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Probabilistic density function method for nonlinear dynamical systems driven by colored noise

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We present a probability density function (PDF) method for a system of nonlinear stochastic ordinary differential equations driven by colored noise. The method provides an integro-differential equation for the temporal evolution of the joint PDF of the system's state, which we close by means of a modified Large-Eddy-Diffusivity (LED) closure. In contrast to the classical LED closure, the proposed closure takes into account the advective transport of the PDF in the approximate temporal deconvolution of the integro-differential equation. Additionally, we introduce the generalized local linearization (LL) approximation for deriving a computable PDF equation in the form of a second-order partial differential equation (PDE). We demonstrate the proposed closure and localization accurately describe the dynamics of the PDF in phase space for systems driven by noise with arbitrary auto-correlation time. We apply the proposed PDF method to the analysis of a set of Kramers equations driven by exponentially auto-correlated Gaussian colored noise to study nonlinear oscillators and the dynamics and stability of a power grid. Numerical experiments show that the PDF method is accurate when the noise auto-correlation time is either much shorter or much longer than the system's relaxation time, with the accuracy decreasing as the ratio of the two time scales approaches unity. Similarly, the PDF method accuracy decreases with increasing standard deviation of the noise.

I. INTRODUCTION

A variety of important physical systems in physics and engineering can be modeled as nonlinear dynamical systems driven by fluctuations with non-trivial auto- and cross-correlation time scales [1–3]. Applications include reaction kinetics [4], electronic systems subject to phase noise [5], and electro-mechanical power systems driven by ucertain renewable power input [6]. For such systems there is no clear time scale separation between the system's relaxation and oscillation time scales and the characteristic time scales of the driving noise, so that a white noise model for the driving fluctuations is inadequate. In fact, these time scales may interact, resulting in dynamic behavior that cannot be predicted by white noise models. It is therefore important to employ models that accurately capture the effect of colored fluctuations.

Nonlinear stochastic processes driven by fluctuations correlated in time ("colored noise") are non-Markovian and thus not amenable to treatment by means of the Fokker-Planck equation (FPE). If the "colored noise" can be modeled by a Langevin stochastic differential equation (SDE) driven by "white noise", then one may reformulate the problem as an expanded Markovian process (i.e., expand the phase space to include the fluctuations) and formulate the FPE for the joint noise-state PDF. Nevertheless, such an approach may be undesirable if the dimension of the phase space and the number of driving processes is large, thus resulting in an even larger, less amenable expanded system. Also, not every noise correlation structure can be readily described by a SDE.

As an alternative, various projection approaches, or PDF methods, have been proposed for deriving an integro-differential conservation equation, or quasi-Fokker-Planck equation, for the evolution of the joint PDF of the system's state (e.g., [7–10]). The nonlocal nature of the resulting PDF equation reflects the non-Markovian character of the nonlinear stochastic process. Nevertheless, obtaining computable coefficients for the PDF equation for the entire range of correlation times of interest in applications remains an open challenge, and additional approximations are necessary. The so-called Best Fokker-Planck Approximation (BFPA) can be employed for an arbitrary number of SDEs, but it is valid only for correlation times short relative to the characteristic time scale of the system, and thus of limited use. Alternative approximations have been successfully employed for a single ODE and a system of two SDEs, such as the local linearization (LL) of [10] for the Langevin equation, and the decoupling theory of [8, 9] for the Langevin and Kramers equations.

In this manuscript, we present a PDF method for systems of nonlinear SDEs driven by colored noise of arbitrarily long auto-correlation time. Our method can be employed for systems of an arbitrary number of SDEs, and results in a quasi-Fokker-Planck equation with computable coefficients. We derive our method by formulating a modified Large-Eddy-Diffusivity (LED) closure for closing the stochastic flux term of the PDF equation. LED closures were originally introduced in the context of stochastic averaging of advective velocity fluctuations for scalar transport [11, 12], and have been extensively employed for the analysis of advection-diffusion and advection-reaction transport processes [13–19]. More recently, the LED closure has been employed in the context of nonlinear Langevin equations driven by colored

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noise with short to moderately long auto-correlation time scale [1, 6].

The classical LED theory results in a time-convoluted integro-differential equation for the PDF, which is transformed into a PDE by introducing a classical localization. Such a localization nevertheless is ill-suited for treating systems characterized by a mean-field velocity with non-zero divergence and long noise auto-correlation time with respect to the systems' relaxation time. In order to address this shortcoming, we introduce a modified localization which employs the history of the advective dynamics of the PDF to deconvolve the integral expression for the stochastic flux. Finally, we propose a generalization of the LL approximation of [10] in order to obtain a computable expression for the stochastic flux applicable to an arbitrary number of SDEs.

The manuscript is structured as follows: The PDF method is introduced in Section II. In Section III, we outline the LED theory, discuss the shortcomings of the classical theory, and introduce our modified localization. Stochastic diffusion coefficients are computed in Section IV by means of our generalized LL approximation. The resulting PDF method is applied in Section V to a set of M Kramers equations. In particular we discuss the overdamped and general case for $M = 1$, and the general case for $M > 1$. Approximate analytical solutions for the stationary joint PDF are presented for $M = 1$, and a Gaussian approximation is presented for $M > 1$. Finally, conclusions are given in Section VI.

II. PDF METHOD

We consider a dynamical system described by the nonlinear initial-value problem (IVP) in N dimensions

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = v_i(\mathbf{x}, t) = \langle v_i(\mathbf{x}, t)\rangle_0 + v_i'(\mathbf{x}, t), \tag{1}$$

$$x_i(0) = x_i^0, \tag{2}$$

for $i = 1, \ldots, N$, where $\mathbf{v} = [v_1(\mathbf{x}, t), \ldots, v_N(\mathbf{x}, t)]^\top$ is a random function with known statistics. Each $v_i(\mathbf{x}, t)$ is decomposed into a deterministic function or "mean-field velocity", $\langle v_i(\mathbf{x}, t)\rangle_0$, and a stochastic fluctuation term, $v_i'(\mathbf{x}, t)$, with zero mean for fixed $\mathbf{x}$ and t, and characterized by its correlation time, λ, and its characteristic amplitude $\sigma < \infty$, i.e., $\sigma^2 \equiv \sup_{i,j,\mathbf{x},t}\langle v_i'(\mathbf{x}, t) v_j'(\mathbf{x}, t)\rangle$, where $\langle\cdot\rangle$ denotes ensemble average. In this manuscript, we study systems for which the effect of non-zero correlation time of the fluctuations is important and cannot be disregarded.

Let $\mathbf{x}(t) = [x_1(t), \ldots, x_N(t)]^\top \in A$ be the system's state vector, where $A \subseteq \mathbb{R}^N$ is the phase space. For simplicity we assume that $A \equiv \mathbb{R}^N$, although different supports for the state variables can be considered. Additionally, let $\mathbf{X} = [X_i, \ldots, X_N]^\top \in A$ denote a variable in phase space. In order to derive the PDE governing the evolution of the one-point joint PDF of the system's state, $p(\mathbf{X}; t)$, we define the auxiliary "raw" PDF, $\Pi(\mathbf{X}; t)$, given by

$$\Pi(\mathbf{X}; t) = \delta[\mathbf{x}(t) - \mathbf{X}] = \prod_{i=1}^{N} \delta[x_i(t) - X_i]. \tag{3}$$

For a given time t, $\Pi(\mathbf{X}; t)$ is a Dirac delta function in phase spaced centered around $\mathbf{X} = \mathbf{x}(t)$. The raw PDF can be decomposed into its ensemble average and a zero-mean scalar fluctuation, i.e., $\Pi = \langle\Pi\rangle + \Pi'$. The ensemble average of $\Pi(\mathbf{X}; t)$ over all realizations $\mathbf{x}(t)$, $\langle\Pi(\mathbf{X}; t)\rangle$, is equal to the PDF $p(\mathbf{X}; t)$, i.e., $p(\mathbf{X}; t) \equiv \langle\Pi(\mathbf{X}; t)\rangle$ [20]. To see this, we recall the definition of the ensemble average of an arbitrary function Q of $\mathbf{x}(t)$, $\langle Q(\mathbf{x}(t))\rangle \equiv \int_A Q(\mathbf{Y}) p(\mathbf{Y}; t) \mathrm{d}\mathbf{Y}$. Substituting $\delta[\mathbf{x}(t) - \mathbf{X}]$ for $Q(\mathbf{x}(t))$, we obtain the relation

$$\langle\Pi(\mathbf{X}; t)\rangle \equiv \int_A \delta(\mathbf{Y} - \mathbf{X}) p(\mathbf{Y}; t)\, \mathrm{d}\mathbf{Y} = p(\mathbf{X}; t). \tag{4}$$

The raw PDF obeys the conservation law (see Appendix A)

$$L\Pi = \frac{\partial\Pi}{\partial t} + \nabla_{\mathbf{X}} \cdot (\langle\mathbf{v}\rangle_0 \Pi) = -\nabla_{\mathbf{X}} \cdot (\mathbf{v}'\Pi), \tag{5}$$

where $\langle\mathbf{v}(\mathbf{X}, t)\rangle_0 = [\langle v_1(\mathbf{X}, t)\rangle_0, \ldots, \langle v_N(\mathbf{X}, t)\rangle_0]^\top$ is the mean-field velocity, and $\mathbf{v}' = [v_1'(\mathbf{X}, t), \ldots, v_N'(\mathbf{X}, t)]^\top$ is the zero-mean velocity fluctuation, with initial condition given by (2) and (3), namely,

$$\Pi(\mathbf{X}; 0) = \delta(\mathbf{x}^0 - \mathbf{X}), \tag{6}$$

where $\mathbf{x}^0 = [x_1^0, \ldots, x_N^0]^\top$.

Taking the ensemble average of (5)–(6), employing the decomposition $\Pi = p + \Pi'$, and recalling that $\langle\mathbf{v}'\rangle = 0$, we obtain the boundary value problem (BVP) for $p(\mathbf{X}; t)$,

$$\frac{\partial p}{\partial t} + \nabla_{\mathbf{X}} \cdot (\langle\mathbf{v}\rangle_0 p) + \nabla_{\mathbf{X}} \cdot \langle\mathbf{v}'\Pi'\rangle = 0, \tag{7}$$

with initial conditions

$$p(\mathbf{X}; 0) = \delta(\mathbf{x}^0 - \mathbf{X}), \tag{8}$$

and vanishing free space boundary conditions for $x_i \to \pm\infty$, which correspond to $A = \mathbb{R}^N$. For periodic state variables with bounded support, the boundary conditions for the BVP are periodic.

The cross-covariance $\langle\mathbf{v}'\Pi'\rangle$ can be understood as a stochastic flux in addition to the deterministic advective flux induced by mean-field velocity $\langle\mathbf{v}\rangle_0$. This flux is unknown *a priori* and requires full knowledge of the solution of the nonlinear IVP (1)–(2) in order to be evaluated; therefore, the governing PDE (7) is unclosed. An appropriate closure must be provided so that (7) can be utilized to solve for the dynamic behavior of the joint PDF p. For this purpose, we propose employing a modified Large-Eddy-Diffusivity (LED) closure, presented in the following section.

