(s,t,t - \tau) \Big|_{s=0}. \end{aligned} \quad (3.10)$$

(In the case of a PDMP, stochasticity for fixed σ arises from the random distribution of initial conditions.) However, in order to determine statistics of the doubly stochastic process, we also need to take expectations with respect to realizations σ of the gate:

$$\langle\langle \mathcal{T}^k(\tau) \rangle\rangle = \mathbb{E}_\sigma[\langle \mathcal{T}^k \rangle] = (-1)^k \frac{d^k}{ds^k} \mathbb{E}_\sigma[Q(s,t,t - \tau)] \Big|_{s=0}, \quad (3.11)$$

assuming we can reverse the order of expectation and differentiation. Hence, calculating the moments of \mathcal{T} with respect to the doubly stochastic process requires determining $\mathbb{E}_\sigma[Q]$. The latter is the generator of moments of \mathcal{T} averaged with respect to realizations of the discrete Markov process.

For calculational purposes, it will be simpler to fix the initial state $X(0) = x_0$ by taking $p_0(y) = \delta(y - x_0)$ and working directly with the corresponding SPDE for $Q = Q(s,t|x_0,t_0)$. Setting $t_0 = t - \tau$, it is straightforward to show that Q satisfies the ‘‘backward’’ SPDE

$$\frac{\partial Q}{\partial \tau} = F_{n(t-\tau)}(x_0) \frac{\partial Q}{\partial x_0} - sU(x_0)Q, \quad (3.12)$$

which is supplemented by the ‘‘final’’ condition $Q(s,t|x_0,t) = 1$. That is, from properties of the propagator G we can write

$$Q(s,t|x_0,t_0) = \int_\Sigma dx \int_\Sigma dx' G(s,x,t|x',t') G(x',t'|x_0,t_0).$$

Differentiating both sides with respect to the intermediate time t' and using the forward equation for G yields

$$\begin{aligned} 0 &= \int_{\Sigma} dx \int_{\Sigma} dx' [\partial_{t'} G(s, x, t | x', t') G(x', t' | x_0, t_0) \\ &\quad + G(s, x, t | x', t') \partial_{t'} G(x', t' | x_0, t_0)] \\ &= \int_{\Sigma} dx \int_{\Sigma} dx' [\partial_{t'} G(s, x, t | x', t') G(x', t' | x_0, t_0) \\ &\quad + G(s, x, t | x', t') (-\partial_{x'} F_{n(t')}(x') - sU(x')) G(x', t' | x_0, t_0). \end{aligned}$$

Integrating by parts with respect to x' , reversing the order of integration, and using the relationship between Q and G shows that

$$\int_{\Sigma} dx' G(x', t' | x_0, t_0) [\partial_{t'} + F_{n(t')}(x') \partial_{x'} - sU(x')] Q(s, t | x', t').$$

Finally, setting $t' = t_0 = t - \tau$ and using $G(x', t' | x_0, t') = \delta(x' - x_0)$ yields the backward equation for Q .

The next step is to average over different realizations σ . As in our study of stochastically gated Brownian functionals [32], we will proceed by adapting our recent work on stochastic diffusion equations in randomly switching environments [33]. Since Q is a random field with respect to realizations of the discrete Markov process $n(t)$, there exists a probability density functional ϱ that determines the distribution of the densities $q(x_0, \tau) = Q(s, t | x_0, t - \tau)$ for fixed s, t . The expectation $\mathbb{E}_{\sigma}[Q]$ then corresponds to the first moment of this density functional. (This is distinct from the first moment of \mathcal{T} generated by Q .) Rather than dealing with the probability density functional directly, we spatially discretize the piecewise deterministic backward FPE (3.12) using a finite-difference scheme and use this to derive corresponding differential equations for $\mathbb{E}_{\sigma}[Q]$. More precisely, we will derive equations for $E_{\sigma}[Q]$ conditioned on the initial state $n(t_0) = n$.

B. Dynamical equations for $\mathbb{E}_{\sigma}[Q]$

Introduce the lattice spacing ℓ and set $x_j = j\ell, j \in \mathbb{Z}$. Let $Q_j(\tau) = Q(s, t | j\ell, t - \tau)$, $U_j = U(j\ell)$, and $F_{j,n} = F(j\ell, n)$, $j \in \mathbb{Z}$. (For the moment, we take $\Sigma = \mathbb{R}$. If Σ is a proper subset of \mathbb{R} , then j will be restricted to some subset of the integers. Also note that here we are discretizing the continuous variable x rather than time.) Equation (3.12) then reduces to the piecewise deterministic ODE (for fixed s, t)

$$\frac{dQ_i}{d\tau} = F_{i,n} \sum_{j \in \mathbb{Z}} K_{ij} Q_j - sU_i Q_i, \quad \text{if } n(t - \tau) = n \quad (3.13)$$

with

$$K_{ij} = \frac{1}{\ell} [\delta_{i,j-1} - \delta_{i,j}]. \quad (3.14)$$

Let $\mathbf{Q}(\tau) = \{Q_j(\tau), j \in \mathbb{Z}\}$ and introduce the probability density

$$\text{Prob}\{\mathbf{Q}(\tau) \in (\mathbf{Q}, \mathbf{Q} + d\mathbf{Q}), n(t - \tau) = n\} = \varrho_n(\mathbf{Q}, \tau) d\mathbf{Q}, \quad (3.15)$$

where we have dropped the explicit dependence on initial conditions. The resulting CK equation for the discretized

piecewise deterministic PDE is [1,34]

$$\begin{aligned} \frac{\partial \varrho_n}{\partial \tau} &= - \sum_{i \in \mathbb{Z}} \frac{\partial}{\partial Q_i} \left[F_{i,n} \left(\sum_{j \in \mathbb{Z}} K_{ij} Q_j \right) \varrho_n(\mathbf{Q}, \tau) \right] \\ &\quad + \sum_{m \in \Gamma} A_{nm}^{\top} \varrho_m(\mathbf{Q}, \tau). \end{aligned} \quad (3.16)$$

Since the Liouville term in the CK equation is linear in \mathbf{Q} , we can derive a closed set of equations for the first-order (and higher-order) moments of the density ϱ_n .

Let

$$Q_{k,n}(s, \tau) = \mathbb{E}[Q_k(s, \tau) 1_{n(t-\tau)=n}] = \int \varrho_n(\mathbf{Q}, \tau) Q_k d\mathbf{Q}, \quad (3.17)$$

where

$$\int \mathcal{F}(\mathbf{Q}) d\mathbf{Q} = \left[\prod_j \int_0^{\infty} dQ_j \right] \mathcal{F}(\mathbf{Q})$$

for any \mathcal{F} . Multiplying both sides of Eq. (3.16) by Q_k and integrating with respect to \mathbf{Q} gives [after integrating by parts the right-hand side and assuming that $\varrho_n(\mathbf{Q}, \tau) \rightarrow 0$ as $\mathbf{Q} \rightarrow \infty$]

$$\frac{dQ_{j,n}}{d\tau} = F_{j,n} \sum_{l \in \mathbb{Z}} K_{jl} Q_{l,n} - sU_j Q_{j,n} + \sum_{m \in \Gamma} A_{nm}^{\top} Q_{m,k}. \quad (3.18)$$

If we now retake the continuum limit $\ell \rightarrow 0$ and set

$$Q_n(x; s, \tau) = \mathbb{E}_{\sigma}[Q(s, t | x, t - \tau) 1_{n(t-\tau)=n}] \quad (3.19)$$

for fixed t , then we obtain the system of equations

$$\frac{\partial Q_n}{\partial \tau} = F_n(x) \frac{\partial Q_n}{\partial x} - sU(x) Q_n + \sum_{m \in \Gamma} A_{mn}^{\top}(x) Q_m. \quad (3.20)$$

We have dropped the subscript on the initial position x_0 . Also note that taking expectation with respect to realizations σ eliminates the dependence on the final time t . Equation (3.20) is the desired Feynman-Kac formula. In the above derivation, we have assumed that integrating with respect to \mathbf{Q} and taking the continuum limit commute. (One can also avoid the issue that \mathbf{Q} is an infinite-dimensional vector by carrying out the discretization over the finite domain $[-L, L]$ and taking the limit $L \rightarrow \infty$ once the moment equations have been derived.) Finally, applying the final condition $Q(s, t | x, t) = 1$ implies that $Q_n(x; s, 0) = 1$.

