Sensitivity analysis of colored-noise-driven interacting particle systems

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We propose an efficient sensitivity analysis method for a wide class of colored-noise-driven interacting particle systems (IPSs). Our method is based on unperturbed simulations and significantly extends the Malliavin weight sampling method proposed by Szamel [Europhys. Lett. **117**, 50010 (2017)] for evaluating sensitivities such as linear response functions of IPSs driven by simple Ornstein-Uhlenbeck processes. We show that the sensitivity index depends not only on two effective parameters that characterize the variance and correlation time of the noise, but also on the noise spectrum. In the case of a single particle in a harmonic potential, we obtain exact analytical formulas for two types of linear response functions. By applying our method to a system of many particles interacting via a repulsive screened Coulomb potential, we compute the mobility and effective temperature of the system. Our results show that the system dynamics depend, in a nontrivial way, on the noise spectrum.

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I. INTRODUCTION

Sensitivity analysis methods were initially developed for stochastic processes used in financial engineering, specifically in dealing with price sensitivities of financial products often referred to as "Greeks" (see, for instance, [1, Chapter 7] and [2]). Over the last decade, applications of these methods have emerged in the physics literature for nonequilibrium systems. They address the sensitivities of complex, white, and colored-noise-driven systems (e.g., active matter) with respect to certain types of perturbations [3–5]. In this area, a fundamental problem is to characterize the sensitivity of complex systems to perturbations by an external force from their steady state. Understanding the changes of a physical system in response to an internal or external perturbation can give crucial insights into the underlying physics, as evidenced by [5–10]. Our goal is to show that it is possible to answer these questions from unperturbed simulations even when the system and the driving noise are complex. It should also be pointed out that sensitivity indices, such as linear response functions for equilibrium systems, can be obtained from the fluctuation-dissipation relations (FDRs) and correlation functions evolving with unperturbed dynamics [11,12]. We further mention that techniques that allow one to calculate the sensitivity indices with simulations of the unperturbed system have been proposed [13–15] in a different context, that of Ising spin systems (discrete in space or time).

A. Review of fundamental work

A considerable leap forward in this direction of research has been made with the work of Warren and Allen [4]. They introduce a simple computational approach for responses to infinitesimal changes in internal or external parameters in stochastic Brownian dynamics simulations, which may be in or out of equilibrium. The method is closely related to the methods developed for the "Greeks," particularly those related to likelihood ratios and Malliavin calculus. Indeed, the method does not require simulating the perturbed system, but in addition to simulating the unperturbed system, it requires following extra stochastic variables. The latter corresponds to the derivatives of the probability density with respect to the parameter of interest. Warren and Allen have coined the term "Malliavin weight" for these variables. They consider a cluster of N particles, each in $\mathbb{R}^d$, $x_\lambda = (x_{1,\lambda}, \dots, x_{N,\lambda})$ satisfying

$$\dot{x}_\lambda = \frac{D}{k_B T_{\rm eff}^{\rm sp}} F_\lambda(x_\lambda) + \sqrt{2D}\dot{w}, \tag{1}$$

where $\dot{w}$ is an n-dimensional Gaussian white noise (time derivative of a n-dimensional Wiener process w), $n = Nd$, $D > 0$ is the diffusion coefficient (assumed to be the same for all particles), k_B is the Boltzmann constant, and $T_{\rm eff}^{\rm sp}$ is the single-particle effective temperature. Here λ is a scalar (real) parameter of interest for sensitivity analysis, and the function $F_\lambda = (F_{1,\lambda}, \dots, F_{N,\lambda})$ specifies the external forces. The Malliavin weight is the real-valued random process q_λ given by

$$\forall t \geqslant 0, \;\; q_\lambda(t) = \frac{\sqrt{D}}{\sqrt{2}k_B T_{\rm eff}^{\rm sp}} \int_0^t \frac{\partial F_\lambda}{\partial \lambda}[x_\lambda(s)] \cdot {\rm d}w(s). \tag{2}$$

The notation $\cdot$ is the inner product in $\mathbb{R}^n$, and the equation should be understood as an Itô's stochastic integral. Warren and Allen have shown that for any test function $\Phi : \mathbb{R}^n \to \mathbb{R}$:

$$\forall t \geqslant 0, \;\; \frac{\rm d}{{\rm d}\lambda} \langle \Phi[x_\lambda(t)] \rangle_\lambda |_{\lambda=0} = \langle \Phi[x_0(t)] q_0(t) \rangle. \tag{3}$$

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They have applied their method to a nonequilibrium-driven steady state formed by a cluster of particles in a two-dimensional harmonic trap under shear. Here $\langle \cdots \rangle_\lambda$ denotes averaging for the system prepared at $t = 0$ in the steady state corresponding to the force F_0 and then evolving for $t > 0$ under the influence of the modified force F_λ. The notation $\langle \cdots \rangle$ is for the unperturbed steady state average $\langle \cdots \rangle_0$. Equation (3) shows that the estimation of the sensitivity index can be carried out with trajectories of the unperturbed dynamics (1) at $\lambda = 0$, only, together with the Malliavin weight (2) at $\lambda = 0$. Warren and Allen's technique has been employed in [5] to test analytical predictions with new Green-Kubo-like expressions for the diffusivity and mobility with unperturbed simulations. It has also been used in [16] to complete an experimental study on the effective temperature via the violation of FDRs for a system of active Brownian particles (ABP) with inertia. The authors have investigated theoretically and numerically the linear response and effective temperature for a single particle. It should be noted that beyond the scope of sensitivity analysis, significant applications of (3) have been proposed for optimizing the steady state of a self-assembling colloid [6]. This formula makes it possible to obtain an explicit formula for gradients used in the optimization procedure, thus avoiding errors in approximations such as with finite differences [17].

Another success in this line of research is a nontrivial generalization of the Malliavin Weight Sampling (MWS) method as proposed by Szamel [3]. He introduced a method for calculating sensitivities of statistics for nonequilibrium systems expressed as colored noise-driven systems. In particular, he studied the evolution of a cluster of particles under the influence of self-propulsion represented by a colored noise. The components of the particles are driven by independent, identically distributed stationary Gaussian noises with a correlation time $\tau_p > 0$. The driving process f (taking values in $\mathbb{R}^n$, $n = Nd$) is of the form

$$\tau_p \mathrm{d}f = -f \mathrm{d}t + \sigma \mathrm{d}w, \tag{4}$$

where w is a n-dimensional Wiener process and $\sigma > 0$ is the noise strength. More precisely, $\sigma = \sqrt{2\xi_0 T_{\mathrm{eff}}^{\mathrm{sp}}} = \xi_0\sqrt{2D_0}$ where ξ_0 is the viscous friction coefficient and $D_0 = T_{\mathrm{eff}}^{\mathrm{sp}}\xi_0^{-1}$. The resulting state variable describing the cluster of particles x (taking values in $\mathbb{R}^n$) satisfies

$$\dot{x} = \xi_0^{-1}[F(x) + f]. \tag{5}$$

Since Szamel is interested in sensitivities (under steady state) in response to drift perturbations, he replaces F by $F_\lambda = F + \lambda\hat{F}$ for some function $\hat{F}$ and he studies the derivative with respect to λ at $\lambda = 0$ of some moments. With F_λ, the state variable is denoted by $x_\lambda^{\tau_p}$. The sensitivity of its statistics can be computed using the following formula valid for any test function $\Phi : \mathbb{R}^n \to \mathbb{R}$:

$$\begin{aligned}\forall t \geqslant 0,\ & \frac{\mathrm{d}}{\mathrm{d}\lambda}\big\langle \Phi\big[x_\lambda^{\tau_p}(t)\big]\big\rangle_\lambda|_{\lambda=0} \\ &= \big\langle \Phi\big[x_0^{\tau_p}(t)\big]\big[q_0^{\tau_p}(t) + p_0^{\tau_p}(t)\big]\big\rangle + \tau_p\big\langle \dot{\Phi}\big[x_0^{\tau_p}(t)\big] q_0^{\tau_p}(t)\big\rangle,\end{aligned} \tag{6}$$

where the auxiliary variables $p_0^{\tau_p}$ and $q_0^{\tau_p}$ are called Malliavin weights and satisfy

$$\begin{aligned} q_0^{\tau_p}(t) &= \frac{1}{\xi_0\sigma}\int_0^t \hat{F}\big[x_0^{\tau_p}(s)\big]\cdot \mathrm{d}w(s), \\ p_0^{\tau_p}(t) &= \frac{\tau_p}{\xi_0^2\sigma}\int_0^t \big[\big(\big\{F\big[x_0^{\tau_p}(s)\big] \\ &\qquad + f(s)\big\}\cdot\nabla_x\big)\hat{F}\big[x_0^{\tau_p}(s)\big]\big]\cdot \mathrm{d}w(s). \end{aligned}$$

Here $\dot{\Phi}[x_0^{\tau_p}(t)]$ means $\mathrm{d}\{\Phi[x_0^{\tau_p}(t)]\}/\mathrm{d}t$. When τ_p vanishes in Szamel's formula (6), the second term and $p_0^{\tau_p}$ vanish as well, leaving a term that is equivalent to Warren and Allen's formula (3). In addition to several examples given by Szamel that we shall examine in this paper, noticeable applications of his method have been given by Maggi *et al.* [18] in which they focused on the dynamics of active particles self-propelled by (4). This system falls within the framework of Szamel, where for each $1 \leqslant i \leqslant N$, $F_i(x) = -\sum_j \nabla_{x_i}\phi(\|x_i - x_j\|)$ and $\|x_i - x_j\|$ is the distance between two particles x_i and x_j. The repulsive interaction potential between two particles is $\phi(r) = \beta r^{-\alpha}$, $\alpha, \beta > 0$. All particles are in $\mathbb{R}^d$ with $d = 2$ or 3. Such an active matter system driven out of thermal equilibrium is a fundamental model for the physics of self-propelled particles (natural or artificial) and has been studied by many authors [7–10].