III. MODIFIED LED CLOSURE

Various closures have been proposed for expressing the stochastic flux $\langle \mathbf{v}'\Pi' \rangle$ in terms of the joint PDF p [8–10, 21, 22]. In the present work, we introduce the family of so-called Large-Eddy-Diffusivity (LED) closures [11–13], and propose a modified LED closure appropriate for deriving a localized PDF equation for nonlinear dynamical systems.

The stochastic flux $\langle \mathbf{v}'\Pi' \rangle$ can be written in terms of the deterministic operator L's Green's function $G(\mathbf{X}, t|\mathbf{Y}, s)$, defined as the solution to the adjoint problem

$$\hat{L}G = -\frac{\partial G}{\partial s} - \langle \mathbf{v} \rangle_0 \cdot \nabla_{\mathbf{Y}} G = \delta(\mathbf{X} - \mathbf{Y})\delta(t - s), \quad (9)$$

with homogeneous free space boundary conditions and terminal condition $G(\mathbf{X}, t|\mathbf{Y}, t) = 0$, where $\hat{L}$ is the adjoint of the operator L introduced in (5). In terms of $G(\mathbf{X}, t|\mathbf{Y}, s)$, $\langle \mathbf{v}'\Pi' \rangle$ can be written as (see Appendix B)

$$\langle \mathbf{v}'\Pi' \rangle(\mathbf{X}, t) = -\int_0^t \int_A G(\mathbf{X}, t|\mathbf{Y}, s) \times \nabla_{\mathbf{Y}} \cdot \left\langle \Pi(\mathbf{Y}, s)\mathbf{v}'(\mathbf{X}, t)\mathbf{v}'^{\top}(\mathbf{Y}, s) \right\rangle \mathrm{d}\mathbf{Y}\mathrm{d}s. \quad (10)$$

This expression is exact but unclosed, as it depends on the unknown moment $\langle \Pi(\mathbf{Y}, s)\mathbf{v}'(\mathbf{X}, t)\mathbf{v}'^{\top}(\mathbf{Y}, s) \rangle$. In order to proceed, we use the standard LED closure

$$\int_0^t \int_A f(\mathbf{Y}) \nabla_{\mathbf{Y}} \cdot \left\langle \mathbf{v}'(\mathbf{X}, t)\mathbf{v}'^{\top}(\mathbf{Y}, s)\Pi(\mathbf{Y}; s) \right\rangle \mathrm{d}\mathbf{Y}\mathrm{d}s \approx \int_0^t \int_A f(\mathbf{Y}) \nabla_{\mathbf{Y}} \cdot \left\langle \mathbf{v}'(\mathbf{X}, t)\mathbf{v}'^{\top}(\mathbf{Y}, s) \right\rangle p(\mathbf{Y}; s)\, \mathrm{d}\mathbf{Y}\mathrm{d}s, \quad (11)$$

for an arbitrary function $f : A \to \mathbb{R}$. Approximation (11) disregards the contribution to the stochastic flux due to the third moment $\langle \Pi'(\mathbf{Y}, s)\mathbf{v}'(\mathbf{X}, t)\mathbf{v}'^{\top}(\mathbf{Y}, s) \rangle$, as it is assumed to be much smaller than the second-order term:

$$\int_0^t \int_A f(\mathbf{Y}) \nabla_{\mathbf{Y}} \cdot \left\langle \mathbf{v}'(\mathbf{X}, t)\mathbf{v}'^{\top}(\mathbf{Y}, s) \right\rangle p(\mathbf{Y}; s)\, \mathrm{d}\mathbf{Y}\mathrm{d}s \gg \int_0^t \int_A f(\mathbf{Y}) \nabla_{\mathbf{Y}} \cdot \left\langle \Pi'(\mathbf{Y}, s)\mathbf{v}'(\mathbf{X}, t)\mathbf{v}'^{\top}(\mathbf{Y}, s) \right\rangle \mathrm{d}\mathbf{Y}\mathrm{d}s,$$

The disregarded contributions are of order $(\sigma\lambda)^3$, so that the approximation is second-order accurate in $\sigma\lambda$ [7].

Applying this approximation to Eq. (10) and substituting Green's function (B8) into the resulting expression, we obtain the following Lagrangian form for the (unclosed) stochastic flux in terms of the PDF p (see Appendix B):

$$\langle \mathbf{v}'\Pi' \rangle(\mathbf{X}, t) \approx -\int_0^t \mathcal{J}(s|\mathbf{X}, t) \times \nabla_{\boldsymbol{\chi}} \cdot \left[\left\langle \mathbf{v}'(\mathbf{X}, t)\mathbf{v}'^{\top}(\boldsymbol{\chi}(s|\mathbf{X}, t), s) \right\rangle \times p(\boldsymbol{\chi}(s|\mathbf{X}, t); s) \right] \mathrm{d}s, \quad (12)$$

where $\boldsymbol{\chi}(s|\mathbf{X}, t) \in A$ is the solution to the terminal value problem,

$$\frac{\mathrm{d}}{\mathrm{d}s}\boldsymbol{\chi}(s|\mathbf{X}, t) = \langle \mathbf{v}(\boldsymbol{\chi}(s|\mathbf{X}, t), s) \rangle_0, \quad s < t, \quad (13)$$

$$\boldsymbol{\chi}(t|\mathbf{X}, t) = \mathbf{X}, \quad (14)$$

and $\mathcal{J}(s|\mathbf{X}, t)$ is the Jacobian determinant of the (reverse) flow $(\mathbf{X}, t) \mapsto \boldsymbol{\chi}(s|\mathbf{X}, t)$, given by the Liouville-Ostrogradski formula

$$\mathcal{J}(s|\mathbf{X}, t) = \left| \frac{\partial \boldsymbol{\chi}(s|\mathbf{X}, t)}{\partial \mathbf{X}} \right| = \exp\left(-\int_s^t \nabla_{\boldsymbol{\chi}} \cdot \langle \mathbf{v}(\boldsymbol{\chi}(s'|\mathbf{X}, t), s') \rangle_0 \, \mathrm{d}s' \right). \quad (15)$$

Here, $\boldsymbol{\chi}(s|\mathbf{X}, t)$ can be interpreted as the Lagrangian coordinate in phase space at time $s < t$, defined by the mean-field velocity $\langle \mathbf{v} \rangle_0$, which coincides with the Eulerian coordinate $\mathbf{X}$ at time t.

Substituting (12) into (7), we obtain a time-convoluted integro-differential equation for p. The temporal convolution reflects the non-Markovian character of the stochastic process $\mathbf{x}(t)$ when driven by colored noise.

For the particular case of temporally uncorrelated velocity fluctuations, (i.e., Gaussian white noise), we have $\langle \mathbf{v}'(\mathbf{X}, t)\mathbf{v}'^{\top}(\mathbf{Y}, s) \rangle = \delta(t - s)\mathbf{G}(\mathbf{X}, \mathbf{Y})$, with $\mathbf{G}(\mathbf{X}, \mathbf{Y})$ the cross-covariance tensor of the velocity fluctuations, for which (12) reduces to

$$\langle \mathbf{v}'\Pi' \rangle(\mathbf{X}, t) \approx -\nabla_{\mathbf{X}} \cdot \mathbf{D}(\mathbf{X})p(\mathbf{X}; t), \quad (16)$$

where the diffusion tensor is simply

$$\mathbf{D}(\mathbf{X}) \equiv \mathbf{G}(\mathbf{X}, \mathbf{X}). \quad (17)$$

Then, substituting (16)–(17) into (7) we recover the Fokker-Planck equation.

Although the integro-differential BVP (7), (8) and (12) for p, resulting from the classical LED theory, may be solved numerically as is, it is much more desirable to transform said problem into a partial differential BVP by means of an appropriately chosen approximate deconvolution or "localization". Such a localization consists of approximating $p(\boldsymbol{\chi}(s|\mathbf{X}, t); s)$ and $\nabla_{\boldsymbol{\chi}}$in terms of $p(\mathbf{X}; t)$ and ∇ over the correlation time-span $(t - \lambda, t)$ for which the contribution of the cross-correlation term $\langle \mathbf{v}'(\mathbf{X}, t)\mathbf{v}'^{\top}(\boldsymbol{\chi}(s|\mathbf{X}, t), s) \rangle$ to the integral in (12) is nontrivial.

A possible approach to formulate a localization is the one provided by the classical LED theory [1, 13, 15, 18, 19], which assumes that p and its spatial derivatives are approximately uniform over the timespan $(t - \lambda, t)$. Under this assumption, we can replace $p(\boldsymbol{\chi}(s|\mathbf{X}, t); s)$ with $p(\mathbf{X}; t)$ and $\nabla_{\boldsymbol{\chi}} p(\boldsymbol{\chi}(s|\mathbf{X}, t); s)$ with $\nabla_{\mathbf{X}} p(\mathbf{X}; t)$ in the integrand of (12), resulting in the classical closed-form LED expression for the stochastic flux

$$\langle \mathbf{v}'\Pi' \rangle(\mathbf{X}, t) \approx \left[\mathbf{v}^{\mathrm{L}}(\mathbf{X}, t) - \mathbf{D}^{\mathrm{L}}(\mathbf{X}, t)\nabla_{\mathbf{X}} \right] p(\mathbf{X}; t), \quad (18)$$

where $\mathbf{v}^L$ and $\mathbf{D}^L$ are the classical LED drift velocity and diffusion tensor, given by

$$\mathbf{v}^{\mathrm{L}}(\mathbf{X},t) \equiv -\int_0^t \mathcal{J}(s|\mathbf{X},t) \times \langle \mathbf{v}'(\mathbf{X},t)\nabla_\chi \cdot \mathbf{v}'(\boldsymbol{\chi}(s|\mathbf{X},t),s)\rangle \,\mathrm{d}s, \tag{19}$$

$$\mathbf{D}^{\mathrm{L}}(\mathbf{X},t) \equiv \int_0^t \mathcal{J}(s|\mathbf{X},t) \times \left\langle \mathbf{v}'(\mathbf{X},t)\mathbf{v}'^{\top}(\boldsymbol{\chi}(s|\mathbf{X},t),s)\right\rangle \mathrm{d}s. \tag{20}$$

The classical LED localization disregards two important effects:

1. The expansion (or contraction) rate of the PDF p from $t-\lambda$ to t due to non-zero divergence of the mean-field velocity, $\nabla\cdot\langle\mathbf{v}\rangle_0 \neq 0$, which may play a significant role if the inverse of the divergence rate is much shorter than the noise correlation time.

2. The divergence operator $\nabla_{\boldsymbol{\chi}}$ may not be collinear with $\nabla_{\mathbf{X}}$ at time $s<t$, so that significant directional contributions to the gradient may be underestimated or disregarded altogether.