IV. OCCUPATION TIME OF A TWO-STATE VELOCITY JUMP PROCESS

As an illustration of the above analysis, consider the velocity jump process

$$\frac{dx}{dt} = \xi(t) \equiv [v_+ + v_-]n(t) - v_-, \quad n(t) \in \{0, 1\}. \quad (4.1)$$

The term $\xi(t)$ is often referred to in the physics literature as dichotomous noise [35]. The discrete state $n(t)$ evolves

according to a two-state Markov chain with matrix generator

$$\mathbf{A} = \begin{pmatrix} -\beta & \alpha \\ \beta & -\alpha \end{pmatrix}. \quad (4.2)$$

If $P_{nn_0}(t) = \mathbb{P}[N(t) = n | N(0) = n_0]$, then the master equation for $n(t)$ takes the form

$$\frac{dP_{nn_0}}{dt} = \sum_{m=0,1} A_{nm} P_{mn_0}.$$

Using the fact that $P_{0n_0}(t) + P_{1n_0}(t) = 1$, we can solve this pair of equations to give

$$P_{0n_0}(t) = \delta_{0,n_0} e^{-t/\tau_c} + \tau_c k_- (1 - e^{-t/\tau_c}), \quad \tau_c = \frac{1}{\alpha + \beta}.$$

We deduce that τ_c is the relaxation time of the Markov chain with $P_{mn_0}(t) \rightarrow \rho_m$ in the limit $t \rightarrow \infty$ and

$$\rho_0 = \frac{\alpha}{\alpha + \beta}, \quad \rho_1 = \frac{\beta}{\alpha + \beta}. \quad (4.3)$$

Suppose that the dichotomous noise term $\xi(t)$ is unbiased so in the stationary state $\langle \xi(t) \rangle = 0$. One then finds that the stationary autocorrelation function is

$$\langle \xi(t) \xi(t') \rangle = \frac{D}{\tau_c} e^{-|t-t'|/\tau_c}, \quad (4.4)$$

with noise amplitude $D = \alpha\beta\tau_c^3(v_+ + v_-)^2$. This shows that dichotomous noise is a form of colored noise.

In terms of the piecewise deterministic ODE (2.1), we have $F_1(x) = v_+$ and $F_0(x) = -v_-$. The corresponding CK equation (2.4) reduces to

$$\frac{\partial p_0}{\partial t} = v_- \frac{\partial p_0}{\partial x} + \alpha p_1 - \beta p_0, \quad (4.5a)$$

$$\frac{\partial p_1}{\partial t} = -v_+ \frac{\partial p_1}{\partial x} + \beta p_0 - \alpha p_1. \quad (4.5b)$$

Similarly, the backwards CK equation (3.12) for Q_n reduces to the pair of equations

$$\frac{\partial Q_0}{\partial \tau} = -v_- \frac{\partial Q_0}{\partial x} - sU(x)Q_0 - \beta Q_0 + \alpha Q_1, \quad (4.6a)$$

$$\frac{\partial Q_1}{\partial \tau} = v_+ \frac{\partial Q_1}{\partial x} - sU(x)Q_1 + \alpha Q_0 - \alpha Q_1. \quad (4.6b)$$

Laplace transforming these equation with respect to τ by setting

$$\begin{aligned} \tilde{Q}_n(x; s, z) &= \int_0^\infty e^{-z\tau} Q_n(x, s, \tau) d\tau \\ &= \int_0^\infty \int_0^\infty e^{-z\tau - sT} \\ &\quad \times \mathbb{E}_\sigma [P(\mathcal{T}, t | x, t - \tau) 1_{n(t-\tau)=n}] d\mathcal{T} d\tau, \end{aligned} \quad (4.7)$$

we have

$$-1 = -v_- \frac{\partial \tilde{Q}_0}{\partial x} - sU(x)\tilde{Q}_0 - (z + \beta)\tilde{Q}_0 + \beta\tilde{Q}_1, \quad (4.8a)$$

$$-1 = v_+ \frac{\partial \tilde{Q}_1}{\partial x} - sU(x)\tilde{Q}_1 + \alpha\tilde{Q}_0 - (z + \alpha)\tilde{Q}_1. \quad (4.8b)$$

A. Infinite line

Suppose that $x(t) \in \mathbb{R}$ and consider the occupation time \mathcal{T} defined by Eq. (3.3) with $U(x) = \Theta(x)$. For the given choice of $U(x)$, we have to solve Eqs. (4.8) separately in the two regions $x > 0$ and $x < 0$ and then impose continuity of the solutions at the interface $x = 0$. In order to determine the far-field boundary conditions for $x \rightarrow \pm\infty$, we note that if the system starts at $x = \pm\infty$, then it will never cross the origin a finite time τ in the future, that is,

$$P(\mathcal{T}, t | \infty, t - \tau) = \delta(t - \mathcal{T}), \quad P(\mathcal{T}, t | -\infty, t - \tau) = \delta(\mathcal{T}).$$

Substituting this into the definition of \tilde{Q}_n shows that

$$\tilde{Q}_n(\infty; s, z) = \frac{1}{z + s}, \quad \tilde{Q}_n(-\infty; s, z) = \frac{1}{z}. \quad (4.9)$$

Therefore, setting

$$\tilde{Q}_n(x; s, z) = u_n^+(x; s, z) + \frac{1}{z + s}, \quad x > 0,$$

$$\tilde{Q}_n(x; s, z) = u_n^-(x; s, z) + \frac{1}{z}, \quad x < 0,$$

we have

$$0 = -v_- \frac{\partial u_0^+}{\partial x} - (z + s + \beta)u_0^+ + \beta u_1^+, \quad (4.10a)$$

$$0 = v_+ \frac{\partial u_1^+}{\partial x} + \alpha u_0^+ - (z + s + \alpha)u_1^+, \quad (4.10b)$$

and

$$0 = -v_- \frac{\partial u_0^-}{\partial x} - (z + \beta)u_0^- + \beta u_1^-, \quad (4.10c)$$

$$0 = v_+ \frac{\partial u_1^-}{\partial x} + \alpha u_0^- - (z + \alpha)u_1^-, \quad (4.10d)$$

with corresponding boundary conditions $u_n^\pm(\pm\infty; s, z) = 0$. Equations (4.10) can be rewritten in the matrix forms

$$\frac{\partial}{\partial x} \begin{pmatrix} u_0^+ \\ u_1^+ \end{pmatrix} + \mathbf{M}(z + s) \begin{pmatrix} u_0^+ \\ u_1^+ \end{pmatrix} = 0, \quad x \in (0, \infty) \quad (4.11)$$

and

$$\frac{\partial}{\partial x} \begin{pmatrix} u_0^- \\ u_1^- \end{pmatrix} + \mathbf{M}(z) \begin{pmatrix} u_0^- \\ u_1^- \end{pmatrix} = 0, \quad x \in (-\infty, 0), \quad (4.12)$$

with

$$\mathbf{M}(z) = \begin{pmatrix} \frac{z+\beta}{v_-} & -\frac{\beta}{v_-} \\ \frac{\alpha}{v_+} & -\frac{z+\alpha}{v_+} \end{pmatrix}. \quad (4.13)$$