B. Our contribution: Sensitivity analysis with general spectra

In Sec. III we propose new formulas for the sensitivity indices of complex systems: complex systems such as interacting particle systems (IPSs) modeled by an equation of the form (5), where the driving noise (self-propulsion) f is a stationary Gaussian noise with mean zero and with a general spectrum. Our motivations for extending Szamel's sensitivity analysis [3] to noise with arbitrary spectra arise from the following observations. (1) The Ornstein-Uhlenbeck (OU) process (4) used in [3] has the same regularity whatever the correlation time τ_p, which is the regularity of a standard Wiener process. It is of interest to explore which quantities of interest could be sensitive to the noise regularity. Smoother processes are addressed in this paper. In particular, Matérn processes [19] with regularity parameters larger than 1/2 are addressed. Rougher processes can also be addressed by using Markovian approximations of rough fractional processes by sums of OU processes as in [20]. (2) The OU noise has a spectrum with Lorentzian form and a correlation function with an exponential form whatever the correlation time. It is of interest to explore which quantities of interest could be sensitive to the form of the noise spectrum or correlation function (which is the inverse Fourier transform of the noise spectrum), and not only the correlation time. One natural way to depart from the exponential structure for the correlation function is to consider the product between an exponential and a polynomial (such as Matérn correlation functions) or between an exponential and a periodic function (such as Kanai-Tajimi correlation functions). (3) Experimentally it is possible to generate noise with arbitrary spectrum and regularity for example with optical-tweezers-type techniques [21,22]. It should be pointed out that references on active systems whose driving forces have nonexponential correlation functions are still very few in numbers. However, it is worth mentioning that there are natural physical systems (though far from active systems) whose forces have a non-exponential correlation, for instance, Kanai-Tajimi processes in earthquake dynamics [23], also called harmonic noise as in [24,25], (Chapter 8), that can simply be produced by the response of a white-noise-driven linear oscillator. In addition, we obtain, in each of these cases, formulas generalizing (6). Naturally, in the same spirit as the works of Warren and Allen and Szamel, these formulas allow for the evaluation of sensitivities such as time-dependent linear response functions for active particle systems propelled by persistent (colored) noise from unperturbed simulations. To compare results and to clarify the role of the noise spectrum, we calibrate the parameters of the noise spectra to keep the same amplitude (temperature) and correlation time for the different types of noise. In doing so, we will be able to ascertain whether these parameters are sufficient to determine the sensitivity indices. Furthermore, our formulas agree with Szamel's formulas when the noise takes the form of a simple OU process as in (4). In Sec. IV we consider a single particle in a harmonic potential and obtain exact analytical formula for two types of perturbations (linear response functions). Finally, in Sec. V we apply our method to compute the mobility function and effective temperature of a system of many particles interacting via a repulsive screened Coulomb potential. Our study shows that the sensitivity indices also depend on the noise spectrum, not only on the two effective parameters that characterize the amplitude and correlation time of the noise. Coupled with the general need to accurately capture the physical impacts of perturbations on IPSs driven by colored noise, these findings demonstrate the usefulness and relevance of our sensitivity analysis method.

II. NOISE STRUCTURES

In Sec. II A we give the general form of driving noise for which we propose new representation formulas for the sensitivity indices in Sec. III. In Sec. II B we provide a few explicit examples of noise spectra that turn out to give different sensitivity indices despite having identical variance and correlation time.

A. General formulation

We consider the system for the state variable x driven by the noise $f = Cy$:

$$\dot{x} = \xi_0^{-1}[F(x) + Cy], \tag{7}$$

$$\dot{y} = -Ay + B\dot{w}. \tag{8}$$

This is the unperturbed dynamics. The perturbed dynamics are obtained by replacing F with F_λ. Here

(i) The state variable $x(.)$ takes values in $\mathbb{R}^n$, the driving noise process $y(.)$ takes values in $\mathbb{R}^q$, and the Wiener process $w(.)$ is p-dimensional, $n, q, p \geqslant 1$,

(ii) $F_\lambda = F + \lambda\hat{F}$ for $\lambda \in \mathbb{R}$, where $F, \hat{F}$ are functions from $\mathbb{R}^n$ to $\mathbb{R}^n$,

(iii) A, B, C are matrices: $A \in \mathbb{R}^{q\times q}$, $B \in \mathbb{R}^{q\times p}$, $C \in \mathbb{R}^{n\times q}$.

The matrices A, B, C and the function $\hat{F}$ are assumed to satisfy the following hypotheses:

(i) All eigenvalues of A have positive real parts (equivalently, $-A$ is a stable matrix).

(ii) The matrix BB^T is nonsingular, or BB^T is singular but A, B, and C have the Brunowski form [26]: There exist integers $n', q' \geqslant 1$, matrices $A_k \in \mathbb{R}^{q'\times q'}$ for $k = 1, \dots, n'$, a matrix $\bar{B} \in \mathbb{R}^{q'\times p}$, and a matrix $\bar{C} \in \mathbb{R}^{n\times q'}$, such that $q = n'q'$,

$$A = \begin{pmatrix} O_{q'} & -I_{q'} & O_{q'} & \cdots & O_{q'} \\ O_{q'} & O_{q'} & -I_{q'} & \cdots & O_{q'} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ O_{q'} & O_{q'} & O_{q'} & \cdots & -I_{q'} \\ A_1 & A_2 & A_3 & \cdots & A_{n'} \end{pmatrix}, \quad B = \begin{pmatrix} O_{q'\times p} \\ O_{q'\times p} \\ \vdots \\ O_{q'\times p} \\ \bar{B} \end{pmatrix},$$
$$C = \begin{pmatrix} \bar{C} & O_{n\times q'} & \cdots & O_{n\times q'} \end{pmatrix}, \tag{9}$$

and $\bar{B}\bar{B}^T \in \mathbb{R}^{q'\times q'}$ is nonsingular (here $O_{p\times q}$ denotes the null matrix of size $p \times q$, $O_p = O_{p\times p}$, and I_p is the identity matrix of size p).

(iii) $\hat{F} \in \mathrm{Im(C)}$, more exactly, there exists a function E from $\mathbb{R}^n$ to $\mathbb{R}^q$ such that $\hat{F} = CE$ when BB^T is nonsingular, or there exists a function $\bar{E}$ from $\mathbb{R}^n$ to $\mathbb{R}^{q'}$ such that $\hat{F} = \bar{C}\bar{E}$ when A, B, C have the Brunowski form (9) and $\bar{B}\bar{B}^T$ is nonsingular.

The first condition ensures the ergodicity of the driving noise y. The second condition ensures that the stationary distribution has a multivariate Gaussian density [with the asymptotic variance matrix $\int_0^\infty \exp(-As)BB^T \exp[-A^T s]\, ds$], and it is also used to get a simple enough representation formula of the sensitivity index (a more general hypothesis such as the Kalman rank condition that "the augmented matrix $(B\, AB\, A^2B\, \cdots\, A^{q-1}B)$ has rank q" could be considered but it would lead to complicated formulas that go beyond the scope of this paper). The third condition guarantees that the derivative of F_λ with respect to λ belongs to the space explored by the noise. This is an important property that allows us to get an expression for a sensitivity index with respect to λ in terms of an expectation that involves only the unperturbed trajectory at $\lambda = 0$ and a Malliavin weight. The model above is versatile, as it covers the case of one one-dimensional particle and the case of many multidimensional particles, as we will see below.

In the next subsection, we present examples of colored noise with general spectra that satisfy the above assumptions: the Gaussian processes with n independent and identically distributed (i.i.d.) components with power spectral density (11) are known as Kanai-Tajimi processes and belong to the first case (BB^T is nonsingular) while the Gaussian processes with n i.i.d. components with power spectral density (14) are known as Matérn processes and belong to the second case (BB^T is singular but A, B, C have the Brunowski form). The first case corresponds to noise with the same regularity as Wiener process (Brownian motion) and the second case corresponds to noise with more regularity.

B. Particular colored-noise-structures and spectra

For a n-dimensional OU process f defined by (4), the correlation function of each component is

$$c_{\rm ou}(t) = \frac{\xi_0 T_{\rm eff}^{\rm sp}}{\tau_p} \exp\left(-\frac{|t|}{\tau_p}\right),$$

and the corresponding power spectral density (PSD) is

$$\hat{c}_{\rm ou}(\omega) \triangleq \int_{-\infty}^{\infty} e^{-i\omega t} c_{\rm ou}(t) {\rm d}t = \frac{2\xi_0 T_{\rm eff}^{\rm sp}}{1+\omega^2\tau_p^2}. \tag{10}$$

The OU process f defined by (4) belongs to the first case described in Sec. II A (BB^T is nonsingular) because (4) reads as (8) with $A = \tau_p^{-1} I_n$, $B = \sigma\tau_p^{-1} I_n$, and $C = I_n$.