It follows that the localization approximation provided by the classical LED theory is only accurate for short correlation time scales and negligible divergence of the mean-field velocity.

We propose an alternative localization approximation that addresses the aforementioned limitations of the classical LED theory. Our approximation consists of assuming that the contribution to the dynamics of p over the time-span $(t-\lambda,t)$ due to mean-field advective transport is much larger than that due to stochastic transport; therefore, it suffices to capture the average-flow advective dynamics of p from $t-\lambda$ to t for the purpose of localization.

In order to formulate such an approximation, we consider the solution of the purely mean-field advective transport problem

$$\frac{\partial p}{\partial s} + \nabla_{\mathbf{X}}\cdot(\langle\mathbf{v}\rangle_0 p) = 0, \quad s<t \tag{21}$$

with terminal condition $p(\mathbf{X},t)$, which has the the solution

$$p(\boldsymbol{\chi}(s|\mathbf{X},t);s) = \mathcal{J}^{-1}(s|\mathbf{X},t)p(\mathbf{X};t). \tag{22}$$

The expression (22) serves as our localization approximation for p. Substituting (22) into (12) we obtain the partially localized expression

$$\langle\mathbf{v}'\Pi'\rangle(\mathbf{X};t) \approx -\int_0^t \mathcal{J}(s|\mathbf{X},t) \times \nabla_{\boldsymbol{\chi}}\cdot\left\{\left\langle\mathbf{v}'(\mathbf{X},t)\mathbf{v}'^{\top}(\boldsymbol{\chi}(s|\mathbf{X},t),s)\right\rangle \times\mathcal{J}^{-1}(s|\mathbf{X},t)p(\mathbf{X};t)\right\}\,\mathrm{d}s. \tag{23}$$

where the PDF p in the integrand has been localized from $(\boldsymbol{\chi}(s|\mathbf{X},t),s)$ to $(\mathbf{X},t)$, but the Lagrangian gradient $\nabla_{\boldsymbol{\chi}}$ has been not. Note that the map $(\mathbf{X},t)\mapsto\boldsymbol{\chi}(s|\mathbf{X},t)$ implies that the Lagrangian gradient $\nabla_{\boldsymbol{\chi}}$ acts on $p(\mathbf{X};t)$ and thus $p(\mathbf{X},t)$ cannot be taken outside the integral in Eq. (23).

Eq. (23) for the stochastic flux, and its generalized LL approximation, presented in the following section, are the main results of this manuscript, and form our PDF method. Eq. (23) is also important because it bridges the more general LED theory with the second-order cumulant expansion of [7], indicating that both theories are equivalent for nonlinear SDEs.

The Lagrangian gradient operator can be re-written in Eulerian coordinates by virtue of the chain rule:

$$\nabla_{\boldsymbol{\chi}} = \left(\frac{\partial\mathbf{X}}{\partial\boldsymbol{\chi}(s|\mathbf{X},t)}\right)^{\top}\nabla_{\mathbf{X}} = \boldsymbol{\Psi}^{\top}(t|\boldsymbol{\chi}(s|\mathbf{X},t),s)^{\top}\nabla_{\mathbf{X}}, \tag{24}$$

where $\boldsymbol{\Psi}^{\top}(t|\boldsymbol{\chi}(s|\mathbf{X},t)$ is the sensitivity matrix of the flow $(\mathbf{X},t)\mapsto\boldsymbol{\chi}(s|\mathbf{X},t)$ with respect to $\boldsymbol{\chi}(s|\mathbf{X},t)$, defined as follows: Consider the flow $(\mathbf{Z},s')\mapsto\boldsymbol{\chi}(t'|\mathbf{Z},s')$ between time s' and $t'>s'$, with initial condition $\mathbf{Z}$. We define the sensitivity matrix $\boldsymbol{\Psi}$ of the flow with respect to $\mathbf{Z}$ as

$$\boldsymbol{\Psi}(t'|\mathbf{Z},s') = \frac{\partial\boldsymbol{\chi}(t'|\mathbf{Z},s')}{\partial\mathbf{Z}}. \tag{25}$$

The sensitivity matrix $\boldsymbol{\Psi}$ satisfies the variational equation

$$\frac{\mathrm{d}}{\mathrm{d}t'}\boldsymbol{\Psi}(t'|\mathbf{Z},s') = \mathbf{J}(\boldsymbol{\chi}(t'|\mathbf{Z},s'),t')\boldsymbol{\Psi}(t'|\mathbf{Z},s'), \tag{26}$$

$$\boldsymbol{\Psi}(s'|\mathbf{Z},s') = \mathbf{I}, \tag{27}$$

where $\mathbf{I}$ is the $N\times N$ identity matrix. Eq (26) is obtained by differentiating (13) with respect to $\mathbf{Z}$, where the $\mathbf{J}(\mathbf{X},t) = \{J_{ij}(\mathbf{X},t)\}$ is the Jacobian of the mean-field velocity, with components $J_{ij}(\mathbf{X},t) = \partial\langle v_i(\mathbf{X},t)\rangle_0/\partial X_j$.

Although Equations (23) and (24) provide a closed expression for the stochastic flux, its exact analytical evaluation requires analytical expressions for the sensitivity matrix $\boldsymbol{\Psi}(t|\boldsymbol{\chi}(s|\mathbf{X},t))$ and the Jacobian $\mathcal{J}(s|\mathbf{X},t)$, which are only available for special cases. As an alternative, in the next section we present an approximate scheme for the analytical evaluation of the stochastic flux.

IV. COMPUTING LED DIFFUSION COEFFICIENTS

In this section we consider the evaluation of the approximate stochastic flux (23) obtained via our modified LED closure. We restrict our attention to additive noise problems for which the mean-field flow is autonomous, and

$$\nabla_{\mathbf{X}}\cdot\langle\mathbf{v}\rangle_0 = -\gamma, \tag{28}$$

with γ a positive constant. This family of problems include Brownian motion [1, 23], the Kramers equation [6, 8, 24], power grid systems driven by uncertain power input [6], and other similar stochastic processes. The SDEs for such systems read

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \langle v_i(\mathbf{x})\rangle_0 + \xi_i(t;\tilde{\omega}), \quad i = 1,\ldots,N. \tag{29}$$

Furthermore, we assume that the velocity fluctuations are stationary.

Various approximations have been proposed for obtaining closed-form expressions for the stochastic flux, applicable to particular cases. For $N = 1$, the stochastic flux was evaluated in [10] by employing the so-called "linear localization" (LL) approximation. For the Kramers equation ($N = 2$), an approximate stochastic flux was obtained in [8]. In this section we propose a generalization of the LL approximation for arbitrary N.

Substituting (28) into (15), and then into (23), we obtain the stochastic flux for additive noise

$$\langle \boldsymbol{\xi}\Pi'\rangle(\mathbf{X};t) \approx -\mathbf{D}^{\mathrm{M}}(\mathbf{X},t)\nabla_{\mathbf{X}}\, p(\mathbf{X};t), \tag{30}$$

with diffusion tensor

$$\mathbf{D}^{\mathrm{M}}(\mathbf{X},t) \equiv \int_0^t \left\langle \boldsymbol{\xi}(t)\boldsymbol{\xi}^\top(s)\right\rangle \times \boldsymbol{\Psi}^\top(t|\boldsymbol{\chi}(s|\mathbf{X},t),s)\,\mathrm{d}s. \tag{31}$$

Note the differences between the diffusion tensors obtained via the classical LED theory (20) and the modified theory (31). We now proceed to propose a computable approximation to the sensitivity matrix. The solution of (26) is

$$\boldsymbol{\Psi}(t|\boldsymbol{\chi}(s|\mathbf{X},t),s) = \mathcal{T}\exp\left(\int_s^t \mathbf{J}(\boldsymbol{\chi}(s_1|\mathbf{X},t))\,\mathrm{d}s_1\right) \equiv 1 + \int_s^t \mathbf{J}(\boldsymbol{\chi}(s_1|\mathbf{X},t))\,\mathrm{d}s_1 + \int_s^t\int_{s_1}^t \mathbf{J}(\boldsymbol{\chi}(s_2|\mathbf{X},t))\mathbf{J}(\boldsymbol{\chi}(s_1|\mathbf{X},t))\,\mathrm{d}s_1\mathrm{d}s_2 + \cdots, \tag{32}$$

where $\mathcal{T}\exp$ denotes the time-ordered exponential function [25]. Instead of evaluating the time-ordered exponential in (32), we propose to linearize the variational equation (26)–(27) for the flow $(\mathbf{X},t)\mapsto\boldsymbol{\chi}(s|\mathbf{X},t)$ around $(\mathbf{X},t)$, so that $\mathbf{J}(\boldsymbol{\chi}(s'|\mathbf{X},t))$, $s<s'<t$ in (32) can be approximated by $\mathbf{J}(\mathbf{X})$, and the time-ordered exponential can be replaced by a matrix exponential, resulting in the approximation

$$\boldsymbol{\Psi}(t|\boldsymbol{\chi}(s|\mathbf{X},t),s) = \mathcal{T}\exp\left(\int_s^t \mathbf{J}(\boldsymbol{\chi}(s_1|\mathbf{X},t))\,\mathrm{d}s_1\right) \approx \exp((t-s)\mathbf{J}(\mathbf{X})). \tag{33}$$

The approximation to the sensitivity matrix of Eq. (33), together with the modified LED closure expression for the stochastic flux [given by Eq. (23)], are the main contributions of this manuscript, as they lead to a fully localized quasi-Fokker-Planck PDE. This approximation can be interpreted as the multi-dimensional generalization of the (LL) approximation introduced in [10]. Substituting (33) into (31) and introducing the lag variable $\tau = t - s$, the generalized LL approximation leads to a computable expression for the stochastic diffusion tensor

$$\mathbf{D}^{\mathrm{M}}(\mathbf{X},t) = \int_0^t \left\langle \boldsymbol{\xi}(0)\boldsymbol{\xi}^\top(\tau)\right\rangle \exp(\tau\mathbf{J}^\top(\mathbf{X}))\,\mathrm{d}\tau. \tag{34}$$

This integral can be evaluated analytically in the stationary limit $t\to\infty$ for exponentially auto-correlated, mutually uncorrelated velocity fluctuation components, i.e.,

$$\langle\xi_i(0)\xi_i(\tau)\rangle = \sigma_i^2\exp(-|\tau|/\lambda_i),$$
$$\langle\xi_i(0)\xi_j(\tau)\rangle = 0, \quad i\neq j,$$

whereby $\mathbf{D}^{\mathrm{M}}(\mathbf{X},t\to\infty) = \mathbf{D}^{\mathrm{M,st}}(\mathbf{X})$ obeys the Sylvester equation

$$\boldsymbol{\Lambda}^{-1}\mathbf{D}^{\mathrm{M,st}} - \mathbf{D}^{\mathrm{M,st}}\mathbf{J}^\top = \boldsymbol{\Sigma}, \tag{35}$$

with $\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1,\ldots\lambda_N)$ and $\boldsymbol{\Sigma} = \mathrm{diag}(\sigma_1^2,\ldots,\sigma_N^2)$.