The matrix $\mathbf{M}(z)$ has eigenvalues

$$\lambda_\pm(z) = -\Gamma \pm \sqrt{\Gamma^2 + \frac{z^2 + (\alpha + \beta)z}{v_- v_+}}, \quad (4.14)$$

where

$$\Gamma = \frac{(z + \alpha)v_- - (z + \beta)v_+}{2v_- v_+}. \quad (4.15)$$

The corresponding eigenvectors are

$$\mathbf{w}^\pm(z) = \begin{pmatrix} \frac{z+\alpha}{v_+} + \lambda_\pm(z) \\ \frac{\alpha}{v_+} \end{pmatrix}. \quad (4.16)$$

In order that the solutions u_n^\pm vanish in the limits $x \rightarrow \pm\infty$, they have to take the form

$$u_n^+(x; s, z) = Aw_n^+(z+s)e^{-\lambda_+(z+s)x}, \quad x \in (0, \infty), \quad (4.17a)$$

$$u_n^-(x; s, z) = Bw_n^-(z)e^{-\lambda_-(z)x}, \quad x \in (-\infty, 0). \quad (4.17b)$$

We thus have two unknown coefficients A, B , which are determined by imposing continuity of the solutions \tilde{Q}_n^\pm , $n = 0, 1$, at $x = 0$. This yields the two conditions ($n = 0, 1$)

$$Aw_0^+(z+s) + \frac{1}{z+s} = Bw_0^-(z) + \frac{1}{z}, \quad (4.18a)$$

$$Aw_1^+(z+s) + \frac{1}{z+s} = Bw_1^-(z) + \frac{1}{z}. \quad (4.18b)$$

Adding and subtracting these equations gives

$$AD_+(z+s) = BD_-(z)$$

$$AS_+(z+s) = BS_-(z) + \frac{2}{z} - \frac{2}{z+s},$$

where

$$S_\pm(z) = w_0^\pm(z) + w_1^\pm(z), \quad D_\pm(z) = w_0^\pm(z) - w_1^\pm(z).$$

Hence

$$A = \left[S_+(z+s) - \frac{S_-(z)D_+(z+s)}{D_-(z)} \right]^{-1} \left[\frac{2}{z} - \frac{2}{z+s} \right], \quad (4.19a)$$

$$B = \left[\frac{S_+(z+s)D_-(z)}{D_+(z+s)} - S_-(z) \right]^{-1} \left[\frac{2}{z} - \frac{2}{z+s} \right]. \quad (4.19b)$$

In general it is not possible to derive an exact analytical expression for the double-inverse Laplace transform of $\tilde{Q}(x_0; s, z)$. However, we can determine the behavior of the averaged probability density $\mathbb{E}_\sigma[P(\mathcal{T}, t|x, t-\tau)]$ in the large-time limits $\mathcal{T}, \tau \rightarrow \infty$; this corresponds to taking the limits $s, z \rightarrow 0$ in Laplace space. [Note that a natural time scale is $\tau_c = 1/\alpha$ (for $\alpha < \beta$) so the large-time regime is characterized by $\tau \gg \tau_c$.] For example, suppose that the mean-field version of Eq. (4.1),

$$\frac{d\bar{x}}{dt} = (v_+ + v_-)\rho_1 - v_- = \rho_1 v_+ - \rho_0 v_-,$$

represents unbiased motion. That is, $\beta v_+ - \alpha v_- = 0$. In particular, take $v_+ = v_- = v$ and $\alpha = \beta$ so $\Gamma = 0$ and $\lambda_\pm(z) = \pm\lambda(z)$ with

$$\lambda(z) = \sqrt{\frac{z^2 + 2\alpha z}{v^2}}.$$

In the asymptotic limit $s, z \rightarrow 0$ we then find that $\lambda(z) \rightarrow \sqrt{2\alpha z}/v$, $S_\pm(z) \rightarrow 2\alpha/v$, and $D_\pm(z) \rightarrow \pm\lambda(z)$. Therefore, the leading-order approximation of the coefficients is

$$A \sim \frac{v}{\alpha} \frac{\sqrt{z}}{(\sqrt{z+s} + \sqrt{z})} \left[\frac{1}{z} - \frac{1}{z+s} \right]. \quad (4.20)$$

The corresponding asymptotic solution for $\tilde{Q}_n(0; s, z)$ becomes

$$\tilde{Q}_n(0; s, z) \sim \frac{\sqrt{z}}{(\sqrt{z+s} + \sqrt{z})} \frac{1}{z} + \frac{\sqrt{z+s}}{(\sqrt{z+s} + \sqrt{z})} \frac{1}{z+s}$$

$$= \frac{1}{\sqrt{z(z+s)}}. \quad (4.21)$$

Finally, inverting the double Laplace transform with respect to s and then z gives

$$\mathbb{E}_\sigma[P(\mathcal{T}, t|x, t-\tau)] \sim \frac{1}{\pi\sqrt{\mathcal{T}(\tau-\mathcal{T})}}, \quad 0 \ll \mathcal{T} < \tau, \quad (4.22)$$

which is independent of x, t . This is identical to the well-known ‘‘arcsine’’ law [29] for the probability density of the occupation time for pure Brownian motion starting at the origin (see also Sec. V C).

The asymptotic connection to Brownian motion is not surprising, given the relationship of the two-state velocity jump process to the telegrapher’s equation. Setting $v_\pm = v$ and $\alpha = \beta$ and adding Eqs. (4.5a) and (4.5b) shows that the marginal probability density $p(x, t) = p_0(x, t) + p_1(x, t)$ satisfies the telegrapher’s equation [36,37]

$$\left[\frac{\partial^2}{\partial t^2} + 2\alpha \frac{\partial}{\partial t} - v^2 \frac{\partial^2}{\partial x^2} \right] p(x, t) = 0. \quad (4.23)$$

(The individual densities $p_{0,1}$ satisfy the same equation.) One finds that the short-time behavior (for $t \ll \tau_c = 1/2\alpha$) is characterized by wavelike propagation with $\langle x(t) \rangle^2 \sim (vt)^2$, whereas the long-time behavior ($t \gg \tau_c$) is diffusive with $\langle x^2(t) \rangle \sim 2Dt$, $D = v^2/2\alpha$. For certain initial conditions, one can solve the telegrapher’s equation explicitly. In particular, if $p(x, 0) = \delta(x)$ and $\partial_t p(x, 0) = 0$, then

$$p(x, t) = \frac{e^{-\alpha t}}{2} [\delta(x-vt) + \delta(x+vt)]$$

$$+ \frac{\alpha e^{-\alpha t}}{2v} \left[I_0(\alpha\sqrt{t^2 - x^2/v^2}) \right.$$

$$\left. + \frac{t}{\sqrt{t^2 - x^2/v^2}} I_1(\alpha\sqrt{t^2 - x^2/v^2}) \right]$$

$$\times [\Theta(x+vt) - \Theta(x-vt)],$$

where I_n is the modified Bessel function of n th order and Θ is the Heaviside function. The first two terms represent the ballistic propagation of the initial data along characteristics $x = \pm vt$, whereas the Bessel function terms asymptotically approach Gaussians in the large time limit. In particular, $p(x, t) \rightarrow 0$ pointwise when $t \rightarrow 0$.