We want to consider more general situations in which f is an n-dimensional process whose components are i.i.d. and belong to a class of zero-mean stationary Gaussian processes (SGP) with a PSD which we denote $\hat{c}(\omega)$. We want to compare situations with the same effective temperature $T_{\rm eff}^{\rm sp}$, which is given in terms of the PSD by

$$2\xi_0 T_{\rm eff}^{\rm sp} = \hat{c}(0) = \int_{-\infty}^{\infty} c(t)\, {\rm d}t.$$

For white noise forces $f = f_{\rm wn}$, a comparable situation is $f_{\rm wn} = \sqrt{2\xi_0 T_{\rm eff}^{\rm sp}}\,\dot{w}$ (where $\dot{w}$ is an n-dimensional white noise) so that $\hat{c}_{\rm wn}(\omega) = 2\xi_0 T_{\rm eff}^{\rm sp}$, but here the correlation time is 0. When dealing with persistent/colored noise with PSD $\hat{c}(\omega)$, in addition to having the same $T_{\rm eff}^{\rm sp}$, we want to compare situations with the same correlation time τ_c. We propose to define it as the root-mean-square (rms) width of the correlation function through the relation

$$\tau_c^2 \triangleq -\frac{\hat{c}''(0)}{\hat{c}(0)} = \frac{\int_{-\infty}^{\infty} t^2 c(t) {\rm d}t}{\int_{-\infty}^{\infty} c(t) {\rm d}t}.$$

For an n-dimensional OU process f defined by (4), this gives $\tau_c = \sqrt{2}\tau_p$. We want to check whether the form of the PSD is important or whether the knowledge of $T_{\rm eff}^{\rm sp}$ and τ_c is sufficient to characterize the dynamics and the sensitivity of a system driven by such a colored noise. Although the results on the sensitivity indices will be established for general noise models, in the numerical applications, we will consider two special forms of PSD that we describe now.

(1) First, we will consider a PSD of the form

$$\hat{c}(\omega) \triangleq \frac{1}{2}\sum_{k=1}^{r} \frac{\sigma_k^2}{1+(\omega-\omega_k)^2/\ell_k^2} + \frac{\sigma_k^2}{1+(\omega+\omega_k)^2/\ell_k^2}. \tag{11}$$

Its corresponding correlation function is

$$c(t) = \frac{1}{2}\sum_{k=1}^{r} \sigma_k^2 \ell_k e^{-|t|\ell_k} \cos(\omega_k t).$$

When $r = 1$, we can consider parameters $(\sigma_1, \omega_1, \ell_1)$ satisfying

$$\hat{c}(0) = \frac{\sigma_1^2}{1+\gamma_1^2} = 2\xi_0 T_{\rm eff}^{\rm sp} \quad \text{and} \quad -\frac{\hat{c}''(0)}{\hat{c}(0)} = \frac{p_1\sigma_1^2/\ell_1^2}{2\xi_0 T_{\rm eff}^{\rm sp}} = \tau_c^2,$$

where $p_1 \triangleq 2(1-3\gamma_1^2)/(1+\gamma_1^2)^3$ and $\gamma_1 \triangleq \omega_1/\ell_1$, so that the effective temperature is $T_{\rm eff}^{\rm sp}$ and the correlation time is τ_c. As an example, we will take

$$\sigma_1 \triangleq \frac{\sqrt{5}}{2}\sqrt{2\xi_0 T_{\rm eff}^{\rm sp}}, \quad \ell_1 \triangleq \frac{2\sqrt{2}}{5}\tau_c^{-1}, \quad \omega_1 \triangleq \ell_1/2, \tag{12}$$

and we then have

$$\hat{c}(\omega) = \frac{2\xi_0 T_{\rm eff}^{\rm sp}\left(1+5\omega^2\tau_c^2/2\right)}{1+3\omega^2\tau_c^2+25\omega^4\tau_c^4/4}. \tag{13}$$

The noise with the spectral density (13) is generated by $\{\sigma_1 y_1(t), t \geqslant 0\}$ where $\dot{y}_1(t) = -\ell_1 y_1(t) + \omega_1 y_2(t) + \ell_1 \dot{w}_1(t)$, $\dot{y}_2(t) = -\omega_1 y_1(t) - \ell_1 y_2(t) + \ell_1 \dot{w}_2(t)$ with its steady state as initial condition at $t = 0$.

(2) Second, for $\nu > 0$, we will consider a PSD of the Matérn form [19], (Sec. 4.2.1)

$$\hat{c}(\omega) \triangleq \sigma_\nu^2 \frac{2\pi^{\frac{1}{2}}\Gamma\left(\nu+\frac{1}{2}\right)(2\nu)^\nu}{\Gamma(\nu)\tau_\nu^{2\nu}} \left(\frac{2\nu}{\tau_\nu^2}+\omega^2\right)^{-\nu-\frac{1}{2}}, \tag{14}$$

where we recall the definition of the Gamma function $\Gamma(\mathfrak{z}) \triangleq \int_0^\infty t^{\mathfrak{z}-1}e^{-t}\,{\rm d}t$. Note that with the regularity parameter $\nu = 1/2$ we recover the PSD of an OU process similar to (10). When the regularity parameter ν is larger, we deal with a smoother noise, whose trajectories can be differentiable up to the order $\lfloor \nu \rfloor$. We have $\hat{c}(0) = \sigma_\nu^2\tau_\nu\sqrt{2\pi}\Gamma(\nu+1/2)/[\sqrt{\nu}\Gamma(\nu)]$, $\tau_c^2 = \tau_\nu^2(2\nu+1)/(2\nu)$. Therefore, we have to take

$$\tau_\nu \triangleq \tau_c\sqrt{2\nu/(2\nu+1)}$$
$$\text{and } \sigma_\nu^2 \triangleq \xi_0 T_{\rm eff}^{\rm sp}\sqrt{2\nu+1}\,\Gamma(\nu)/[\Gamma(\nu+1/2)\sqrt{\pi}\tau_c],$$

so that the effective temperature is $T_{\rm eff}^{\rm sp}$ and the correlation time is τ_c. As an example, we will take $\nu = 3/2$, $\sigma_\nu^2 = \xi_0 T_{\rm eff}^{\rm sp}\tau_c^{-1}$, $\tau_\nu = \tau_c\sqrt{3}/2$, and we then have

$$\hat{c}(\omega) = \frac{2\xi_0 T_{\rm eff}^{\rm sp}}{\left(1+\omega^2\tau_c^2/4\right)^2}. \tag{15}$$

The corresponding correlation function is

$$c(t) = \frac{\xi_0 T_{\rm eff}^{\rm sp}}{\tau_c} e^{-\frac{2|t|}{\tau_c}}\left(\frac{2|t|}{\tau_c}+1\right).$$

The noise with the spectral density (15) is generated by $\{\sqrt{2\xi_0 T_{\rm eff}^{\rm sp}}y_1(t), t \geqslant 0\}$ where $\dot{y}_1(t) = 2\tau_c^{-1}y_2(t)$, $\dot{y}_2(t) = -2\tau_c^{-1}[y_1(t)+2y_2(t)] + 2\tau_c^{-1}\dot{w}(t)$ with its steady state as initial condition at $t = 0$.

In Fig. 1 we plot the PSDs (10), (13), and (15) and the corresponding correlation functions. On the one hand, PSDs (13) and (15) decrease faster to 0 than PSD (10), as $|\omega| \to \infty$, with PSD (15) decreasing even faster than PSD (13). On the other hand, the correlation function corresponding to (10) decreases faster than its counterparts for (13) and (15) as $t \to \infty$.

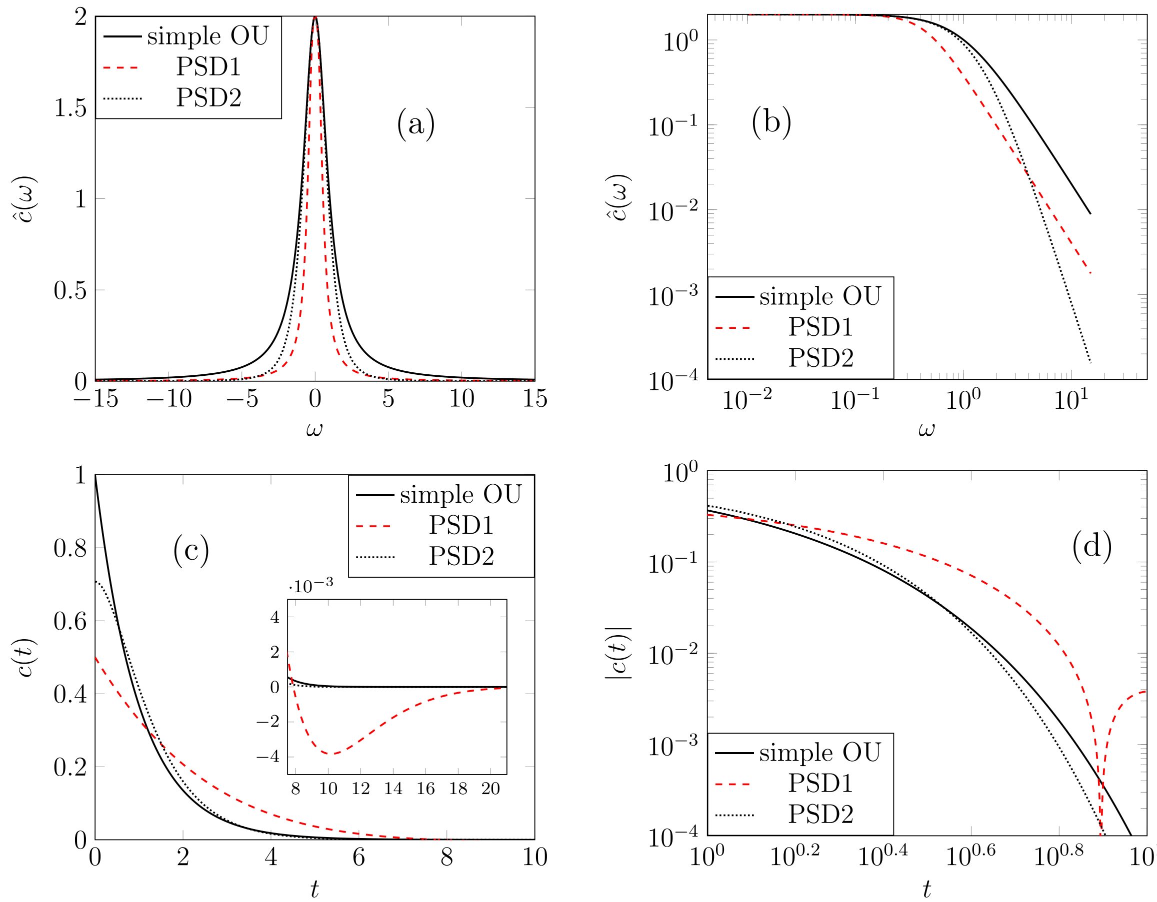

FIG. 1. The solid, dashed, and dotted lines represent, respectively, the PSD (10) of a OU process, PSD1 (13) and PSD2 (15) in all panels. Panels (a) and (b) represent the PSDs for $\omega \in [-15, 15]$ and for $\omega \in [0, 50]$ in loglog scale, respectively. Panels (c) and (d) represent the corresponding correlation functions for $t \in [0, 1]$ and for $t \in [1, 10]$ in loglog scale, respectively [the inset in panel (c) plots the tails of the correlation functions]. Here $\xi_0 = T_{\rm eff}^{\rm sp} = 1$ and $\tau_c = \sqrt{2}$.