Replacing the approximate equality in (30) with an equality, and substituting into (7), we obtain the PDF equation

$$\frac{\partial p}{\partial t} + \nabla_{\mathbf{X}}\cdot(\langle\mathbf{v}\rangle_0 p) = \nabla\cdot\mathbf{D}^{\mathrm{M}}\nabla p. \tag{36}$$

V. APPLICATIONS TO KRAMERS EQUATIONS

In this section we present the application of the proposed modified LED theory to a set of coupled Kramers equations. The Kramers equation is widely used to model reaction kinetics [24], oscillatory dynamics [8, 23], electromechanical power systems [6], among other phenomena of interest in engineering and physics. We consider the set of M coupled Kramers equations

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = v_\mathrm{B} v_i, \tag{37}$$

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = F_i - S_i(x_1, \ldots, x_M) - \gamma v_i + \Gamma_i(t), \tag{38}$$

for $i = 1, \ldots, M$. For each i, $x_i \in A_i^X$ is the position variable, either periodic ($A_i^X \equiv [-\pi, \pi)$) or free-space ($A_i^X \equiv (-\infty, \infty)$), and $v_i \in (-\infty, \infty)$ is the (dimensionless) momentum variable (not to be confused with the RHS of the nonlinear SDEs (1); additionally, v_B is the momentum scale, F_i is a deterministic force, $\Gamma_i(t)$ is a zero-mean stochastic force, γ is the relaxation rate, and $S_i(x_1, \ldots, x_N)$ is the position-dependent recovery force. For periodic coordinates, the functions S_i satisfy

$$S_i(x_1, \ldots, x_j, \ldots, x_n) \\ = S_i(x_i, \ldots, x_j + \pi, x_n), \quad i, j = 1, \ldots, M.$$

We assume that the driving stochastic forces are stationary and mutually uncorrelated, with auto-correlation structure

$$\langle \Gamma_i(0)\Gamma_i(\tau)\rangle = \sigma_i^2 \exp(-|\tau|/\lambda_i). \tag{39}$$

Let $A^X \equiv \prod_{i=1}^M A_i^X$ and $A^V \equiv \mathbb{R}^M$ denote the position and momentum phase spaces, respectively, and let $(\mathbf{X}, \mathbf{V}) \in A^X \times A^V$. Then, the PDF equation (36) for the joint PDF $p(\mathbf{X}, \mathbf{V}; t)$ reads

$$\frac{\partial p}{\partial t} + v_\mathrm{B} V_i \frac{\partial p}{\partial X_i} + \frac{\partial}{\partial V_i}\left(F_i - S_i - \gamma V_i\right) p \\ = \frac{\partial}{\partial V_i}\left(D_{ij}^X \frac{\partial p}{\partial X_j} + D_{ij}^V \frac{\partial p}{\partial V_j}\right). \tag{40}$$

Along the X_i directions, $i = 1, \ldots, N$, Eq. (40) is subject to either periodic or free-space boundary conditions, namely

$$p([X_1, \ldots, X_i, \ldots, X_N]^\top, \mathbf{V}; t) \\ = p([X_1, \ldots, X_i + \pi, \ldots, X_N]^\top, \mathbf{V}; t), \tag{41}$$

for periodic coordinates, or

$$p([X_1, \ldots, X_i = \pm\infty, \ldots, X_N]^\top, \mathbf{V}; t) = 0, \tag{42}$$

for free-space coordinates. Along the V_i directions, $i = 1, \ldots, N$, we have vanishing conditions

$$p(\mathbf{X}, [V_1, \ldots, V_i = \pm\infty, \ldots, V_N]^\top; t) = 0. \tag{43}$$

The deterministic initial condition is

$$p(\mathbf{X}, \mathbf{V}; 0) = \delta(\mathbf{x}^0 - \mathbf{X})\delta(\mathbf{V}), \tag{44}$$

where $\mathbf{x}^0 \in A^X$. Additionally, we have the probability conservation relation

$$\int_{A^X}\int_{A^V} p(\mathbf{X}, \mathbf{V}; t)\, \mathrm{d}\mathbf{V}\mathrm{d}\mathbf{X} = 1, \quad t > 0. \tag{45}$$

The diffusion tensors $\mathbf{D}^X(\mathbf{X})$ and $\mathbf{D}^V(\mathbf{X})$ are given by Eq (35). The Jacobian of the mean-field flow is

$$\mathbf{J}(\mathbf{X}) = \begin{bmatrix} \mathbf{0} & v_\mathrm{B}\mathbf{I} \\ -\mathbf{H}(\mathbf{X}) & -\gamma\mathbf{I} \end{bmatrix}, \tag{46}$$

where $\mathbf{0}$ and $\mathbf{I}$ are the zero and unit order-M second-rank tensors, and $\mathbf{H}(\mathbf{X}) = \{H_{ij}(\mathbf{X})\}$ is the matrix with components $H_{ij} = \partial S_i/\partial x_j$. Substituting (39) and (46) into (35), and computing the block-wise matrix inversion, we obtain the following relations for the stationary diffusion tensors $\mathbf{D}^X(\mathbf{X})$ and $\mathbf{D}^V(\mathbf{X})$,

$$[\mathbf{I} + (\gamma\mathbf{\Lambda})^{-1}]\mathbf{D}^V + (\gamma)^{-1} v_\mathrm{B}\mathbf{\Lambda}\mathbf{D}^V\mathbf{H}^\top = (\gamma)^{-1}\mathbf{\Sigma}, \tag{47}$$

$$\mathbf{D}^X = v_\mathrm{B}\mathbf{\Lambda}\mathbf{D}^V. \tag{48}$$

The PDF equation (40) makes clear the limitations of the classical LED theory. Most evidently, the classical theory (e.g., [1]) predicts a stationary diffusion term of the form

$$\frac{\partial}{\partial V_i}\langle \Gamma_i \Pi' \rangle = -\bar{D}_{ij}^{V,\mathrm{st}} \frac{\partial^2 p}{\partial V_i \partial V_j},$$

with constant diffusion coefficients

$$\bar{D}_{ii}^{V,\mathrm{st}} = \frac{\sigma_i^2 \lambda_i}{1 - M\gamma\lambda_i}, \qquad i = 1, \ldots, M,$$

$$\bar{D}_{ij}^{V,\mathrm{st}} = 0, \qquad i \neq j,$$

given by (20), (28), and (39). The classical theory disregards both the variability in phase space of the diffusion coefficients predicted by the modified theory, and the cross-derivative diffusion term $\partial(D_{ij}^X \partial p/\partial X_j)/\partial V_i$; additionally, the limit of $\bar{D}_{ii}^{V,\mathrm{st}}$ for $\lambda \to \infty$ is negative, which is non-physical. As a consequence, the classical LED theory is unable to predict some key dynamic behavior of the system in the intermediate-to-long auto-correlation time scale regime, as is discussed in Section V B.

Unfortunately there is no general solution to (40)–(44) for a general choice of recovery forces S_i, stochastic parameters, and number of equations. Nevertheless, we can derive approximate analytical expressions for some particular cases. In particular, we discuss the overdamped case and general case for $M = 1$ in Sections V A and V B, respectively, and the general case for $M > 1$ in Section V C.

A. Overdamped Kramers equation

For $M = 1$, we can write the net force $F - S(x)$ in (38) as $F - S(x) = -\mathrm{d}U^\mathrm{eff}/\mathrm{d}x$, i.e., as stemming from the effective tilted potential $U^\mathrm{eff}(x) = -Fx + U(x)$, where $U(x)$ is a potential function. For periodic coordinates, we assume $U(x)$ is a periodic metastable potential with a single minimum over the period $[-\pi, \pi)$ at the attractor x^0 (Figure 1).

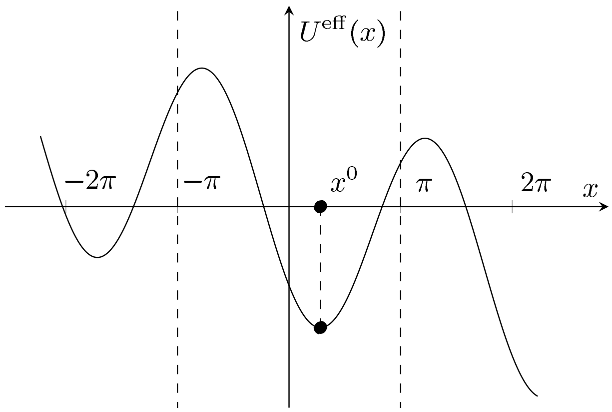


FIG. 1. Example of effective tilted metastable potential $U^{\rm eff}(x)$, with stable equilibrium at $x = x^0$.

In this section we consider the case of the overdamped Kramers equation. Consider a system oscillating around the equilibrium position x^0 due to the stochastic forcing $\Gamma(t)$, and let $v_{\rm s}$ be the natural frequency of oscillations around this equilibrium. If $\gamma \gtrsim v_{\rm s}$, there is a clear separation between the time scales of the dynamics of the position and momentum variables, with the momentum variable relaxing towards its equilibrium value $v = 0$ faster than the position variable. Setting $M = 1$, combining Eqs (37) and (38) as

$$\frac{1}{v_{\rm B}}\frac{{\rm d}^2x}{{\rm d}t^2} + \frac{\gamma}{v_{\rm B}}\frac{{\rm d}x}{{\rm d}t} = F - S(x) + \Gamma(t),$$

and disregarding the acceleration term ${\rm d}^2x/{\rm d}t^2$, we obtain the reduced SDE

$$\frac{\gamma}{v_{\rm B}}\frac{{\rm d}x}{{\rm d}t} = F - \frac{{\rm d}U(x)}{{\rm d}x} + \Gamma(t), \tag{49}$$

where $S = {\rm d}U/{\rm d}x$. The corresponding quasi-Fokker-Planck equation for the PDF $p(X,t)$ reads

$$\frac{\gamma}{v_{\rm B}}\frac{\partial p}{\partial t} + \frac{\partial}{\partial X}\left(F - \frac{{\rm d}U}{{\rm d}x}\right)p + \frac{\partial}{\partial X}\langle\Gamma\Pi'\rangle = 0, \tag{50}$$

where the stochastic flux can be computed by means of (23), namely,

$$\langle\Gamma\Pi'\rangle(X,t) = -\frac{v_{\rm B}}{\gamma}\int_0^t \langle\Gamma(t)\Gamma(s)\rangle\frac{\partial\chi(s|X,t)}{\partial X} \times \frac{\partial}{\partial\chi(s|X,t)}\left[\frac{\partial X}{\partial\chi(s|X,t)}p(X,t)\right]{\rm d}s.$$

We can apply the chain rule to the previous expression in order to obtain the closed LED approximation

$$\langle\Gamma\Pi'\rangle(X,t) = -\frac{v_{\rm B}}{\gamma}\frac{\partial}{\partial X}D(X)p(X,t), \tag{51}$$

$$D(X,t) = \int_0^t \langle\Gamma(t)\Gamma(s)\rangle\frac{\partial X}{\partial\chi(s|X,t)}\,{\rm d}s. \tag{52}$$

Also, employing the LL approximation (33), we have

$$\frac{\partial X}{\partial\chi(s|X,t)} \approx \exp\left(-(t-s)\frac{v_{\rm B}}{\gamma}\frac{{\rm d}^2U}{{\rm d}x^2}\right). \tag{53}$$

Finally, substituting (53) and (39) into (51)–(52), combining the resulting expression with (50), and disregarding transient behavior of the diffusion coefficient, we obtain the approximate PDF equation

$$\frac{\gamma}{v_{\rm B}}\frac{{\rm d}p}{{\rm d}t} + \frac{\partial}{\partial X}\left(F - \frac{{\rm d}U}{{\rm d}x}\right)p = \frac{v_{\rm B}}{\gamma}\frac{\partial}{\partial X}\left[\frac{\lambda\sigma^2}{1+\lambda v_{\rm B}U''(X)/\gamma}\frac{\partial p}{\partial X}\right], \tag{54}$$

where $U''(X)$ denotes ${\rm d}^2U/{\rm d}X^2$. This result was obtained by [10], where the LL approximation was originally proposed for an overdamped oscillator; therefore, it is shown that our generalized LL approximation coincides with the original LL approximation for the particular case of a single nonlinear SDE.