Using similar arguments, we can also determine what happens in the case of a biased velocity jump process for $x(0) = 0$. If $\beta v_+ > \alpha v_-$, then we expect the system to be located in \mathbb{R}^+ at large times t and so $\mathcal{T} \approx t$, whereas if $\beta v_+ < \alpha v_-$ then we expect the system to be located in \mathbb{R}^- at large times t and so $\mathcal{T} \approx 0$. In order to construct a nontrivial example of biased motion, we consider a velocity jump process on the semi-infinite line \mathbb{R}^+ .

B. Semi-infinite line

One well-known example of a two-state velocity jump process on the semi-infinite line is the Dogterom-Leibler model of microtubule catastrophes [5,38]. This is a probabilistic model of the length $x(t)$ of a microtubule, which switches between growth and shrinkage phases according to a two-state Markov process with generator (4.2), and v_{\pm} represent the corresponding elongation and shrinkage velocities. A nontrivial steady-state solution can be obtained on the semi-infinite line, $x > 0$, for $v_{+} \neq v_{-}$. This can be established by adding equations (4.5a) and (4.5b) and setting $\partial_t p_{0,1} = 0$. This gives $v_{+}p_1'(x) - v_{-}p_0'(x) = 0$, and thus $v_{+}p_1(x) - v_{-}p_0(x) = \text{const}$. Integrability of $p_{0,1}(x)$ means that the constant must be zero and, hence, $p_1(x) = P(x)/v_{+}$, $p_0(x) = P(x)/v_{-}$ with P satisfying the equation

$$\frac{dP(x)}{dx} = \left[\frac{\beta}{v_{-}} - \frac{\alpha}{v_{+}} \right] P(x) = -\frac{V}{\kappa} P(x),$$

where

$$V = \rho_0 v_{-} - \rho_1 v_{+}, \quad \kappa = \frac{v_{+}v_{-}}{\alpha + \beta}.$$

Here $-V$ is the mean velocity and κ has the units of diffusivity. It immediately follows that there exists a steady-state solution, $P(x) = P(0)e^{-Vx/\kappa}$, $0 < x < \infty$, if and only if $V > 0$. In the regime $V < 0$, catastrophe events are relatively rare and the microtubule continuously grows with mean speed $|V|$, whereas, for $V > 0$, the catastrophe events occur much more frequently so there is a balance between growth and shrinkage that results in a steady-state distribution of microtubule lengths.

Let us now introduce an occupation time for the interval $[L, \infty)$, $L > 0$, given by

$$\mathcal{T}(t) = \int_0^t \Theta(X_{\sigma}(\tau) - L) d\tau. \quad (4.24)$$

Here $\mathcal{T}(t)$ is the amount of time up to time t that the continuous variable $X_{\sigma}(\tau)$ spends in the region $x > L$, given a particular realization σ of the discrete Markov process $n(t) \in \{0, 1\}$. Following a similar argument to the analysis of Brownian functionals in Ref. [39], we assume that in the large time limit we can replace averaging over different realizations of the stochastic process by averaging with respect to the stationary density $p_n(x)$. That is, for large τ ,

$$\mathbb{E}[\Theta(X_{\sigma}(\tau) - L)], \quad (4.25)$$

$$\rightarrow Z(L) \equiv \int_L^{\infty} [p_0(x) + p_1(x)] dx = e^{-VL/\kappa}. \quad (4.26)$$

Therefore, the average occupation time $\langle\langle \mathcal{T}(t) \rangle\rangle$ scales linearly with time t for $t \rightarrow \infty$:

$$\langle\langle \mathcal{T}(t) \rangle\rangle \equiv \int_0^t \mathcal{T} \mathcal{P}(\mathcal{T}, t) d\mathcal{T} \rightarrow Z(L)t, \quad (4.27)$$

where

$$\mathcal{P}(\mathcal{T}, t) = \mathbb{E}_{\sigma} [P(\mathcal{T}, t | x_0, t_0)].$$

From the central limit theorem, we expect that in the large time limit the probability density \mathcal{P} will take the form of a Gaussian

distribution of \mathcal{T} around the mean value $\langle\mathcal{T}\rangle$:

$$\mathcal{P}(\mathcal{T}, t) \sim \exp\left(-\frac{[\mathcal{T} - \langle\mathcal{T}(t)\rangle]^2}{2\Sigma^2(t)}\right), \quad (4.28)$$

with the variance $\Sigma^2 = \langle\langle \mathcal{T}^2 \rangle\rangle - \langle\langle \mathcal{T} \rangle\rangle^2$.

One can calculate the variance using Eq. (3.11) for $k = 2$, with the Laplace transforms of $\mathcal{Q}_{0,1}$ satisfying Eqs. (4.8) on $x \in \mathbb{R}^+$ for $U(x) = \Theta(x - L)$. Modifying the analysis of the infinite line case accordingly, we find that

$$\tilde{\mathcal{Q}}_n(x; s, z) = A_{+} w_n^{+}(z + s) e^{-\lambda_{+}(z+s)x} + \frac{1}{z + s}, \quad L < x < \infty, \quad (4.29a)$$

$$\tilde{\mathcal{Q}}_n(x; s, z) = B_{+} w_n^{+}(z) e^{-\lambda_{+}(z)x} + B_{-} w_n^{-}(z) e^{-\lambda_{-}(z)x} + \frac{1}{z}, \quad (4.29b)$$

for $0 < x < L$. Conditions on the coefficients A_{\pm}, B_{\pm} are obtained by a reflecting boundary condition at $x = 0$,

$$B_{+} w_0^{+}(z) + B_{-} w_0^{-}(z) = B_{+} w_1^{+}(z) + B_{-} w_1^{-}(z), \quad (4.30a)$$

and the two matching conditions at $x = L$ for $n = 0, 1$:

$$\begin{aligned} A_{+} w_n^{+}(z + s) e^{-\lambda_{+}(z+s)L} + \frac{1}{z + s} \\ = B_{+} w_n^{+}(z) e^{-\lambda_{+}(z)L} + B_{-} w_n^{-}(z) e^{-\lambda_{-}(z)L} + \frac{1}{z}. \end{aligned} \quad (4.30b)$$