The n-dimensional zero-mean SGPs with power spectral density (11) and (14) have the same distribution as the random processes $f \triangleq Cy$ with y taking values in $\mathbb{R}^q$ and solving (8), with $A \in \mathbb{R}^{q\times q}$, $B \in \mathbb{R}^{q\times p}$, $C \in \mathbb{R}^{n\times q}$, and w is a p-dimensional Wiener process. In the particular cases of the PSDs defined by (11) and (14), the matrices A, B, C have the following forms.

(1) Case of PSD defined by (11):

$$A = \oplus_{k=1}^{r}\begin{pmatrix} \ell_k I_n & -\omega_k I_n \\ \omega_k I_n & \ell_k I_n \end{pmatrix}, \quad B = \oplus_{k=1}^{r}\begin{pmatrix} \ell_k I_n & O_n \\ O_n & \ell_k I_n \end{pmatrix},$$
$$C = (\sigma_1 I_n \quad O_n \quad \cdots \quad \sigma_r I_n \quad O_n), \tag{16}$$

where $p = q = rn$.

(2) Case of PSD defined by (14) with $\nu = r - 1/2$ for a positive integer r:

$$A = \ell \begin{pmatrix} O_n & -I_n & O_n & \dots & O_n \\ O_n & O_n & -I_n & \dots & O_n \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ O_n & O_n & O_n & \dots & -I_n \\ \alpha_0 I_n & \alpha_1 I_n & \cdots & \cdots & \alpha_{r-1} I_n \end{pmatrix}, \quad B = \ell \begin{pmatrix} O_n \\ O_n \\ \vdots \\ O_n \\ I_n \end{pmatrix},$$
$$C = \sigma (I_n \quad O_n \quad \cdots \quad O_n), \tag{17}$$

where $p = n$, $q = rn$, $\alpha_k \triangleq \binom{r}{k} = \frac{r!}{k!\,(r-k)!}$,

$$\ell = 2\tau_\nu^{-1}\sqrt{(2\nu+1)/(2\nu)} = 2\tau_c^{-1} \quad \text{and} \quad \sigma^2 = 2\xi_0 T_{\rm eff}^{\rm sp}. \tag{18}$$

III. SENSITIVITY INDICES OF COLORED-NOISE-DRIVEN SYSTEMS

We recall that $\langle\cdots\rangle_\lambda$ denotes averaging for the system prepared at $t = 0$ in the steady state corresponding to the force $F(x)$ and then evolving for $t > 0$ under the influence of the modified force $F_\lambda(x)$.

A. The case where BB^T is nonsingular

If (x, y) satisfies (7) and (8) with a nonsingular matrix BB^T, and $\Phi(.)$ is a continuously differentiable function, then

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\Phi[x(t)]\rangle_\lambda|_{\lambda=0} = \langle\Phi[x(t)][p_{0,0}(t) + p_{1,0}(t)]\rangle + \langle\dot{\Phi}[x(t)]\; p_{1,1}(t)\rangle, \tag{19}$$

where the $p_{j,k}(t)$ evolve according to the following equations of motion

$$\dot{p}_{0,0} = E(x)\cdot A^T(BB^T)^{-1}B\dot{w},$$
$$\dot{p}_{1,0} = \nabla E(x)\xi_0^{-1}[F(x)+Cy]\cdot(BB^T)^{-1}B\dot{w},$$
$$\dot{p}_{1,1} = E(x)\cdot(BB^T)^{-1}B\dot{w}, \tag{20}$$

with initial conditions $p_{j,k}(0)=0$ for each $0\leqslant k\leqslant j\leqslant 1$ (here $\nabla E(x)\in\mathbb{R}^{q\times n}$ for all $x\in\mathbb{R}^n$). Here the notation $\cdot$ is the inner product in $\mathbb{R}^q$. The proof is shown in Appendix A 1. This is the first generalization of Szamel's formula.

B. The case where BB^T is singular but A, B, C have the Brunowski form

If (x, y) satisfies (7) and (8) where A, B, C have the Brunowski form (9), and $\Phi(\cdot)$ is a function continuously differentiable at the order n', then

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\Phi[x(t)]\rangle_\lambda|_{\lambda=0} = \sum_{k=0}^{n'}\left\langle\frac{\mathrm{d}^k\Phi[x(t)]}{\mathrm{d}t^k}\left[\sum_{j=k}^{n'}\binom{j}{k}p_{j,k}(t)\right]\right\rangle. \tag{21}$$

For $j, k\in\mathbb{N}$ such that $0\leqslant k\leqslant j\leqslant n'$, the function $p_{j,k}(t)$ evolves according to the following equation of motion:

$$\dot{p}_{j,k}(t) = \frac{\mathrm{d}^{(j-k)}\bar{E}[x(t)]}{\mathrm{d}t^{(j-k)}}\cdot(A_{j+1})^T(\bar{B}\bar{B}^T)^{-1}\bar{B}\dot{w}(t), \tag{22}$$

with initial condition $p_{j,k}(0)=0$ and with $A_{n'+1} := I_{q'}$. Here the notation $\cdot$ is the inner product in $\mathbb{R}^{q'}$, and $\binom{j}{k}$ is for $\frac{j!}{k!(j-k)!}$. The proof is given in Appendix A 2. This is the second generalization of Szamel's formula.

Remark 1. Suppose we have matrices of the form ℓA and ℓB, then the functions $p_{j,k}(t)$ become

$$\dot{p}_{j,k}(t) = \frac{\mathrm{d}^{(j-k)}\bar{E}[x(t)]}{\mathrm{d}t^{(j-k)}}\cdot\frac{1}{\ell^j}(A_{j+1})^T(\bar{B}\bar{B}^T)^{-1}\bar{B}\dot{w}(t),$$
$$\text{for}\quad 0\leqslant j\leqslant n'. \tag{23}$$

Remark 2. The first formula (19) covers a noise structure for Cy that is appropriate to describe the PSD (10) or (11), for instance. In general, when BB^T is nonsingular, then the sample paths of Cy have the same regularity as the Brownian paths. The second formula (21) covers a noise structure for Cy that is appropriate to describe the PSD (14), for instance. In general, when A, B, C have the Brunowski form and $\bar{B}\bar{B}^T$ is nonsingular, then the sample paths of Cy are smooth. Indeed, this is equivalent to considering a time-dependent $\mathbb{R}^{q'}$-valued variable $z(t)$ that satisfies

$$z^{(n')} = -\sum_{j=0}^{n'-1}A_{j+1}z^{(j)} + \bar{B}\dot{w},$$

where the notation $(.)^{(j)}$ represents the derivative at the order j with respect to time and $Cy=\bar{C}z$.

IV. EXPLICIT SENSITIVITY FORMULAS FOR A PARTICLE IN A HARMONIC POTENTIAL

In this section, we consider examples in a similar configuration to that of Szamel in [3]. The correlation time is $\tau_c = \sqrt{2}\tau_p$, and τ_p will take the same range of values given in [3]. We consider the case of a single one-dimensional particle in a harmonic potential. The real-valued state variable x satisfies

$$\dot{x} = \xi_0^{-1}(-kx+f), \tag{24}$$

where $k>0$ and f is a real-valued Gaussian process with PSD (13) or (15). We recall that when f corresponds to (13), then $f=Cy$ and (x, y) satisfies (7) and (8) with $F(x)=-kx$ and parameters from (16) as follows: $n=r=1$, $p=q=2$,

$$A = \ell_1\begin{pmatrix}1 & -1/2\\ 1/2 & 1\end{pmatrix},\quad B=\ell_1 I_2,\quad C=(\sigma_1\quad 0),$$

with the value of (σ_1, ℓ_1) is given in (12).

Similarly, when f corresponds to (15), (x, y) also satisfies (7) and (8) with $F(x)=-kx$ and parameters from (17) as follows: $n=1$, $r=2$, $p=1$, $q=2$,

$$A = \ell\begin{pmatrix}0 & -1\\ 1 & 2\end{pmatrix},\quad B=\ell\begin{pmatrix}0\\ 1\end{pmatrix},\quad C=(\sigma\quad 0),$$

with the value of (σ, ℓ) is given in (18).

We perturb the system in two different ways:

(I) By a constant force λ_1, i.e., $-kx$ is replaced by $-kx+\lambda_1$ in (24). We can write $-kx+\lambda_1$ as $F(x)+\lambda_1\hat{F}(x)$ where $\hat{F}(x)=1$,

(II) By a force constant λ_2, $-kx$ is replaced by $-kx+\lambda_2 x$ in (24). We can write $-kx+\lambda_2 x$ as $F(x)+\lambda_2\hat{F}(x)$ where $\hat{F}(x)=x$.