B. Single Kramers equation

For $M = 1$, (37)–(38) read

$$\frac{{\rm d}x}{{\rm d}t} = v_{\rm B}v, \tag{55}$$

$$\frac{{\rm d}v}{{\rm d}t} = F - \frac{{\rm d}U(x)}{{\rm d}x} - \gamma v + \Gamma(t), \tag{56}$$

where $S(x) = {\rm d}U(x)/{\rm d}x$, and $U(x)$ is the potential introduced in Section V A.

For arbitrary values of the relaxation rate γ, the time scale separation argument presented in Section V A is not applicable, and, therefore, we cannot consider the momentum as a fast variable. Nevertheless, a different time scale separation argument appears to be valid. It was noted in [6] that Monte Carlo (MC) simulation experiments show a clear time scale separation between the dynamics of the momentum and position variables for $\gamma\lambda \gtrsim 1$, i.e, when the auto-correlation time scale of the driving force fluctuations is approximately equal or larger than the relaxation time scale. Over the span of the correlation time, for which the noise fluctuation Γ varies slowly, the momentum variable is observed to relax to its stationary value $v = 0$, while the position variable stabilizes towards the root of $F - {\rm d}U(x)/{\rm d}x + \Gamma = 0$. Therefore, we can employ a separation of variables ansatz in order to obtain an approximate analytical solution to the stationary joint distribution.

Setting $M = 1$, (40) reads

$$\frac{\partial p}{\partial t} + v_{\rm B}V\frac{\partial p}{\partial X} + \frac{\partial}{\partial V}\left(F - \frac{{\rm d}U}{{\rm d}x} - \gamma V\right)p = \frac{\partial}{\partial V}\left(D^X\frac{\partial p}{\partial X} + D^V\frac{\partial p}{\partial V}\right), \tag{57}$$

with stationary stochastic diffusion coefficients given by (47)–(48),

$$D^V(X) = \frac{\sigma^2/\gamma}{1 + 1/(\gamma\lambda) + \lambda v_{\mathrm{B}} U''(X)/\gamma}, \tag{58}$$

$$D^X(X) = \lambda v_{\mathrm{B}} D^V(X). \tag{59}$$

The decoupling theory of [8] results in the same expressions for diffusion coefficients, but with $\langle U''(x(t))\rangle$ used instead of $U''(X)$. In [9], $\langle U''(x(t))\rangle$ was computed using white driving noise in order to calculate the diffusion coefficients. On the other hand, the position-dependent diffusion coefficients (58)–(59) proposed here can be directly calculated, because $U''(X)$ is a known function of X.

The joint PDF of the state of the Kramers equation with a tilted metastable potential is characterized by two modes. The main mode corresponds to "locked solutions", or realizations of the stochastic process that oscillate around the the stable equilibrium. The secondary mode corresponds to "running solutions", or realizations that "slide" between equilibrium positions due to the tilting of the effective potential [23].

For the remainder of this section we are interested in deriving an approximation to the quasi-stationary distribution of locked solutions. We can write the joint PDF as $p^{\mathrm{st}}(X, V) = p^X(X)\tilde{p}^V(V|X)$, where $p^X(X)$ denotes the marginal distribution of x, and $\tilde{p}^V(V|X)$ denotes the conditional probability density of v given $x = X$. The mode of locked solutions is characerized by $\langle v(t)\rangle \approx 0$; therefore, we assume that the conditional PDF $\tilde{p}^V$ satisfies

$$-\gamma\frac{\partial}{\partial V} V\tilde{p}^V = D^V(X)\frac{\partial^2}{\partial V^2}\tilde{p}^V, \tag{60}$$

together with the conservation relation

$$\int_{A^V} \tilde{p}^V(V|X)\,\mathrm{d}V = 1. \tag{61}$$

and natural boundary conditions at $V \to \pm\infty$. Note that by construction, the net probability flux of p^{st} along the V direction is zero. Equations (60)–(61) have the solution

$$\tilde{p}^V = (2\pi D^V/\gamma)^{-1/2} \exp\left(-\frac{\gamma V^2}{2D^V}\right), \tag{62}$$

which obeys the property

$$\int_{A^V} V^n \tilde{p}^V\,\mathrm{d}V = 0, \quad n \text{ odd}, \tag{63}$$

Substituting (62) into (57), integrating over V, and recalling the property (63), we obtain the first-order equation for p^X

$$-v_{\mathrm{B}}\sigma^2\frac{\lambda}{\gamma}\frac{\partial}{\partial X}\left[\frac{1 + 1/(\gamma\lambda)}{1 + 1/(\gamma\lambda) + \lambda v_{\mathrm{B}} U''(X)/\gamma} p^X\right] + \left[F - \frac{\mathrm{d}U}{\mathrm{d}x}\right] p^X = f(X), \tag{64}$$

where $f(X)$ is the probability flux in X direction (appearing as an integration constant with respect to V). Given that at the steady-state, the probability flux is divergence-free and the probability flux in V direction is zero, the probability flux $f(X)$ must be constant.

An interesting feature of the proposed analytical approximation is that it shows that the time scale separation argument advanced in this section is essentially equivalent to the time scale separation shown by an overdamped oscillator. This can be seen by taking the limit $\gamma\lambda \to \infty$ in (62) and (64), for which $p^{\mathrm{st}} \to p^X\delta(V)$, and (64) reduces to the stationary form of (54). Therefore, it can be said that a system with a long auto-correlation timescale behaves similarly to an overdamped system.

The well-known periodic solution to (64) over the domain $[-\pi, \pi)$ reads [26]

$$p^X(X) = C\frac{e^{-V(X)}}{D(X)}\int_X^{X+2\pi} e^{V(X')}\,\mathrm{d}X', \tag{65}$$

where

$$V(X) = \int^X \frac{U'(X')}{D(X')}\,\mathrm{d}X', \tag{66}$$

$$D(X) = v_{\mathrm{B}}\sigma^2\frac{\lambda}{\gamma}\frac{1 + 1/(\gamma\lambda)}{1 + 1/(\gamma\lambda) + \lambda v_{\mathrm{B}} U''(X)/\gamma}, \tag{67}$$

and C is a constant chosen such that $\int_{A^X} p^X \mathrm{d}X = 1$. Similarly, for free-space coordinates, the solution to (64) reads

$$p^X(X) = Ce^{-V(X)}/D(X). \tag{68}$$

Having obtained $\tilde{p}^V$ and p^X, the marginal distribution of v can be computed using the relation

$$p^V(V) = \int_{A^X} p^X(X)\tilde{p}^V(V|X)\,\mathrm{d}X. \tag{69}$$

Alternatively to the approximate marginal distributions (65) and (69), one can compute a Gaussian approximation to the solution of (57) if the stationary joint PDF is unimodal. Such an approximation violates the periodic boundary conditions in the case of periodic coordinates. The corresponding approximate marginal distributions read

$$p_{\mathrm{g}}^X(X) = [2\pi s^2]^{-1/2}\exp\left[-\frac{(X - x^0)^2}{2s^2}\right], \tag{70}$$

$$p_{\mathrm{g}}^V(V) = \tilde{p}^V(V, x^0), \tag{71}$$

where $s^2 = D(x_0)/U''(x_0)$, with $D(X)$ given by (67), and x_0 is the system's deterministic equilibrium position.

We validate the analytical approximations (65), (68) and (69) by comparing them with MC estimators of the marginal distributions for two choices of potential functions: the periodic cosine potential

$$U(x) = -d\cos(x), \tag{72}$$

for $x \in [-\pi, \pi)$, and the bistable potential

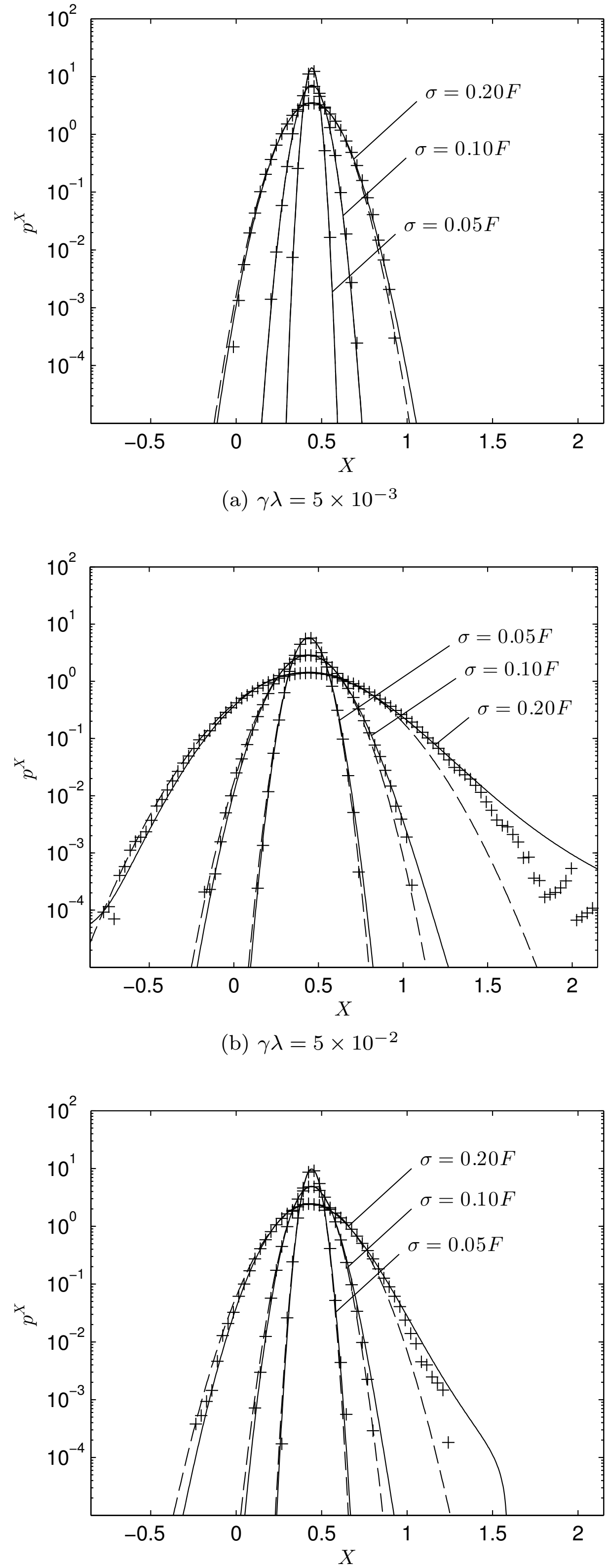
$$U(x) = -\frac{\alpha}{2}x^2 + \frac{\beta}{4}x^4, \tag{73}$$

for $x \in (-\infty, \infty)$. In order to generate the MC samples, the SDEs (55)–(56) are integrated numerically using a second-order strong RK scheme [27], together with an evolution equation for the Ornstein-Uhlenbeck (O-U) process that generates the exponentially-correlated fluctuation Γ. The initial value of the fluctuation is drawn directly from the stationary distribution of the O-U process.