In the asymptotic limit $z \rightarrow 0$, we have

$$\Gamma(z) \sim \frac{V}{2\kappa}, \quad \lambda_{+}(z) \sim \frac{z}{V}, \quad \lambda_{-}(z) \sim -\frac{V}{\kappa},$$

and

$$w_0^{+}(z) \sim \frac{\alpha}{v_{+}} + \frac{z}{V}, \quad w_0^{-} \sim \frac{\beta}{v_{-}},$$

while $w_1^{\pm}(z) = \alpha/v_{+}$ for all z , see Eqs. (4.14) and (4.16). Hence, taking $s, z \rightarrow 0$ in Eq. (4.30a) shows that

$$B_{-} \sim \frac{\kappa z}{V^2} B_{+}, \quad (4.31)$$

whereas subtracting the pair of Eqs. (4.30b) for $n = 0, 1$ shows that

$$B_{-} \sim \frac{\kappa z}{V^2} e^{-VL/\kappa} (B_{+} - A_{+}). \quad (4.32)$$

Comparing Eqs. (4.31) and (4.32) yields the asymptotic relationship

$$B_{+} \sim -\frac{e^{-VL/\kappa} A_{+}}{1 - e^{-VL/\kappa}}.$$

Finally, substituting for B_{+} in Eq. (4.30b) gives to leading order

$$\begin{aligned} \frac{\alpha}{v_{+}} A_{+} &\sim (1 - e^{-VL/\kappa}) \left(\frac{1}{z} - \frac{1}{z + s} \right), \quad s, z \rightarrow 0 \\ \frac{\alpha}{v_{+}} B_{+} &\sim -e^{-VL/\kappa} \left(\frac{1}{z} - \frac{1}{z + s} \right), \quad s, z \rightarrow 0. \end{aligned}$$

Combining these various results establishes that the leading-order asymptotic behavior of the solution $\tilde{Q}_n(x; s, z)$ is

$$\tilde{Q}_n(x; s, z) \sim \frac{1 - e^{-VL/\kappa}}{z} + \frac{e^{-VL/\kappa}}{z + s} \quad (4.33)$$

for all $x \in \mathbb{R}^+$ and $n = 0, 1$. It follows that

$$\left. \frac{\partial \tilde{Q}_n(x; s, z)}{\partial s} \right|_{s=0} \sim -\frac{Z(L)}{z^2}, \quad \left. \frac{\partial^2 \tilde{Q}_n(x; s, z)}{\partial s^2} \right|_{s=0} \sim \frac{2Z(L)}{z^3},$$

and hence

$$\langle\langle T \rangle\rangle \sim Z(L)\tau, \quad \langle\langle T^2 \rangle\rangle \sim Z(L)\tau^2. \quad (4.34)$$

Therefore, the leading-order form of the variance is

$$\Sigma^2 \sim Z(L)(1 - Z(L))\tau^2. \quad (4.35)$$

Note that this result differs from an analogous result obtained for the occupation time of Brownian motion in an attractive or stable potential [39]. In the latter case, one finds that both the mean and variance of the occupation time vary linearly with τ .

V. PATH-INTEGRAL REPRESENTATION OF $\mathbb{E}_\sigma[\mathcal{Q}]$

In our derivation of the Feynman-Kac formula for a stochastic hybrid system, see Sec. III, we considered a particular realization of the discrete Markov process $n(t)$ and obtained a stochastic Liouville equation for the continuous process $x(t)$. We then averaged over different realizations of the discrete process by adapting the moments method of Ref. [33]. Here we explore an alternative approach to the analysis of functionals of stochastic hybrid system based on our recent path-integral representation of PDMPs [26,27].

A. Construction of path integral

In order to derive the Feynman-Kac formula and introduce notation, we first briefly recap the construction of the path-integral representation of stochastic hybrid systems [26,27]. The first step is to discretize time and write down the path-integral representation of $Q(s, t, t_0)$ given by Eq. (3.5). We now note that the joint probability distribution $P_\sigma(x_0, x_1, \dots, x_N)$ for a fixed realization σ can be written as

$$P_\sigma(x_0, x_1, \dots, x_N) = \prod_{j=0}^{N-1} \delta(x_{j+1} - x_j - F_{n_j}(x_j)\Delta t).$$

Inserting the Fourier representation of the Dirac δ function gives

$$P_\sigma(x_0, x_1, \dots, x_N) = \prod_{j=0}^{N-1} \left[\int_{-\infty}^{\infty} e^{-ip_j(x_{j+1} - x_j - F_{n_j}(x_j)\Delta t)} \frac{dp_j}{2\pi} \right].$$

In contrast to our previous approach, Sec. III, we now average with respect to the intermediate states $n_j, j = 1, N-1$ and fix n_N . This gives

$$P(x_0, x_1, \dots, x_N; n_0, n_N) = \sum_{n_1, \dots, n_{N-1}} \left(\prod_{j=0}^{N-1} T_{n_{j+1}, n_j}(x_j) \right) P_\sigma(x_0, x_1, \dots, x_N), \quad (5.1)$$

where

$$\begin{aligned} T_{n_{j+1}, n_j}(x_j) &\sim A_{n_{j+1}, n_j}(x_j)\Delta t + \delta_{n_{j+1}, n_j} \left[1 - \sum_m A_{m, n_j}(x_j)\Delta t \right] \\ &+ o(\Delta t) = [\delta_{n_{j+1}, n_j} + A_{n_{j+1}, n_j}(x_j)\Delta t]. \end{aligned}$$

For a fixed x , we introduce the matrix operator $\mathbf{Q}(x, \phi)$ with ϕ a parameter and [26,27]

$$Q_{nm}(x, \phi) = A_{nm}(x) + \phi \delta_{n,m} F_m(x). \quad (5.2)$$

Let $\Lambda_r(x, \phi), r \in \Gamma$, denote the set of eigenvalues of \mathbf{Q} with corresponding eigenvectors $\mathbf{R}^{(r)}(x, \phi)$ and adjoint eigenvectors $\xi^{(r)}(x, \phi)$. That is,

$$\sum_{m \in \Gamma} [A_{nm}(x) + \phi \delta_{n,m} F_m(x)] R_m^{(r)}(x, \phi) = \Lambda_r(x, \phi) R_n^{(r)}(x, \phi), \quad (5.3)$$

for fixed x, ϕ and

$$\begin{aligned} \sum_r \xi_m^{(r)}(x, \phi) R_n^{(r)}(x, \phi) &= \delta_{m,n} \\ \sum_m \xi_m^{(r)}(x, \phi) R_m^{(s)}(x, \phi) &= \delta_{r,s}. \end{aligned}$$