Below we derive analytically explicit formulas of the sensitivity indices for this example. The first goal is to show by inspection of these explicit formulas that the sensitivity indices depend on the form of the spectrum of the driving noise. The second goal is to check that empirical averages of the right-hand sides of (19) and (21) by Monte Carlo simulations of the unperturbed dynamics give excellent estimates of the sensitivity indices. For more complex examples (see the next section), the sensitivity indices can be obtained only by Monte Carlo estimation of (19) and (21).

Calculations show that the sensitivity of the first (second) moment of $x(t)$ with respect to the second (first) perturbation under the two types of noise (13) and (15) is zero, i.e., $\frac{\mathrm{d}}{\mathrm{d}\lambda_2}\langle x(t)\rangle_{\lambda_2}=0$ at $\lambda_2=0$ and $\frac{\mathrm{d}}{\mathrm{d}\lambda_1}\langle x(t)^2\rangle_{\lambda_1}=0$ at $\lambda_1=0$. To be precise, the calculations are done as follows: we calculate explicitly the solution of the perturbed system and the quantities of interest $\langle x(t)\rangle_{\lambda_2}$ and $\langle x^2(t)\rangle_{\lambda_1}$, then the differentiation with respect to the perturbation parameter is straightforward. Therefore, below, we focus on the sensitivity of the first (second) moment of $x(t)$ with respect to the first (second) perturbation. We have calculated the explicit formula for the first sensitivity index $\mathrm{d}\langle x(t)\rangle_{\lambda_1}/\mathrm{d}\lambda_1$ at $\lambda_1=0$ in two different ways. The first relies on evaluating the weighted averages that appear on the right-hand side (rhs) of (19) and (21) and summing up. The second, for verification, consists of evaluating the first moment of the perturbed dynamics, then differentiating with respect to the perturbation parameters. The evaluation is done by taking the values of these

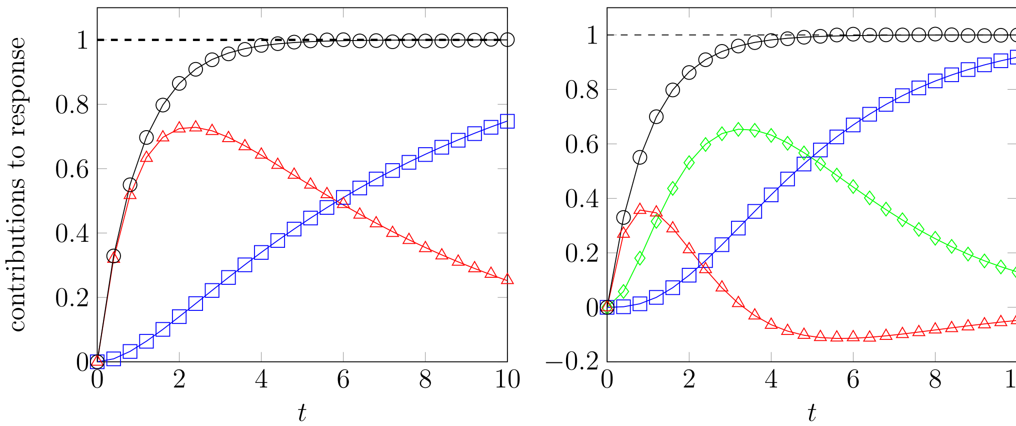

FIG. 2. First sensitivity index in (25) and (26). The solid lines represent the analytical results. The shapes correspond to Monte Carlo simulation results. Left: PSD (13). The blue, red, and black lines correspond to $\langle x(t)p^1_{0,0}(t)\rangle$, $\langle \dot{x}(t)p^1_{1,1}(t)\rangle$, and $\frac{d}{d\lambda_1}\langle x(t)\rangle_{\lambda_1}$ at $\lambda_1 = 0$, respectively. Right: PSD (15). The blue, green, red, and black lines correspond to $\langle x(t)p^2_{0,0}(t)\rangle$, $\langle \dot{x}(t)p^2_{1,1}(t)\rangle$, $\langle \ddot{x}(t)p^2_{2,2}(t)\rangle$, and $\frac{d}{d\lambda_1}\langle x(t)\rangle_{\lambda_1}$ at $\lambda_1 = 0$, respectively.

parameters to 0. Both results agree perfectly of course (see Figs. 2 and 3). We have also estimated the weighted averages with Monte Carlo simulations, and the results follow our analytical predictions. Here, for the two types of noise with PSD (13) and (15), the expression is simple: we get $d\langle x(t)\rangle_{\lambda_1}/d\lambda_1|_{\lambda_1=0} = k^{-1}(1-e^{-k\xi_0^{-1}t})$. Nonetheless, the two decompositions in terms of weighted averages are different. For Eq. (19) that is related to PSD (13), the decomposition is as follows:

$$\frac{d}{d\lambda_1}\langle x(t)\rangle_{\lambda_1}|_{\lambda_1=0} = \langle x(t)p^1_{0,0}(t)\rangle + \langle \dot{x}(t)p^1_{1,1}(t)\rangle, \tag{25}$$

where the Malliavin weights are $p^1_{0,0}(t) = \sigma_1^{-1}w_1(t) + \sigma_1^{-1}\ell_1^{-1}\omega_1 w_2(t)$, and $p^1_{1,1}(t) = \sigma_1^{-1}\ell_1^{-1}w_1(t)$. Note that $p^1_{1,0}(t) = 0$. Then for Eq. (21) that is related to PSD (15) the decomposition is as follows:

$$\frac{d}{d\lambda_1}\langle x(t)\rangle_{\lambda_1}|_{\lambda_1=0} = \langle x(t)p^2_{00}(t)\rangle + \langle \dot{x}(t)p^2_{11}(t)\rangle + \langle \ddot{x}(t)p^2_{22}(t)\rangle, \tag{26}$$

where the Malliavin weights are $p^2_{0,0}(t) = \sigma^{-1}\alpha_0 w(t)$, $p^2_{1,1}(t) = \sigma^{-1}\ell^{-1}\alpha_1 w(t)$, and $p^2_{2,2}(t) = \sigma^{-1}\ell^{-2}w(t)$. See Appendix A 3 for details on the weighted averages. Similarly, we have also calculated the second sensitivity index $d\langle x(t)^2\rangle_{\lambda_2}/d\lambda_2$ at $\lambda_2 = 0$ in two different ways. The counterpart of (25) is

$$\frac{d}{d\lambda_2}\langle x^2(t)\rangle_{\lambda_2}|_{\lambda_2=0} = \langle x^2(t)p^3_{0,0}(t)\rangle + \langle x^2(t)p^3_{1,0}(t)\rangle + \langle \dot{x^2}(t)p^3_{1,1}(t)\rangle, \tag{27}$$

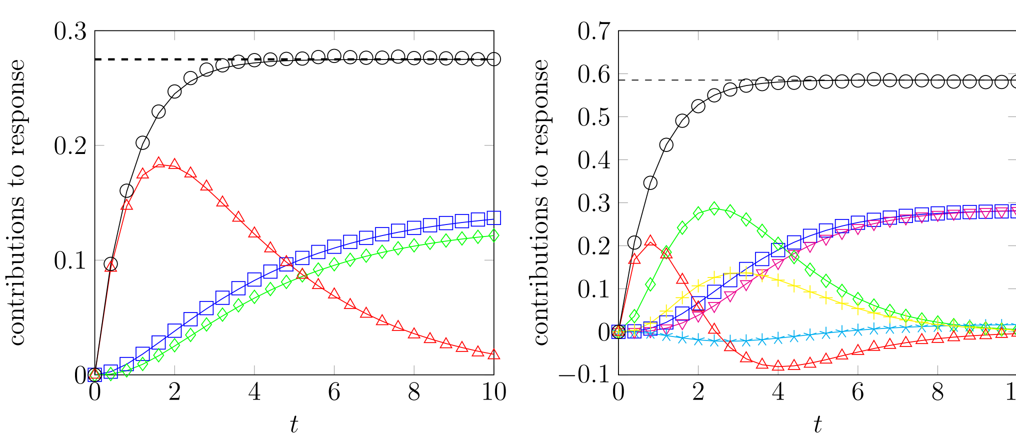

FIG. 3. Second sensitivity index in (27) and (28). The solid lines represent the analytical results. The shapes correspond to Monte Carlo simulation results. Left: PSD (13). The blue, green, red, and black lines correspond to $\langle x^2(t)p^3_{0,0}(t)\rangle$, $\langle x^2(t)p^3_{1,0}(t)\rangle$, $\langle \dot{x^2}(t)p^3_{1,1}(t)\rangle$, and $\frac{d}{d\lambda_2}\langle x^2(t)\rangle_{\lambda_2}$ at $\lambda_2 = 0$, respectively. Right: PSD (15). The blue, magenta, green, cyan, yellow, red, and black lines correspond to $\langle x^2(t)p^4_{0,0}(t)\rangle$, $\langle x^2(t)p^4_{1,0}(t)\rangle$, $\langle \dot{x^2}(t)p^4_{1,1}(t)\rangle$, $\langle x^2(t)p^4_{2,0}(t)\rangle$, $2\langle \dot{x^2}(t)p^4_{2,1}(t)\rangle$, $\langle \ddot{x^2}(t)p^4_{2,2}(t)\rangle$, and $\frac{d}{d\lambda_2}\langle x^2(t)\rangle_{\lambda_2}$ at $\lambda_2 = 0$, respectively.