Figures 2 and 3 show the stationary marginal PDFs $p^X(X)$ and $p^V(V)$ for the cosine potential (72), computed using (65) and (69), and the approximate Gaussian marginals (70)–(71), together with MC simulation results. Stationary marginals are estimated for three values of $\gamma\lambda$, 5×10^{-3}, 5×10^{-2} and 5×10^{-1}, and three values of the standard deviation of fluctuations, $\sigma = 0.05F$, $0.10F$ and $0.20F$. A good agreement is observed between the stationary marginals computed via the proposed separation ansatz and MC simulations for all values of $\gamma\lambda$ and σ considered. Figure 3 shows that the proposed separation ansatz captures accurately the marginal distribution of the momentum, including the tails of the distribution. For the marginal distribution of the position, Figure 2 indicates that the separation ansatz is accurate in the vicinity of the stable equilibrium, and that the agreement with MC simulations deteriorates with increasing X (i.e., in the direction of the tilt of the effective potential U^{eff}). Nevertheless, it can be seen that the separation ansatz captures the non-gaussian behavior of the distribution, and that its agreement with MC simulations improves with increasing $\gamma\lambda$.

It is important to note that the proposed modified LED closure captures the widening and then sharpening of the marginal distributions with increasing auto-correlation time. The stochastic resonance of the system's relaxation rate and the noise auto-correlation time scale can be seen at the level of the PDF equation on the stochastic diffusion coefficients (58)– (59), and occurs for $U''(x^0) \neq 0$. On the other hand, this behavior is not captured by the classical LED theory, which highlights its limitations in the regime $\gamma\lambda \gtrsim 1$.

Figure 4 shows the stationary marginal PDF $p^X(X)$ for the bistable potential (73), computed using (68), together with MC simulation results, for $\sigma = 0.2$, 0.5 and 1.0, and three choices of γ and λ. Additionally, we show the marginal PDF computed using the decoupling theory of [8]. Figure 4a shows that for small $\gamma\lambda$, both our approximation and the decoupling theory result in accurate marginal distributions. As $\gamma\lambda$ increases (Figure 4b), both approximations become significantly less accurate, specially for large σ. Nevertheless, our approximation qualitatively retains the bimodal character of the distribution. Increasing $\gamma\lambda$ further (Figure 4c, achieved by increasing γ from 1.0 to 10.0), both approximations regain accuracy, with our approximation being more accurate

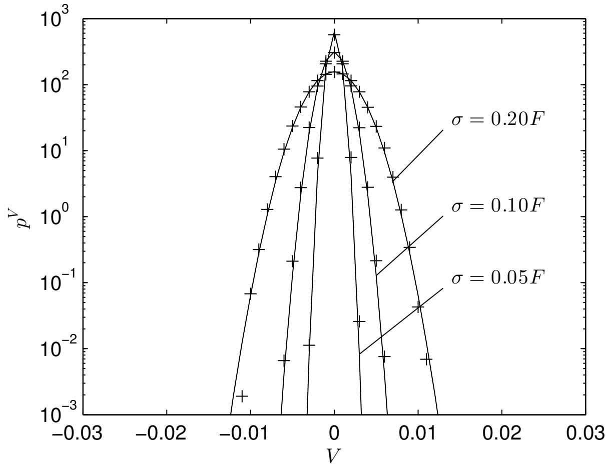


(a) $\gamma\lambda = 5 \times 10^{-3}$

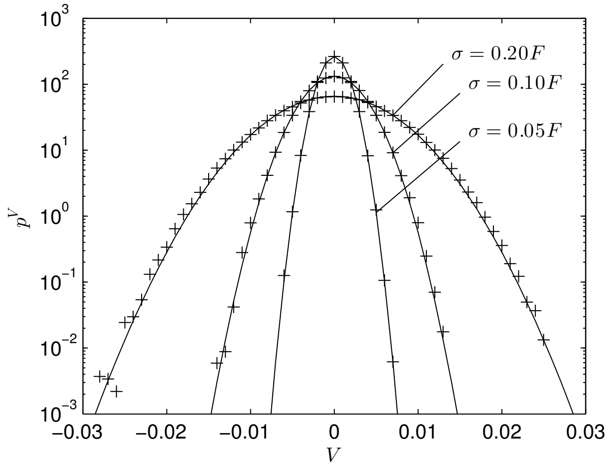
(b) $\gamma\lambda = 5 \times 10^{-2}$

(c) $\gamma\lambda = 5 \times 10^{-1}$

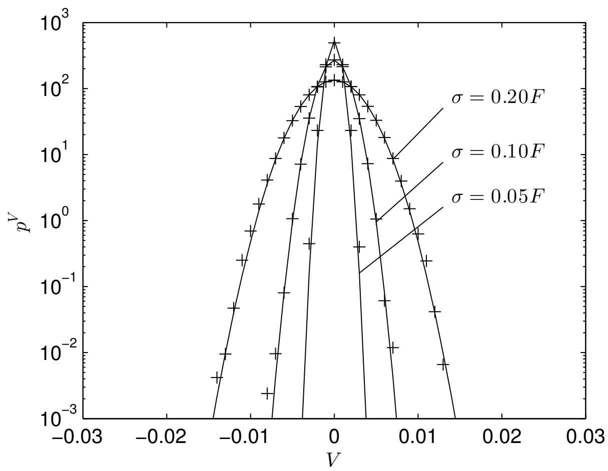
FIG. 2. Stationary marginal distribution of the position variable, $p^X(X)$, for the cosine potential, with $d = 0.21$, $F = 0.09$, $\gamma = 0.5$, $v_{\mathrm{B}} = 120\pi$, and $\sigma = 0.05F$, $0.10F$ and $0.20F$, for various values of $\gamma\lambda$. Continuous lines indicate the analytic approximation (65). Dashed lines indicate the Gaussian approximation to the solution to (70).



(a) $\gamma\lambda = 5 \times 10^{-3}$



(b) $\gamma\lambda = 5 \times 10^{-2}$



(c) $\gamma\lambda = 5 \times 10^{-1}$

FIG. 3. Stationary marginal distribution of the momentum variable, $p^V(V)$, for the cosine potential, with $d = 0.21$, $F = 0.09$, $\gamma = 0.5$, $v_\mathrm{B} = 120\pi$, and $\sigma = 0.05F$, $0.10F$ and $0.20F$, for various values of $\gamma\lambda$. Continuous lines indicate the analytic approximation (69).

than the decoupling theory. This experiment illustrates the limitations of the modified LED theory and our PDF method: it is more accurate for small σ and $\gamma\lambda < 1$ or $\gamma\lambda \gg 1$, and less accurate for large σ, and for $\gamma\lambda \gtrsim 1$.

C. Multiple Kramers equations

In this section we discuss the case $M > 1$, and employ our modified LED theory to approximate the marginal distribution of state variables of an electrical power system governed by coupled Kramers equations.

The separation ansatz presented in the previous section for the case $M = 1$ essentially disregards the cross-correlation between the position and momentum processes. For $M > 1$, the system may exhibit a non-trivial degree of correlation between the various position and momentum coordinates; therefore, it is in general not possible to employ a similar separation ansatz, and we must recur to the full PDF equation (40).

The general solution to (40) is not straightforward and falls outside the scope of this manuscript. Nevertheless, we can evaluate the accuracy of the proposed modified LED closure by computing a Gaussian approximation to the quasi-stationary PDF of locked solutions around a given attractor $(\mathbf{x}^0, 0)$,

$$p^{\mathrm{st}} \propto \exp\left(-\frac{1}{2}\left[(\mathbf{X}-\mathbf{x}^0)^\top \ \ \mathbf{V}^\top\right]\boldsymbol{\Sigma}_S^{-1}\begin{bmatrix}\mathbf{X}-\mathbf{x}^0\\ \mathbf{V}\end{bmatrix}\right) \quad (74)$$

where the cross-covariance matrix $\boldsymbol{\Sigma}_S$ is the symmetric part of the solution $\boldsymbol{\Sigma}$ to the Sylvester equation

$$\mathbf{J}(\mathbf{x}^0)\boldsymbol{\Sigma} + \boldsymbol{\Sigma}\mathbf{J}^\top(\mathbf{x}^0) = -2\begin{bmatrix}\mathbf{0} & \mathbf{0}\\ \mathbf{D}^X(\mathbf{x}^0) & \mathbf{D}^V(\mathbf{x}^0).\end{bmatrix} \quad (75)$$

As an application, we consider an electrical power system consisting of $M+1$ synchronous machine system (Figure 5), driven by renewable mechanical power sources P_i^m, $i = 1, \ldots, M+1$. Such power sources are uncertain and exhibit non-trivial auto-correlation times, and thus are amenable to treatment by means of our theory.