Inserting multiple copies of the above completeness relation with $(x, \phi) = (x_j, \phi_j)$ at the j th time step, we have

$$\begin{aligned} P(x_0, x_1, \dots, x_N; n_N, n_0) &= \sum_{n_1, \dots, n_{N-1}} \prod_{j=0}^{N-1} \int_{-\infty}^{\infty} G_{n_{j+1}, n_j}(x_{j+1}, x_j, q_j, \phi_j) \frac{dq_j}{2\pi} \end{aligned}$$

with [26,27]

$$\begin{aligned} G_{n_{j+1}, n_j}(x_{j+1}, x_j, q_j, \phi_j) &\sim \sum_{r_j, m} R_{n_{j+1}}^{(r_j)}(x_j, \phi_j) \xi_m^{(r_j)}(x_j, \phi_j) T_{m, n_j}(x_j) e^{-iq_j[x_{j+1} - x_j - F_{n_j}(x_j)\Delta t]} \\ &\sim \sum_{r_j} \exp \left\{ \left[\Lambda_{r_j}(x_j, \phi_j) - iq_j \frac{x_{j+1} - x_j}{\Delta t} \right] \Delta t \right\} \exp \{ [iq_j F_{n_j}(x_j) - \phi_j F_{n_j}(x_j)] \Delta t \} \\ &\times R_{n_{j+1}}^{(r_j)}(x_j, \phi_j) \xi_{n_j}^{(r_j)}(x_j, \phi_j), \end{aligned}$$

to leading order in $O(\Delta x, \Delta t)$. Now integrating over intermediate states x_j leads to

$$\begin{aligned}
 P(x_N, n_N | x_0, n_0) &= \left[\prod_{j=1}^{N-1} \int_{-\infty}^{\infty} dx_j \right] P(x_0, x_1, \dots, x_N; n_0, n_N) \\
 &= \left[\prod_{j=1}^{N-1} \int_{-\infty}^{\infty} dx_j \right] \left[\prod_{j=0}^{N-1} \int_{-\infty}^{\infty} \frac{dq_j}{2\pi} \right] \sum_{n_1, \dots, n_{N-1}} \sum_{r_0, \dots, r_{N-1}} \left[\prod_{j=0}^{N-1} R_{n_{j+1}}^{(r_j)}(x_j, \phi_j) \xi_{n_j}^{(r_j)}(x_j, \phi_j) \right] \\
 &\quad \times \exp \left\{ \sum_j \left[\Lambda_{r_j}(x_j, \phi_j) - i q_j \frac{x_{j+1} - x_j}{\Delta t} \right] \Delta t \right\} \exp \{ [i q_j F_{n_j}(x_j) - \phi_j F_{n_j}(x_j)] \Delta t \}. \quad (5.4)
 \end{aligned}$$

By inserting the eigenfunction products and using the Fourier representation of the Dirac δ function, we have introduced sums over the discrete labels r_j and new phase variables q_j . Suppose that we can perform a so-called Wick rotation in the complex q plane so q_j becomes pure imaginary and then perform the change of variables $i q_j \rightarrow q_j$ [40,41]. Noting that the discretized path integral is independent of the ϕ_j , we are free to set $\phi_j = q_j$ for all j , thus eliminating the final exponential factor. This choice means that we can perform the summations with respect to the intermediate discrete states n_j using the orthogonality relation

$$\sum_n R_n^{(r)}(x_j, \phi_{j-1}) \xi_n^{(r')} (x_{j+1}, \phi_j) = \delta_{r,r'} + O(\Delta x, \Delta \phi).$$

We thus obtain the result that $r_j = r$ for all j . Finally, taking the continuum limit of equation (5.4), we obtain the following path integral from $x(0) = x_0$ to $x(\tau) = x$,

$$\begin{aligned}
 P(x, n, \tau | x_0, n_0, 0) &= \sum_r \int_{x(t_0)=x_0}^{x(\tau)=x} \exp \left\{ - \int_0^\tau [q \dot{x} - \Lambda_r(x, q)] dt \right\} \\
 &\quad \times R_n^{(r)}(x, q(\tau)) \xi_{n_0}^{(r)}(x_0, q(t_0)) \mathcal{D}[q] \mathcal{D}[x]. \quad (5.5)
 \end{aligned}$$

Finally, since the generator \mathbf{A} of the Markov chain is assumed to be irreducible, we can apply the Perron-Frobenius theorem [42] to the linear operator on the left-hand side of Eq. (5.3). That is, there exists a real, simple Perron eigenvalue labeled by $r = 0$, say, such that $\Lambda_0 > \text{Re}(\Lambda_r)$ for all $r > 0$. Moreover, $\xi^{(0)}$ is the only positive eigenvector so it can be taken to determine the initial distribution of n_0 and thus we restrict the sum over r in Eq. (5.5) to $r = 0$. [Setting $\phi = 0$ in Eq. (5.3), it can be seen that $R_n^{(r)}(x, 0)$ and $\xi_n^{(r)}(x, 0)$ correspond to the right and left eigenvectors of \mathbf{A} . Hence, $R_n^{(r)}(x, 0) = \rho_n(x)$ and $\xi_n^{(r)}(x, 0) = 1$ for all $n \in \Gamma$.] We thus obtain the following path integral for a

1D stochastic hybrid system [26,27]:

$$\begin{aligned}
 P(x, n, \tau | x_0, n_0, 0) &= \int_{x(0)=x_0}^{x(\tau)=x} D[x] D[q] e^{-S[x, q]} \\
 &\quad \times R_n^{(0)}(x, q(\tau)) \xi_{n_0}^{(0)}(x_0, q(t_0)), \quad (5.6)
 \end{aligned}$$

with the action

$$S[x, q] = \int_{t_0}^t [q \dot{x} - \Lambda_0(x, q)] dt'. \quad (5.7)$$

Although the above derivation uses formal path-integral methods, it generates the same action S obtained rigorously using large deviation theory, as detailed in the monograph by Kifer [25]. Equation (5.6) is the starting point for obtaining a variational principle that can be used to solve first-passage time problems associated with the escape from a fixed-point attractor of the underlying deterministic system (2.6) in the weak noise (fast switching) limit (see also Sec. VC). This involves finding the most probable paths of escape, which minimize the action S with respect to the set of all trajectories emanating from the fixed point. We now have a classical variational problem, in which the Perron eigenvalue $\Lambda_0(x, q)$ is identified as a Hamiltonian and the most probable paths are the zero-energy solutions to Hamilton's equations [26,27]

$$\dot{x} = \frac{\partial \mathcal{H}}{\partial q}, \quad \dot{q} = - \frac{\partial \mathcal{H}}{\partial x}, \quad \mathcal{H}(x, q) = \Lambda_0(x, q). \quad (5.8)$$

B. Derivation of Feynman-Kac formula

Let us now return to the representation of $Q(s, t | x_0, t_0)$ given by Eqs. (3.7) and (3.8) with $p_0(y) = \delta(y - x_0)$. Taking expectations with respect to the realizations σ of the discrete Markov process now yields a path-integral representation of $\mathcal{Q}_n(x_0; s, \tau)$ given by

$$\mathcal{Q}_{n_0}(x_0; s, \tau) = \sum_{n \in \Gamma} \int_{\Sigma} \mathcal{G}_{nn_0}(s, x, q, t | x_0, q_0, t_0) dx dq dq_0, \quad (5.9)$$

with $\tau = t - t_0$ and

$$\mathcal{G}_{nn_0}(s, x, q, t | x_0, q_0, t_0) = R_n^{(0)}(x, q) \left[\int_{x(t_0)=x_0, q(t_0)=q_0}^{x(t)=x, q(t)=q} \exp \left\{ -S[x, q] - s \int_{t_0}^t U[x(\tau)] d\tau \right\} \mathcal{D}[q] \mathcal{D}[x] \right] \xi_{n_0}^{(0)}(x_0, q_0). \quad (5.10)$$