where

$$p^3_{0,0}(t) = \sigma_1^{-1}\int_0^t x(s)\,\mathrm{d}w_1(s) + \sigma_1^{-1}\ell_1^{-1}\omega_1\int_0^t x(s)\,\mathrm{d}w_2(s),$$

$$p^3_{1,0}(t) = \sigma_1^{-1}\ell_1^{-1}\int_0^t \dot{x}(s)\,\mathrm{d}w_1(s)$$

$$\text{and}\quad p^3_{1,1}(t) = \sigma_1^{-1}\ell_1^{-1}\int_0^t x(s)\,\mathrm{d}w_1(s).$$

The counterpart of (26) is

$$\frac{\mathrm{d}}{\mathrm{d}\lambda_2}\langle x^2(t)\rangle_{\lambda_2}|_{\lambda_2=0} = \langle x^2(t)p^4_{0,0}(t)\rangle + \langle x^2(t)p^4_{1,0}(t)\rangle + \langle x^2(t)p^4_{2,0}(t)\rangle + \langle \dot{x^2}(t)p^4_{1,1}(t)\rangle + 2\langle \dot{x^2}(t)p^4_{2,1}(t)\rangle + \langle \ddot{x^2}(t)p^4_{2,2}(t)\rangle, \tag{28}$$

where

$$p^4_{0,0}(t) = \sigma^{-1}\alpha_0\int_0^t x(s)\,\mathrm{d}w(s),\quad p^4_{1,1}(t) = \sigma^{-1}\alpha_1\ell^{-1}\int_0^t x(s)\,\mathrm{d}w(s),$$

$$p^4_{2,2}(t) = \sigma^{-1}\ell^{-2}\int_0^t x(s)\,\mathrm{d}w(s),\quad p^4_{1,0}(t) = \sigma^{-1}\alpha_1\ell^{-1}\int_0^t \dot{x}(s)\,\mathrm{d}w(s),$$

$$p^4_{2,1}(t) = \sigma^{-1}\ell^{-2}\int_0^t \dot{x}(s)\,\mathrm{d}w(s),\quad \text{and}\ p^4_{2,0}(t) = \sigma^{-1}\ell^{-2}\int_0^t \ddot{x}(s)\,\mathrm{d}w(s).$$

In each case, both analytical results agree. We represent our analytical finding in Fig. 3 including Monte Carlo simulations. See Appendix B 1 for further detail on the implementation of the Monte Carlo simulations. Among the two sensitivity indices above, only the second depends on the correlation time. This is consistent with [3] for the case of a simple OU process. We also obtain the long-time asymptotic. In all cases, for the first sensitivity index, we have

$$\lim_{t\to\infty}\frac{\mathrm{d}\langle x(t)\rangle_{\lambda_1}}{\mathrm{d}\lambda_1}\bigg|_{\lambda_1=0} = \frac{1}{k}.$$

In contrast, the long-time asymptotic of the second sensitivity index depends on the type of noise. For (13),

$$\lim_{t\to\infty}\frac{\mathrm{d}\langle x^2(t)\rangle_{\lambda_2}}{\mathrm{d}\lambda_2}\bigg|_{\lambda_2=0} = \frac{\sigma_1^2}{2k^2\xi_0}\frac{[2k(\xi_0\ell_1)^{-1}+1][k(\xi_0\ell_1)^{-1}+1]^2 + \left(\frac{\omega}{\ell_1}\right)^2}{\left\{[(k(\xi_0\ell_1)^{-1}+1]^2 + \left(\frac{\omega}{\ell_1}\right)^2\right\}^2}.$$

For (15),

$$\lim_{t\to\infty}\frac{\mathrm{d}\langle x^2(t)\rangle_{\lambda_2}}{\mathrm{d}\lambda_2}\bigg|_{\lambda_2=0} = \frac{\sigma^2}{4k^2\xi_0}\frac{k/(\xi_0\ell)+2}{[k/(\xi_0\ell)+1]^2} + \frac{\sigma^2}{4k\xi_0^2\ell}\frac{[k/(\xi_0\ell)+2]^2-1}{[k/(\xi_0\ell)+1]^4}.$$

Such a difference in behavior can also be observed in the steady state/long-time asymptotic variance of the response. For (13),

$$\lim_{t\to\infty}\langle x^2(t)\rangle = \frac{\ell_1\left(\frac{k}{\xi_0}+\ell_1\right)\sigma_1^2}{2k\xi_0\left[\left(\frac{k}{\xi_0}+\ell_1\right)^2+\omega_1^2\right]}.$$

For (15),

$$\lim_{t\to\infty}\langle x^2(t)\rangle = \frac{\sigma^2}{4k\xi_0}\frac{2+k\xi_0^{-1}\ell^{-1}}{\left(1+k\xi_0^{-1}\ell^{-1}\right)^2}.$$

When $\tau_c \to 0$, in the first two equations above both rhs converge towards $T^{\mathrm{sp}}_{\mathrm{eff}}k^{-2}$ and in the last two equations above both rhs converge towards $T^{\mathrm{sp}}_{\mathrm{eff}}k^{-1}$. That is consistent with the long-time asymptotic response of a thermal Brownian particle in a harmonic potential.

V. SENSITIVITY ANALYSIS FOR AN INTERACTING PARTICLE SYSTEM IN A SCREENED COULOMB POTENTIAL

We consider N particles in three dimensions interacting via a repulsive screened Coulomb potential, $\forall r > 0,\ V(r) = A_V\exp[-\kappa(r-\sigma_V)]/r$. We consider a periodic domain which is a cube of length L and we use the same parameters as in [3]: $N = 1372, A_V = 475T^{\mathrm{sp}}_{\mathrm{eff}}\sigma_V$, and $\kappa\sigma_V = 24$, at number density $N\sigma_V^3/L^3 = 0.51$ (see Appendix B 2 for further details). The state variable $x = \{x_{i\alpha}\}_{1\leqslant i\leqslant N,\,1\leqslant\alpha\leqslant 3}$ (stacked in one vector of size $n = 3N$) is $n = 4116$ dimensional and satisfies the equation

$$\dot{x} = \xi_0^{-1}[F(x)+f],$$

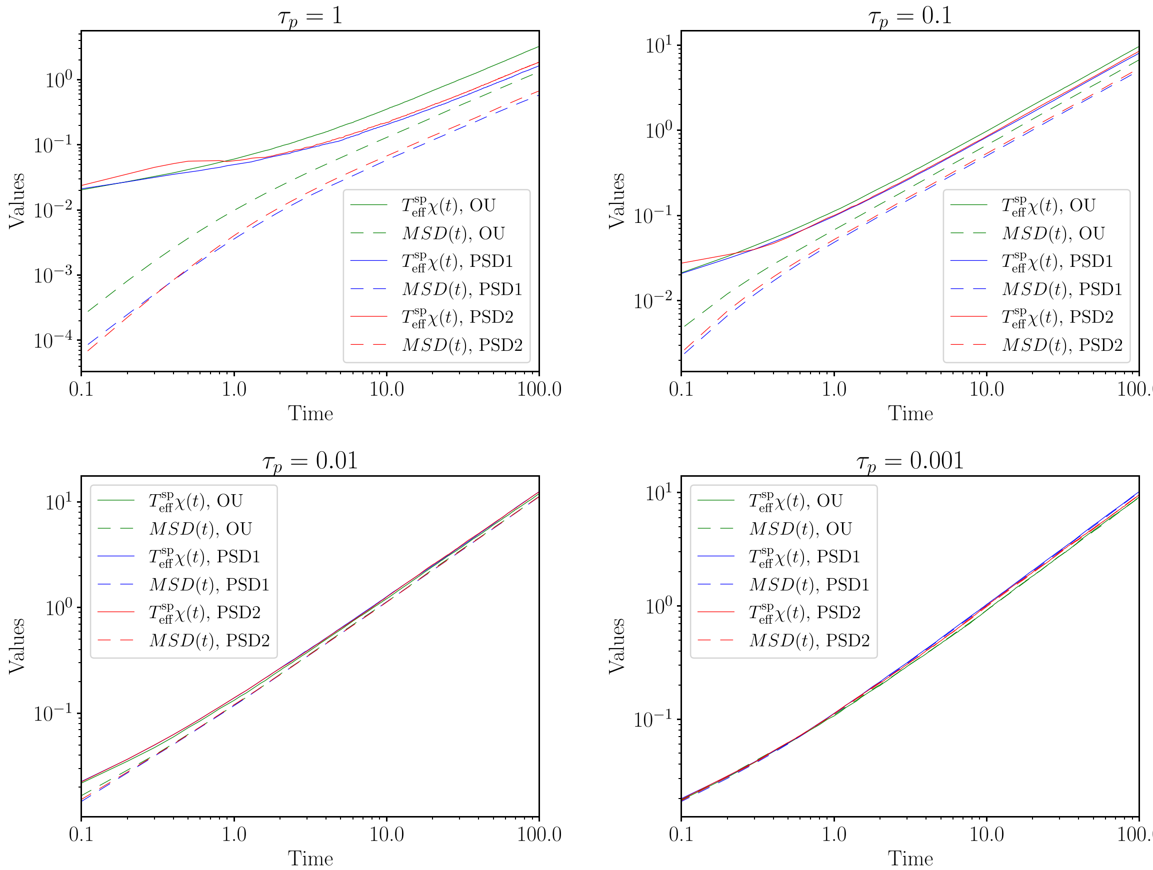

FIG. 4. Mobility function, $T_{\rm eff}^{\rm sp}\chi(t)$, (solid) and mean-square displacement, $MSD(t)$, (dashed) as a function of time, for $\tau_p =$ 1(top left), 0.1(top right), 0.01(bottom left), 0.001(bottom right). Superposition of the results for OU (green), PSD1 (blue), PSD2 (red) with spectra (10), (13), and (15), respectively.