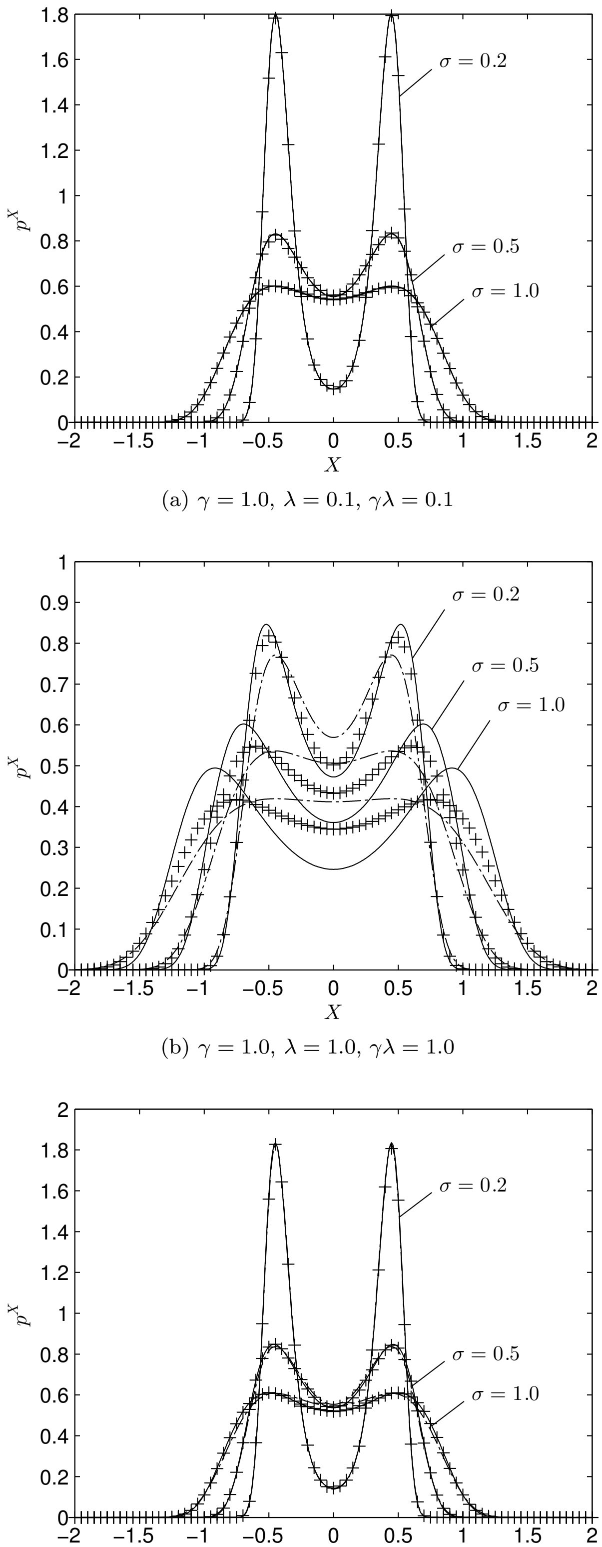
Employing the so-called classical model of synchronous machines [28], such systems can be modeled via a set of $2M$ nonlinear ODEs of the form (37)–(38) , where the position and momentum variables x_i and v_i, $i = 1, \ldots, M$ are the ith generator angular position and velocity with respect to reference machine $i = M+1$ (see Appendix C). The driving mechanical power for the reference machine $i = M+1$ is assumed constant. For machines 1 to M, P_i^m is modeled as stationary stochastic processes with properties

$$P_i^m(t) = \langle P_i^m\rangle(1 + \sigma\Gamma_i), \quad (76)$$

$$\langle\Gamma_i(t)\Gamma_i(s)\rangle = \exp(-|\tau|/\lambda), \quad (77)$$

$$\langle\Gamma_i(t)\Gamma_j(s)\rangle = 0, \quad i \neq j. \quad (78)$$

We approximate the quasi-stationary joint and marginal distributions for the system of Figure 5 ($M =$



(a) $\gamma = 1.0$, $\lambda = 0.1$, $\gamma\lambda = 0.1$

(b) $\gamma = 1.0$, $\lambda = 1.0$, $\gamma\lambda = 1.0$

(c) $\gamma = 10.0$, $\lambda = 1.0$, $\gamma\lambda = 10.0$

FIG. 4. Stationary marginal distribution of the position variable, $p^X(X)$, for the bistable potential, with $F = 0$, $\alpha = 0.2$, $\beta = 1.0$, and $\sigma = 0.2$, 0.5 and 1.0, for various values of γ and λ. Continuous lines indicate the analytic approximation (68), Dash-dotted lines indicate the results of the decoupling theory [8], and crosses denote the results obtained from the MC simulations.

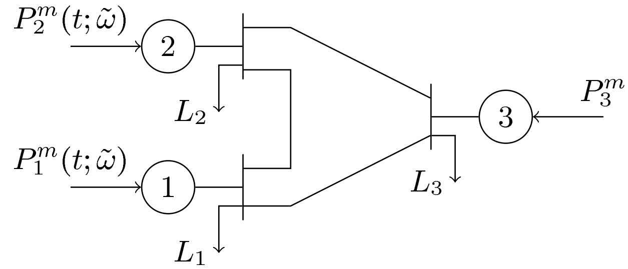


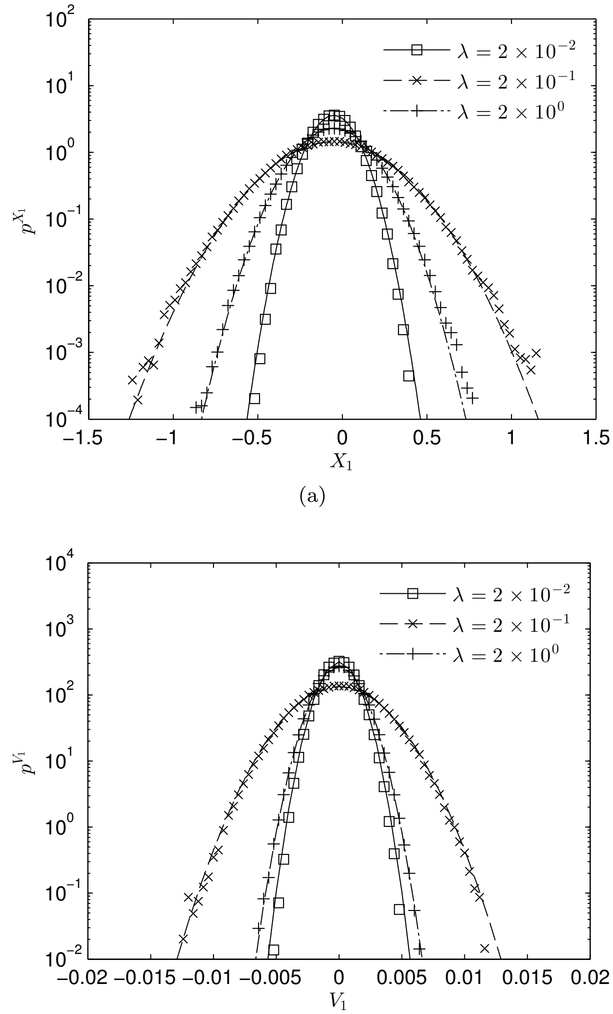
FIG. 5. Schematic for a power system composed of 3 synchronous generators, 3 buses, and 3 loads L_i, $i = 1, 2, 3$. Generators 2 and 3 are driven by stochastic mechanical powers $P_1^m(t;\tilde{\omega})$, $P_2^m(t;\tilde{\omega})$. Generator 3 is driven by the constant mechanical power P_3^m.

2), and parameters given in [29]. Figure 6 shows the marginal distribution for the relative position and velocity variables X_1 and V_1, respectively, for $\sigma = 0.2$, $\gamma = 0.5$, and three values for the auto-correlation time, $\lambda = 2 \times 10^{-2}$, 2×10^{-1} and 2×10^{0}, together with MC simulation results. Good agreement is observed between the approximate solution of the PDF equation and MC simulations for the range of auto-correlation time scales studied, indicating that our modified LED theory captures the dependence of the variance of the stochastic processes on the auto-correlation time scale of the driving colored noise. Additionally, similarly to what was observed in Section V B, the marginal distributions become wider with increasing λ up to a critical value λ^*, and then become sharper with further increase of λ.

Furthermore, the marginal distributions of angular velocity can be employed for evaluating the quality of electric power service in terms of deviations from synchronicity due to mechanical power fluctuations. This can be quantified in terms of the probability of the absolute relative angular velocity exceeding a certain quality threshold v_t. Figure 7 shows the probability $\text{Prob}(|V_1| > v_t)$ as a function of λ, computed using (74), with $v_t = 1 \times 10^{-3}$ (0.1%), and with $\sigma = 5 \times 10^{-2}$, $\sigma = 0.1$ and $\sigma = 0.2$. Again, good agreement is again observed between the analytical results and MC simulations.

VI. CONCLUSIONS

We have presented a PDF method for the analysis of nonlinear dynamic systems driven by colored noise. The method is based on a modified LED closure, and is applicable to systems of an arbitrary number of SDEs characterized by mean-field flow of non-zero divergence, and noise fluctuations of small variance and arbitrarily long correlation time scales. The localization of the modified LED closure takes into account the advective transport of the PDF in the approximate deconvolution of the integro-differential equation governing the dynamics of the PDF. The resulting stochastic flux of the modified LED theory is shown to be equivalent to the second-order cumulant



(a)

(b)

FIG. 6. Stationary marginal distribution of the (a) relative position variable X_1, and (b) relative velocity variable V_1 for the electrical power system of [29], with $\sigma = 0.2$, $\gamma = 0.5$, and $\lambda = 2 \times 10^{-2}$, 2×10^{-1} and 2×10^{0}. Smooth lines indicate the Gaussian approximation (74). Symbols indicate MC simulations.

expansion theory of [7]. Additionally, we have introduced a generalized linear localization (LL) approximation for the evaluation of the diffusion coefficients of the PDF method.

Our method has been applied to the analysis of a set of Kramers equations. We show that the classical LED theory is inaccurate for such systems with $\gamma\lambda \gtrsim 1$; on the other hand, our method successfully captures the stochastic resonance behavior resulting from the interaction between the relaxation time scale of the Kramers system and the auto-correlation time scale of the noise processes.

Given that the LED theory is employed for a variety of applications, the observations made on the properties of the classical LED theory have consequences beyond the study of nonlinear dynamical systems. Future research

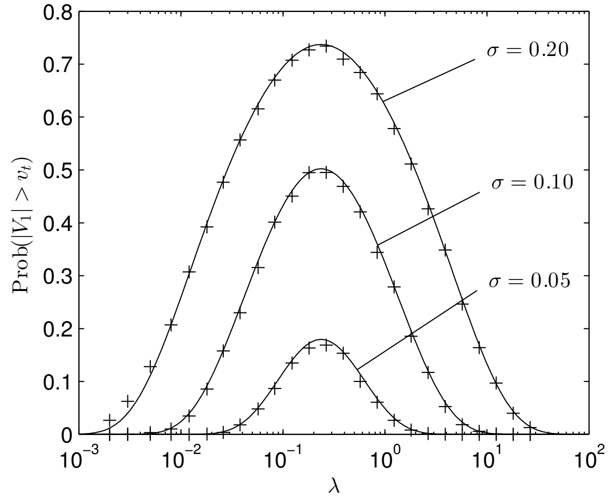


FIG. 7. $\mathrm{Prob}(|V_1| > v_t)$ for the electrical power system of [29] as a function of λ, computed using (74), with $v_t = 1 \times 10^{-3}$, and $\sigma = 0.05$, $\sigma = 0.10$, $\sigma = 0.20$.

will extend our modified LED theory to other applications, such as advection-reaction and advection-diffusion processes for fluctuating advection fields. Our modified LED theory can also be systematically extended by retaining higher orders of $(\sigma\lambda)$ in the equivalent cumulant expansion presented in [7], e.g., as is done in [30] for the deterministic ODE for the mean of linear SDEs.