We can now proceed along analogous lines to the derivation of the Feynman-Kac formula in Sec. III. That is,

$$\begin{aligned} \mathcal{G}_{nn_0}(s, x, q, t + \Delta t | x_0, q_0, t_0) &= e^{-q\Delta x + \Lambda_0(x, q)\Delta t - sU(x)\Delta t} \mathcal{G}_{nn_0}(s, x - \Delta x, t | x_0, q_0, t_0) \\ &\approx \mathcal{G}_{nn_0}(s, x - \Delta x, t | x_0, q_0, t_0) + [\Lambda_0(x, q) - q\Delta(x) - sU(x)\Delta t] \mathcal{G}_{nn_0}(s, x, t | x_0, q_0, t_0) \\ &= \mathcal{G}_{nn_0}(s, x - \Delta x, t | x_0, q_0, t_0) - [q(t)\Delta x + sU(x)\Delta t] \mathcal{G}_{nn_0}(s, x, q, t | x_0, q_0, t_0) \\ &\quad + \sum_{m \in \Gamma} [A_{nm}(x) + q\delta_{n,m} F_m(x)] \mathcal{G}_{mn_0}(s, x, q, t | x_0, q_0, t_0) \Delta t, \end{aligned}$$

where we have used Eq. (5.3). Again, we have split the time interval $[t_0, t + \Delta t]$ into two parts $[t_0, t]$ and $[t, t + \Delta t]$ and introduced the intermediate state $x(t) = x - \Delta x$ with Δx determined by $x = x - \Delta x + F_n(x - \Delta x)\Delta t$. Expressing Δx in terms of Δt and Taylor expanding with respect to Δt , we find that the two multiplicative terms in q cancel. Hence, we obtain the following CK equation in the limit $\Delta t \rightarrow 0$:

$$\frac{\partial \mathcal{G}_{nn_0}}{\partial t} = -\frac{\partial F_n(x) \mathcal{G}_{nn_0}}{\partial x} - sU(x) \mathcal{G}_{nn_0} + \sum_{m \in \Gamma} A_{nm}(x) \mathcal{G}_{mn_0}. \quad (5.11)$$

After integrating with respect to q and q_0 , this is precisely the forward version of the CK equation for \mathcal{Q}_n , see Eq. (3.20). Thus our analysis of Sec. III is equivalent to deriving the Feynman-Kac formula directly from the path-integral representation of stochastic hybrid systems constructed in Refs. [26,27].

C. Gaussian approximation

In Sec. IV, we analyzed the occupation time for a simple two-state velocity jump process. A major simplifying feature

of this model is that the functions F_n and transition rates α, β are independent of x . Solving the Feynman-Kac formula given by Eq. (3.20) or (5.11) for more general two-state stochastic hybrid system is nontrivial. However, progress can be made by carrying out a Gaussian approximation of the stochastic hybrid system in the so-called fast switching regime.

In the case of the unbounded domain $\Sigma = \mathbb{R}$, there is no natural scale for the continuous variable x [except possibly from the particular structure of the functions $F_n(x)$]. Therefore, we are free to fix the units of x by introducing a quantity X_0 such that the transition rates of the discrete Markov process are much faster than \bar{v}/X_0 , where \bar{v} is a typical value of the “velocity” \dot{x} . (For the velocity jump process in Sec. IV, we would have $v_{\pm}/X_0 \ll \alpha, \beta$.) We can interpret the choice of X_0 as defining a fast-switching regime, such that $\Delta X/X_0 \ll 1$ over a time interval Δt for which $\alpha \Delta t \gg 1$. The fast switching regime can be implemented by setting $X_0 = 1$ and introducing the rescaling $\mathbf{A} \rightarrow \mathbf{A}/\varepsilon$ with $0 < \varepsilon \ll 1$ [26]. Repeating the derivation of the propagator (5.10), we obtain the same expression except that $S[x, q] \rightarrow S[x, q]/\varepsilon$. Introduce the modified propagator

$$\mathcal{G}(s, x, q, t | x_0, q_0, t_0) = \sum_{n, n_0} \xi_n^{(0)}(x, q) \mathcal{G}_{nn_0}(s, x, q, t | x_0, q_0, t_0) R_{n_0}^{(0)}(x_0, q_0). \quad (5.12)$$

After performing the rescaling $q \rightarrow -iq/\varepsilon$, Eqs. (5.10) and (5.7) yield the path integral

$$\mathcal{G}(s, x, q, t | x_0, q_0, t_0) = \int_{x(t_0)=x_0, q(t_0)=q_0}^{x(t)=x, q(t)=q} \mathcal{D}[q] \mathcal{D}[x] \exp \left\{ -\frac{1}{\varepsilon} \int_{t_0}^t [i\varepsilon q \dot{x} - \Lambda_0(x, i\varepsilon q)] d\tau - s \int_{t_0}^t U(x) d\tau \right\}. \quad (5.13)$$

The Gaussian approximation involves Taylor expanding the Perron eigenvalue Λ_0 to second order in ε , which yields a quadratic in q :

$$\mathcal{G}(s, x, q, t | x_0, q_0, t_0) \sim \int_{x(t_0)=x_0, q(t_0)=q_0}^{x(t)=x, q(t)=q} \mathcal{D}[q] \mathcal{D}[x] \exp \left(-\int_{t_0}^t \{iq[\dot{x} - A(x)] + \varepsilon q^2 B(x)\} d\tau - s \int_{t_0}^t U(x) d\tau \right),$$

where

$$A(x) = \frac{\partial}{\partial p} \Lambda_0(x, p) \Big|_{p=0}, \quad B(x) = \frac{1}{2} \frac{\partial^2}{\partial p^2} \Lambda_0(x, p) \Big|_{p=0}. \quad (5.14)$$

We can now perform the integration over the “momenta” by defining

$$\mathcal{G}(s, x, t | x_0, t_0) = \int dq dq_0 \int \mathcal{D}(q) \mathcal{G}(s, x, q, t | x_0, q_0, t_0)$$

either directly or by returning to the discretized path integral, Taylor expanding to second order in q_j , and then performing

the Gaussian integration with respect to q_j before taking the continuum limit:

$$\begin{aligned} \mathcal{G}(s, x, t | x_0, t_0) &= \int_{x(0)=x_0}^{x(\tau)=x} \mathcal{D}[x] \exp \left\{ -\int_{t_0}^t \frac{[\dot{x} - A(x)]^2}{4\varepsilon B(x)} d\tau \right\} \\ &\quad \times \exp \left[-s \int_{t_0}^t U(x) d\tau \right]. \end{aligned} \quad (5.15)$$

Finally, noting that $\xi_n^{(0)}(x, 0) = 1$ and $R_n^{(0)}(x, 0) = \rho_n(x)$, and using Eqs. (5.9) and (5.12), we can make the following

identification under the Gaussian approximation:

$$\begin{aligned} \mathcal{Q}(x_0; s, \tau) &\equiv \sum_{n_0} \mathcal{Q}_{n_0}(x_0; s, \tau) \rho_{n_0}(x_0) \\ &\approx \int_{\Sigma} \mathcal{G}(s, x, t | x_0, t - \tau) dx. \end{aligned} \quad (5.16)$$

The path integral in Eq. (5.15) is identical in form to the one obtained in the derivation of the Feynman-Kac formula for the Brownian functional (1.1) of a particle with position $X(t)$ satisfying the Ito SDE [28,31],

$$dX = A(X)dt + \sqrt{2\epsilon B(X)}dW(t). \quad (5.17)$$

Hence, we deduce that in the fast switching regime, the moment generating function \mathcal{Q} of the stochastic hybrid system satisfies the Feynman-Kac formula

$$\begin{aligned} \frac{\partial \mathcal{Q}(x; s, \tau)}{\partial \tau} &= A(x) \frac{\partial \mathcal{Q}(x; s, \tau)}{\partial x} + \epsilon B(x) \frac{\partial^2 \mathcal{Q}(x; s, \tau)}{\partial x^2} \\ &\quad - sU(x)\mathcal{Q}(x; s, \tau). \end{aligned} \quad (5.18)$$