where the unperturbed force for each particle $1 \leqslant i \leqslant N$ can be expressed as

$$F_{i\alpha}(x) = -\partial_{x_{i\alpha}}\left(\sum_{j\neq i} V(\|x_i - x_j\|)\right)$$
$$= -\sum_{j\neq i}(x_{i\alpha} - x_{j\alpha})\frac{V'(\|x_i - x_j\|)}{\|x_i - x_j\|}, \quad \alpha = 1, 2, 3,$$

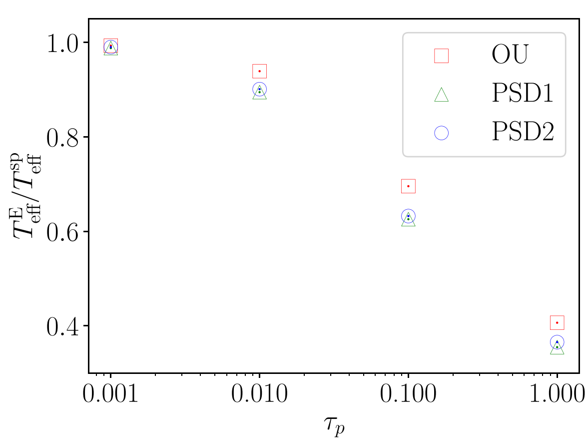

FIG. 5. $T_{\rm eff}^{E}/T_{\rm eff}^{\rm sp}$, as a function of persistence time, τ_p. Superposition of the results for OU (red), PSD1 (green), PSD2 (blue) with spectra (10), (13), and (15), respectively.

and the colored noise f is an n-dimensional zero-mean SGP whose components all have PSD (13) or (15). The matrices A, B, C in Eq. (8) will then be of the form (16) or (17). We use the notation $\|u\| = \sqrt{u_1^1 + u_2^2 + u_3^2}$. When f corresponds to (13), then $f = Cy$ and (x, y) satisfies Eqs. (7) and (8) with matrices A, B, C given in (16) with $n = 4116$, $r = 1$, $p = q = 2rn = 8232$, and the value of (σ_1, ℓ_1) is given in (12). Similarly, when f corresponds to (15), (x, y) also satisfies Eqs. (7) and (8) with matrices A, B, C given in (17) with $n = 4116$, $r = 2$, $p = n = 4116$, $q = 8232$, and the value of (σ, ℓ) is given in (18). Next, we evaluate the time-dependent mobility of a single particle in the system of interacting particles driven by the n-dimensional noise f (self-propulsion) following (13) and (15). Since explicit formulas are unavailable, we perform computations using our sensitivity formula (19) and (20), (21)–(23), and unperturbed simulations. We fix a particle $1 \leqslant i \leqslant N$ and a direction $1 \leqslant \alpha \leqslant 3$, and we perturb the system at $t = 0^+$ as follows: $F_i(x)$ is replaced by $F_i(x) + \lambda \boldsymbol{e}_\alpha$ where $\boldsymbol{e}_\alpha$ is the unit vector in the direction α. Under the influence of the additional constant force, the component α of the particle i moves according to the mobility function $\chi(t)$ as $\langle x_{i\alpha}(t)\rangle_\lambda = \chi(t)\lambda + o(\lambda)$ and thus $\mathrm{d}\langle x(t)\rangle_\lambda/\mathrm{d}\lambda_{|\lambda=0} = \chi(t)$. Moreover, $\lim_{t\to\infty}\chi(t)/t = \mu$, the mobility coefficient. In principle, to estimate $\chi(t)$ we can compute the sensitivity index above with unperturbed averages $\langle x_{i\alpha}(t)p^1_{00;i\alpha}(t)\rangle + \langle \dot{x}_{i\alpha}(t)p^1_{11;i\alpha}(t)\rangle$ or $\langle x_{i\alpha}(t)p^2_{00;i\alpha}(t)\rangle + \langle \dot{x}_{i\alpha}(t)p^2_{11;i\alpha}(t)\rangle + \langle \ddot{x}_{i\alpha}(t)p^2_{22;i\alpha}(t)\rangle$ when the driving noise corresponds to (13) or (15), respectively. Here the corresponding weight functions evolve according to the following equations of motion:

(1) For (13),

$$p^1_{00;i\alpha}(t) = \sigma_1^{-1}(w_{i\alpha})_1(t) + \sigma_1^{-1}\ell_1^{-1}\omega_1(w_{i\alpha})_2(t), \text{ and}$$
$$p^1_{11;i\alpha}(t) = \sigma_1^{-1}\ell_1^{-1}(w_{i\alpha})_1(t).$$

(2) For (15),

$$p^2_{00;i\alpha}(t) = \sigma^{-1}\alpha_0 w_{i\alpha}(t),$$
$$p^2_{11;i\alpha}(t) = \sigma^{-1}\ell^{-1}\alpha_1 w_{i\alpha}(t), \text{ and}$$
$$p^2_{22;i\alpha}(t) = \sigma^{-1}\ell^{-2} w_{i\alpha}(t).$$

For both cases, since the particles are indistinguishable and exhibit isotropic behavior, the mobility function $\chi(t)$ does not depend on (i, α). Then, as inspired by Szamel's computing strategy, we can use all the particles in all Cartesian directions and average over the origins of time. The mobility function $\chi(t)$ can thus be estimated by

$$\frac{1}{3NN_o}\sum_{i=1}^{N}\sum_{\alpha=1}^{3}\sum_{\mathfrak{o}=1}^{N_o}\zeta(i,\alpha,\mathfrak{o},t), \tag{29}$$

where in the case of (13),

$$\zeta(i,\alpha,\mathfrak{o},t) = \langle x_{i\alpha}(t+t_\mathfrak{o})[p^1_{00;i\alpha}(t+t_\mathfrak{o}) - p^1_{00;i\alpha}(t_\mathfrak{o})]\rangle + \langle \dot{x}_{i\alpha}(t+t_\mathfrak{o})[p^1_{11;i\alpha}(t+t_\mathfrak{o}) - p^1_{11;i\alpha}(t_\mathfrak{o})]\rangle$$

and in the case of (15),

$$\zeta(i,\alpha,\mathfrak{o},t) = \langle x_{i\alpha}(t+t_\mathfrak{o})(p^2_{00;i\alpha}(t+t_\mathfrak{o}) - p^2_{00;i\alpha}(t_\mathfrak{o}))\rangle + \langle \dot{x}_{i\alpha}(t+t_\mathfrak{o})(p^2_{11;i\alpha}(t+t_\mathfrak{o}) - p^2_{11;i\alpha}(t+t_\mathfrak{o}))\rangle + \langle \ddot{x}_{i\alpha}(t+t_\mathfrak{o})(p^2_{22;i\alpha}(t+t_\mathfrak{o}) - p^2_{22;i\alpha}(t_\mathfrak{o}))\rangle.$$

Finally, in both cases we can compute an estimation of the mean-square displacement (MSD) defined by

$$\mathrm{MSD}(t) = \langle\|x_1(t) - x_1(0)\|^2\rangle = \frac{1}{N}\sum_{i=1}^{N}\langle\|x_i(t) - x_i(0)\|^2\rangle, \tag{30}$$

which grows as $6D_{\mathrm{sd}}t$, with D_{sd} being the self-diffusion coefficient. The Einstein relation can be used to define the Einstein effective temperature $T^E_{\mathrm{eff}} = D_{\mathrm{sd}}/\mu$ [3]. It can then be estimated by the ratio of $\mathrm{MSD}(t)/6$ over $\chi(t)$ for t large. For four distinct persistence times, we plot, in Fig. 4, the mobility function and mean-square displacement for the systems corresponding to the three noises that we consider. It is known that the Einstein effective temperature can be different from $T^{\mathrm{sp}}_{\mathrm{eff}}$, except in the small correlation time limit. In Fig. 5, we show that the ratio $T^E_{\mathrm{eff}}/T^{\mathrm{sp}}_{\mathrm{eff}}$ decreases when the correlation time increases and that the decay also depends on the form of the PSD. The value is, therefore, a complicated function of the PSD and not only a function of the amplitude and correlation time of the colored noise.

VI. CONCLUSION

In this paper, we have proposed a method of sensitivity analysis for particle systems under colored noise. We have obtained original formulas, generalizing those obtained by Szamel, for the sensitivity indices of the IPS statistics mentioned above with respect to the perturbation of the drift coefficient. The type of colored noise we considered falls into a class of stationary Gaussian processes with zero mean and whose spectra can be general. Both our analytical and numerical calculations show that the sensitivity indices do not depend only on the effective parameters: the amplitude and correlation time of the noise. Instead, it is also dependent on the structure of the spectrum. Moreover, the method that we have developed can be applied beyond the quantities studied in this paper. For example, it can be used to study the structure of correlations in the particle system, as done in [18] (the case of a simple OU). Furthermore, our method can prove effective for gradient calculation in optimization procedures, as was done in [6] (the case of white noise).

The code for this paper is available upon request.

ACKNOWLEDGMENTS

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APPENDIX A: PROOFS AND DETAILS OF WEIGHT FORMULAS

1. Derivation of our first main result

We extend the approach in [3] to compute the derivative of $\langle\Phi[x(t)]\rangle_\lambda$ with respect to λ at $\lambda = 0$.