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Appendix A: Conservation equation for raw PDF

The raw PDF obeys a conservation law with flux $\mathbf{v}\Pi$ [16, 17, 20]. To see this, we differentiate (3) with respect to time, so that we obtain

$$\begin{aligned}\frac{\partial \Pi}{\partial t} &= \frac{\mathrm{d}x_i(t)}{\mathrm{d}t}\delta^{(1)}[x_i(t) - X_i] = -\frac{\mathrm{d}x_i(t)}{\mathrm{d}t}\delta^{(1)}[X_i - x_i(t)] \\ &= -\frac{\mathrm{d}x_i(t)}{\mathrm{d}t}\frac{\partial \Pi}{\partial X_i},\end{aligned}$$

where $\delta^{(1)}$ is the first distributional derivative of the delta function. By virtue of the sifting property of the delta function, we have

$$\Pi(\mathbf{X};t)\frac{\mathrm{d}x_i(t)}{\mathrm{d}t} = \Pi(\mathbf{X};t)v_i(\mathbf{x},t;\tilde{\omega}) = \Pi(\mathbf{X};t)v_i(\mathbf{X},t;\tilde{\omega}),$$

so that we can rewrite the previous equation as

$$\frac{\partial \Pi}{\partial t} + \frac{\partial}{\partial X_i}(v_i\Pi) = \frac{\partial \Pi}{\partial t} + \nabla_{\mathbf{X}}\cdot(\mathbf{v}\Pi) = 0, \tag{A1}$$

thus recovering (5).

Appendix B: Derivation of the modified LED closure

Subtracting (7) from (5), we obtain the governing PDE of Π',

$$L\Pi' = -\nabla_{\mathbf{X}} \cdot (\mathbf{v}'\Pi - \langle \mathbf{v}'\Pi' \rangle), \tag{B1}$$

with homogeneous initial conditions, and vanishing conditions for $x_i \to \pm\infty$.

Rewriting the right-hand side of (B1) in terms of s and $\mathbf{Y}$, multiplying by Green's function $G(\mathbf{X}, t|\mathbf{Y}, s)$, integrating over $(0, t)$ and A, and performing integration by parts, we obtain the reciprocity relation

$$\int_0^t \int_A GL\Pi' \,\mathrm{d}\mathbf{Y}\mathrm{d}s = \int_A (G\Pi')|_0^t \,\mathrm{d}\mathbf{Y} + \int_0^t \int_{\partial A} \mathbf{n} \cdot G\langle \mathbf{v} \rangle_0 \Pi' \,\mathrm{d}\mathbf{Y}\mathrm{d}s + \int_0^t \int_A \Pi' \hat{L} G \,\mathrm{d}\mathbf{Y}\mathrm{d}s,$$

where $\hat{L}$ is the adjoint of L,

$$\hat{L} = -\frac{\partial}{\partial t} - \langle \mathbf{v} \rangle_0 \cdot \nabla_{\mathbf{X}}. \tag{B2}$$

We choose $G(\mathbf{X}, t|\mathbf{Y}, s)$ as the solution of the adjoint problem

$$\hat{L}G = \delta(\mathbf{X} - \mathbf{Y})\delta(t - s), \tag{B3}$$

with homogeneous boundary conditions and terminal condition $G(\mathbf{X}, t|\mathbf{Y}, t) = 0$. Replacing above and recalling the initial and boundary conditions of the Π' problem we obtain

$$\Pi'(\mathbf{X}; t) = -\int_0^t \int_A G(\mathbf{X}, t|\mathbf{Y}, s) \nabla_{\mathbf{Y}} \cdot [\mathbf{v}'(\mathbf{Y}, s)\Pi(\mathbf{Y}; s) - \langle \mathbf{v}'(\mathbf{Y}, s)\Pi'(\mathbf{Y}, s) \rangle] \,\mathrm{d}\mathbf{Y}\mathrm{d}s, \tag{B4}$$

Multiplying (B4) by $\mathbf{v}'(\mathbf{X}, t)$ and taking the ensemble average, we recover (10). Employing the first approximation of the classical LED theory, (11), (10) can be rewritten in terms of the PDF p as

$$\langle \mathbf{v}'(\mathbf{X}, t)\Pi'(\mathbf{X}; t) \rangle = -\int_0^t \int_A G(\mathbf{X}, t|\mathbf{Y}, s) \times \nabla_{\mathrm{Y}} \cdot [\langle \mathbf{v}'(\mathbf{X}, t)\mathbf{v}'(\mathbf{Y}, s) \rangle p(\mathbf{Y}; s)] \,\mathrm{d}\mathbf{Y}\mathrm{d}s. \tag{B5}$$

We can solve for G via the method of characteristics. The characteristics solve the initial value problem

$$\frac{\mathrm{d}}{\mathrm{d}s'} \boldsymbol{\chi}(s'|\mathbf{Y}, s) = \langle \mathbf{v}(\boldsymbol{\chi}(s'|\mathbf{Y}, s), s') \rangle_0, \quad s' \in [s, t], \tag{B6}$$

$$\boldsymbol{\chi}(s|\mathbf{Y}, s) = \mathbf{Y}. \tag{B7}$$

Along characteristics the problem for G is reduced to the terminal value problem

$$\frac{\mathrm{d}}{\mathrm{d}s'} G(\mathbf{X}, t|\boldsymbol{\chi}(s'|\mathbf{Y}, s), s') = -\delta(t - s')\delta(\mathbf{X} - \boldsymbol{\chi}(s'|\mathbf{Y}, s)),$$
$$G(\mathbf{X}, t|\boldsymbol{\chi}(t|\mathbf{Y}, s), t) = 0.$$

Integrating from s to t and recalling the terminal condition, we obtain

$$\begin{aligned} G(\mathbf{X}, t|\mathbf{Y}, s) &= \int_s^t \delta(t - s')\delta(\mathbf{X} - \boldsymbol{\chi}(s'|\mathbf{Y}, s), s') \,\mathrm{d}s' \\ &= \mathcal{H}(t - s)\delta(\mathbf{X} - \boldsymbol{\chi}(t|\mathbf{Y}, s)). \end{aligned} \tag{B8}$$

This result allows us to evaluate integrals over A of G times functions of $\mathbf{Y}$ as follows:

$$\begin{aligned} &\int_A G(\mathbf{X}, t|\mathbf{Y}, s) f(\mathbf{Y}) \,\mathrm{d}\mathbf{Y} \\ &\quad = \mathcal{H}(t - s) \int_A \delta(\mathbf{X} - \boldsymbol{\chi}(t|\mathbf{Y}, s)) f(\mathbf{Y}) \,\mathrm{d}\mathbf{Y} \\ &= \mathcal{H}(t - s) \int_{A'} \mathcal{J}^{-1}(t|\mathbf{Y}, s)\delta(\mathbf{X} - \boldsymbol{\chi}(t|\mathbf{Y}, s)) f(\mathbf{Y}) \,\mathrm{d}\boldsymbol{\chi} \\ &= \begin{cases} \mathcal{H}(t - s)\mathcal{J}(s|\mathbf{X}, t) f(\boldsymbol{\chi}(s|\mathbf{X}, t)) & \text{if } \mathbf{X} \in A', \\ 0 & \text{if } \mathbf{X} \notin A', \end{cases} \end{aligned} \tag{B9}$$

where A' is the image at time t of A at time s, and $\mathcal{J}(s|\mathbf{X}, t)$ is given by (15). Given our choice of support for the stochastic variables, A and A' are equivalent, and thus $\mathbf{X} \in A'$ for any choice of $\mathbf{X}$. Finally, employing (B9) on (B5) we obtain (12).

Appendix C: Equations of the classical model for synchronous machines

Consider a system composed of $M + 1$ synchronous machines. Let $\tilde{x}_i$ and $\tilde{v}_i$ be the angular position and (dimensionless) velocity of the ith machine with respect to a synchronous reference frame. The classical model governing equations for $\tilde{x}_i$ and $\tilde{v}_i$ read

$$\frac{\mathrm{d}\tilde{x}_i}{\mathrm{d}t} = v_{\mathrm{B}} \tilde{v}_i, \tag{C1}$$

$$2H_i \frac{\mathrm{d}\tilde{v}_i}{\mathrm{d}t} = P_i^m - P_i^e - D_i \tilde{v}_i, \tag{C2}$$

for $i = 1, \ldots, M + 1$, where $H_i > 0$, P_i^m, P_i^e, $D_i > 0$ are the ith generator's inertia constant, driving mechanical power, electrical power, and damping constant, respectively, and v_{B} is the velocity scale.

The electrical power P_i^e is a function of the angular positions relative to one another, given by the classical model as

$$P_i^e - E_i^2 G_{ii} = \sum_{\substack{j=1 \\ j \neq i}}^{M+1} \left[D_{ij} \cos(\tilde{x}_i - \tilde{x}_j) + C_{ij} \sin(\tilde{x}_i - \tilde{x}_j) \right], \tag{C3}$$

together with the relations

$$C_{ij} = E_i E_j B_{ij}, \quad D_{ij} = E_i E_j G_{ij},$$

(no index summation implied), where E_i is the ith generator internal voltage, and $\mathbf{G} = \{G_{ij}\}$ and $\mathbf{B} = \{B_{ij}\}$ are the $M+1 \times M+1$ so-called system reduced conductance and susceptance matrices, respectively.

For simplicity, we restrict our attention to the case $D_1/2H_1 = \ldots D_{M+1}/2H_{M+1} = \gamma$. For this case, we can eliminate the equations for the $(M+1)$th machine by dividing (C2) by $2H_i$ and subtracting (C1)–(C2) for $i = M+1$ from (C1)–(C2) for $i = 1, \ldots, M$, obtaining the reduced system of equations

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = v_{\mathrm{B}} v_i, \tag{C4}$$

$$\frac{\mathrm{d}v_i}{\mathrm{d}t} = F_i - S_i - \gamma v_i, \tag{C5}$$

$$F_i = \frac{P_i^m}{2H_i} - \frac{P_{M+1}^m}{2H_{M+1}}, \tag{C6}$$

$$S_i = \frac{P_i^e}{2H_i} - \frac{P_{M+1}^e}{2H_{M+1}}, \tag{C7}$$

for $i = 1, \ldots, M$, thus recovering a system of the form (37)–(38), where $x_i = \tilde{x}_i - \tilde{x}_{M+1}$ and $v_i = \tilde{v}_i - \tilde{v}_{M+1}$ are the angular position and velocity of the ith machine with respect to the $M+1$th machine. Note that the electrical power P_i^e given by (C3) can be written in terms of the relative angular positions x_i, $i = 1, \ldots, M$.

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