Let us apply the above analysis to a two-state version of the stochastic hybrid system (2.1) for which $N_0 = 2$ and the matrix \mathbf{A} is given by Eq. (4.2), with possibly x -dependent transition rates α, β . The eigenvalue equation (5.3) can be written as the two-dimensional system

$$\begin{bmatrix} -\beta(x) + pF_0(x) & \alpha(x) \\ \beta(x) & -\alpha(x) + pF_1(x) \end{bmatrix} \begin{pmatrix} R_0 \\ R_1 \end{pmatrix} = \lambda \begin{pmatrix} R_0 \\ R_1 \end{pmatrix}. \quad (5.19)$$

It follows that the Perron eigenvalue [satisfying $\Lambda_0(x, 0) = 0$] is given by

$$\Lambda_0(x, p) = \frac{1}{2}[\Sigma(x, p) + \sqrt{\Sigma(x, p)^2 - 4\gamma(x, p)}], \quad (5.20)$$

where

$$\Sigma(x, p) = p[F_0(x) + F_1(x)] - [\alpha(x) + \beta(x)]$$

and

$$\gamma(x, p) = [pF_1(x) - \alpha(x)][pF_0(x) - \beta(x)] - \alpha(x)\beta(x).$$

A little algebra shows that

$$\begin{aligned} Z(x, p) &\equiv \Sigma(x, p)^2 - 4\gamma(x, p) \\ &= [p(F_0 - F_1) - (\beta - \alpha)]^2 + 4\alpha\beta > 0 \end{aligned}$$

so, as expected, Λ_0 is real. In order to calculate the terms $A(x)$ and $B(x)$ appearing in the SDE (5.17), we differentiate $\Lambda_0(x, p)$ with respect to p . First,

$$\begin{aligned} \frac{\partial \Lambda_0}{\partial p} &= \frac{F_0 + F_1}{2} + \frac{\partial Z}{\partial p} \frac{1}{4\sqrt{Z}} \\ &= \frac{F_0 + F_1}{2} + \frac{F_0 - F_1}{2} \\ &\quad \times \frac{p(F_0 - F_1) - (\beta - \alpha)}{\sqrt{[p(F_0 - F_1) - (\beta - \alpha)]^2 + 4\alpha\beta}}. \end{aligned}$$

On setting $p = 0$, we have

$$A(x) = \rho_0(x)F_0(x) + \rho_1(x)F_1(x), \quad (5.21)$$

as expected. Similarly,

$$\begin{aligned} \frac{\partial^2 \Lambda_0}{\partial p^2} &= \frac{[F_0 - F_1]^2}{2\sqrt{[p(F_0 - F_1) - (\beta - \alpha)]^2 + 4\alpha\beta}} \\ &\quad - \frac{[F_0 - F_1]^2}{2} \frac{[p(F_0 - F_1) - (\beta - \alpha)]^2}{\{[p(F_0 - F_1) - (\beta - \alpha)]^2 + 4\alpha\beta\}^{3/2}}, \end{aligned}$$

so

$$B(x) = \frac{[F_0(x) - F_1(x)]^2 \alpha(x) \beta(x)}{[\alpha(x) + \beta(x)]^3}. \quad (5.22)$$

In the special case of the unbiased velocity jump process considered in Sec. IV, with $\alpha = \beta$ independent of x and $F_1(x) = v = -F_0(x)$, we recover a diffusion process with effective diffusivity $D = \epsilon v^2 / 2\alpha$ and zero drift.

It is important to note that the fast switching regime is distinct from the large-time regime $t \gg \tau_c = 1/2\alpha$ considered in Sec. IV. In the former case, we fix the scale of the continuous variable x by setting $X_0 = 1$. This means that any important features of the functions $F_n(x)$ at finer spatial scales will be lost. With this caveat, the usefulness of working in the fast switching regime is that we have replaced a system of PDES (3.20) by a scalar PDE (5.18). Such a reduction becomes even more significant when the number of discrete states satisfies $N_0 > 2$. However, solving the scalar equation (5.18) is still a nontrivial problem for general functions $A(x)$ and $B(x)$. On the other hand, it might be possible to adapt recent work on Brownian functionals [39] when $B(x)$ is independent of x . This would occur in the two-state model, for example, if α, β are independent of x and $F_0(x) - F_1(x)$ is a nonzero constant.

VI. DISCUSSION

In this paper we derived a Feynman-Kac formula for functionals \mathcal{T} of a stochastic hybrid system evolving according to a piecewise deterministic Markov process. We considered two complementary approaches. The first involved fixing a particular realization σ of the discrete process, deriving a stochastic Liouville equation for the moment generating function Q of \mathcal{T} and then averaging with respect to σ . This generated a differential CK equation for the σ -averaged moment generating function \mathcal{Q} . The second method derived the CK equation directly by constructing the Feynman-Kac formula for a path-integral representation of the full stochastic hybrid system.

One immediate extension of our theory would be to develop analytical and numerical tools for solving more complicated examples of stochastic hybrid systems than the velocity jump process of Sec. IV. Two simplifying aspects of the latter were the small number of discrete states ($n = 0, 1$) and the x independence of the generator \mathbf{A} and functions F_n . As highlighted in Sec. VC, one possible approach would be to perform a Gaussian approximation in the fast switching regime. In addition to considering more complicated 1D examples, other possible extensions include higher-dimensional piecewise deterministic dynamics ($x \in \mathbb{R}^d$) and stochastic versions of the continuous process. In the last case, the piecewise deterministic ODE (2.1) is replaced by the piecewise SDE,

$$dX = F_n(X)dt + \sqrt{2B_n(X)}dW(t),$$

where $W(t)$ is a Wiener process and $B_n(X)$ is an n -dependent noise amplitude. The corresponding CK equation (2.5) becomes (assuming Ito calculus, say)

$$\mathbb{L}p_n(x,t) = -\frac{\partial F_n(x)p_n(x,t)}{\partial x} + \frac{\partial^2 B_n(x)p_n(x,t)}{\partial x^2} + \sum_{m \in \Gamma} A_{nm}(x)p_m(x,t).$$

It is straightforward to extend the derivation of the Feynman-Kac formula in Secs. III or V to include the intrinsic noise term. For example, the stochastic Liouville equation (3.9) becomes a stochastic Fokker-Planck equation, which after averaging with respect to realizations of the discrete Markov process, yields a generalization of the Feynman-Kac formula (3.20) that includes diffusion terms.

A final issue concerns identifying concrete applications where functionals other than those associated with first-passage time problems might be relevant. One important application area of stochastic hybrid systems is to gene regulatory networks. Hybrid models arise when a partial thermodynamic limit of a biochemical master equation is taken. This yields a piecewise deterministic or stochastic differential equation for the concentrations of proteins and messenger ribonucleic acid, while the remaining discrete variables represent the activation states of one or more genes [17–21]. One quantity of interest is the amount of time that a protein concentration remains above some threshold, which can be formulated in terms of the occupation time of a stochastic hybrid system on \mathbb{R}^+ .

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