Step 1. We start by discretizing the equations of motion (7) and (8), for fixed N_t, over time intervals of length $\Delta t = t/N_t$ to obtain the following limit of integrals:

$$\langle\Phi[x(t)]\rangle_\lambda = \lim_{N_t\to\infty}\int \Phi(x_{N_t})\prod_{i=2}^{N_t} P_{\lambda,i}P_1P^{ss},$$

where $P_{\lambda,i} = P_\lambda(x_i, y_i|x_{i-1}, y_{i-1})$, for $i = 2, \dots, N_t$, are the transition densities of the perturbed system, $P_1 = P(x_1, y_1|x_0, y_0)$ is the transition density of the unperturbed system, and $P^{ss} = P^{ss}(x_0, y_0)$ is the steady state distribution for the unperturbed system. Here the transition densities, for $i = 2, \dots, N_t$, are given by

$$P_\lambda(x_i, y_i|x_{i-1}, y_{i-1}) = \delta_{\mathcal{X}_{\lambda,i}}g(y_i, (I_q - \Delta tA)y_{i-1}, \Delta tBB^T),$$

where $\mathcal{X}_{\lambda,i} = x_i - x_{i-1} - \Delta t\xi_0^{-1}(F_\lambda(x_{i-1}) + Cy_{i-1})$ and $g(y, \mu, \Sigma)$ is the density of the multidimensional Gaussian $\mathcal{N}(\mu, \Sigma)$. We use the notation I_q for the identity matrix of size $q \times q$.

Step 2. To compute the derivative $\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\Phi(x(t))\rangle_\lambda$, we interchange the limit and integral on the rhs of the equation, followed by applying the product rule to obtain the following:

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\Phi[x(t)]\rangle_\lambda\Big|_{\lambda=0} = \lim_{N_t\to\infty}\sum_{i=2}^{N_t}\int\Phi(x_{N_t})P'_{\lambda=0,i} \times\left(\prod_{j=2,j\neq i}^{N_t}P_j\right)P_1P^{ss}.$$

Using the assumption that $\hat{F} = CE$ and the chain rule, it can be shown that

$$P'_{\lambda=0,i} = E(x_{i-1}) \cdot \nabla_{y_{i-1}}(\delta_{\mathcal{X}_{\lambda,i}}) g(y_i, (I_q - \Delta t A)y_{i-1}, \Delta t BB^T).$$

Step 3. By applying integration by parts and rearranging, we have the following:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\Phi[x(t)]\rangle_\lambda\Big|_{\lambda=0} = \lim_{N_t\to\infty}\int \Phi\big(x_{N_t}\big)\prod_{j=1}^{N_t}P_jP^{ss}\Bigg\{ &-\Big[\big(I_q - \Delta t A\big)E\big(x_{N_t-1}\big)\cdot(\Delta t BB^T)^{-1}\big[\big(y_{N_t} - (I_q - \Delta t A)y_{N_t-1}\big]\Big] \\ &+ \sum_{i=1}^{N_t-1}\left[\frac{[E(x_i) - E(x_{i-1})]}{\Delta t}\cdot(\Delta t BB^T)^{-1}[y_i - (I_q - \Delta t A)y_{i-1}]\Delta t\right] \\ &+ \sum_{i=2}^{N_t-1}\left[\Delta t A E(x_{i-1})\cdot(\Delta t BB^T)^{-1}[y_i - (I_q - \Delta t A)y_{i-1}]\right] \\ &+ \left[E(x_0)\cdot(\Delta t BB^T)^{-1}[y_1 - (I_q - \Delta t A)y_0]\right]\Bigg\}.\end{aligned}$$

Note that this equation generalizes Eq. (A.3) in [3].

Step 4. It can be shown that an equivalent identity to Eq. (A.4) in [3] can be derived from the steady-state property, which results in the following:

$$\begin{aligned}&\int \big[\Phi\big(x_{N_t}\big)E(x_0)\cdot(\Delta t BB^T)^{-1}[y_1 - (I_q - \Delta t A)y_0]\cdots \\ &\cdots - \Phi\big(x_{N_t}\big)E\big(x_{N_t-1}\big)\cdot(\Delta t BB^T)^{-1}[y_{N_t} - (I_q - \Delta t A)y_{N_t-1}]\big]\prod_{j=1}^{N_t}P_jP^{ss} \\ &= \int \frac{\Phi\big(x_{N_t}\big) - \Phi\big(x_{N_t-1}\big)}{\Delta t}\left[\sum_{i=1}^{N_t-1}E(x_{i-1})\cdot(BB^T)^{-1}[y_i - (I_q - \Delta t A)y_{i-1}]\right]\prod_{j=1}^{N_t}P_jP^{ss}.\end{aligned}$$

Step 5. The equation can now be written in the form of finite differences as follows:

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\Phi[x(t)]\rangle_\lambda\Big|_{\lambda=0} = \lim_{N_t\to\infty}\int\Bigg\{&\Phi\big(x_{N_t}\big)\left[\sum_{i=2}^{N_t}AE(x_{i-1})\cdot(BB^T)^{-1}[y_i - (I_q - \Delta t A)y_{i-1}]\right] \\ &+ \Phi\big(x_{N_t}\big)\left[\sum_{i=1}^{N_t-1}\nabla E(x_{i-1})\frac{x_i - x_{i-1}}{\Delta t}\cdot(BB^T)^{-1}[y_i - (I_q - \Delta t A)y_{i-1}]\right] \\ &+ \frac{\Phi\big(x_{N_t}\big) - \Phi\big(x_{N_t-1}\big)}{\Delta t}\left[\sum_{i=1}^{N_t-1}E(x_{i-1})\cdot(BB^T)^{-1}[y_i - (I_q - \Delta t A)y_{i-1}]\right]\Bigg\}\prod_{j=1}^{N_t}P_jP^{ss}.\end{aligned}$$

This corresponds to Eq. (A.5) in [3].

Step 6. Assuming that limits can be taken, we obtain (19) and (20).

2. Derivation of our second main result

Our proof is composed of several steps. Starting with the third step, we provide the proof in details for the case $n' = 2$. We give the main formula for the general case $n' \geqslant 1$.

Step 1. We start the perturbation at $x_{n'+1}$. Here the transition densities, for $i = n' + 1, \dots, N_t$, are given by

$$P_\lambda(x_i, y_i|x_{i-1}, y_{i-1}) = \delta_{\mathcal{X}_{\lambda,i}}\left(\prod_{k=1}^{n'-1}\delta_{\mathcal{Y}_{i,k}}\right) g\left(y_{i,n'}, (I_{q'} - \Delta t A_{n'})y_{i-1,n'} - \Delta t\sum_{k=1}^{n'-1}A_k y_{i-1,k}, \Delta t\bar{B}\bar{B}^T\right),$$

where $\mathcal{X}_{\lambda,i}$ is defined as above and $\mathcal{Y}_{i,k} = \{y_{i,k} - y_{i-1,k} - \Delta t y_{i-1,k+1}\}$ and $g(y, \mu, \Sigma)$ is the density of the multidimensional Gaussian $\mathcal{N}(\mu, \Sigma)$. We use the notation $I_{q'}$ for the identity matrix of size $q' \times q'$. The unperturbed transition densities for $i = 1, \dots, n'$ are given by the same formula except that $\lambda = 0$. Below we use the short notation $P_{\lambda,i}$, and P_i for the perturbed and unperturbed transition densities, respectively.

Step 2. To compute the derivative $\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\Phi[x(t)]\rangle_\lambda$ at $\lambda = 0$, we interchange the limit and integral on the rhs of the equation, followed by applying the product rule to obtain the following:

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\Phi[x(t)]\rangle_\lambda\bigg|_{\lambda=0} = \lim_{N_t\to\infty}\sum_{i=n'+1}^{N_t}\int \Phi\big(x_{N_t}\big)P'_{\lambda=0,i}\Bigg(\prod_{j=1,\,j\neq i}^{N_t} P_j\Bigg)P^{ss}.$$

We will use the short notation $\mathcal{X}_i$ for $\mathcal{X}_{0,i}$. Using the assumption that $\hat{F} = \bar{C}\bar{E}$ and the chain rule, it can be shown that

$$P'_{\lambda=0,i} = \bar{E}(x_{i-1})\cdot\nabla_{y_{i-1,1}}(\delta_{\mathcal{X}_i})\Bigg(\prod_{k=1}^{n'-1}\delta_{y_{i,k}}\Bigg)\underbrace{g\Bigg(y_{i,n'},\,(I_{q'}-\Delta t A_{n'})y_{i-1,n'} - \Delta t\sum_{k=1}^{n'-1}A_k y_{i-1,k},\,\Delta t\bar{B}\bar{B}^T\Bigg)}_{g_i:=}.$$

Here we recall that both $\bar{E}(x_{i-1})$ and $\nabla_{y_{i-1,1}}(\delta_{\mathcal{X}_{\lambda,i}})$ take values in $\mathbb{R}^{q'}$. Below we use the notation

$$\mathcal{T}_i \triangleq \int \Phi\big(x_{N_t}\big)P'_{\lambda=0,i}\Bigg(\prod_{j=1,\,j\neq i}^{N_t}P_j\Bigg)P^{ss}. \tag{A1}$$

a. Case $n' = 2$ in detail

In this subsection we consider the case $n' = 2$. In order to alleviate the notation, we denote $\nabla_u(\cdot)$ as $(\cdot)_u$. We reformulate $\mathcal{T}_i$ using several integration by parts (IBPs). We use the notation

$$\zeta = \Phi\big(x_{N_t}\big)\Bigg(\prod_{j=1}^{N_t}P_j\Bigg)P^{ss} \text{ and } \bar{E}_i = \bar{E}(x_i),$$

and then $\mathcal{T}_i$ can be expressed as

$$\mathcal{T}_i = \frac{1}{\Delta t}\int \zeta\bar{E}_{i-1}([\log(g_{i-1}g_i)]_{y_{i-1,2}} - [\log(g_{i-2}g_{i-1})]_{y_{i-2,2}}) + \int\zeta\bar{E}_{i-1}\,[-\log(g_i)]_{y_{i-1,1}}. \tag{A2}$$

The transition from (A1) to (A2) is given in Lemma 3. Then calculations yield

$$\begin{aligned}
[-\log(g_i)]_{y_{i-1,1}} &= A_1^T(\bar{B}\bar{B}^T)^{-1}\theta_i,\\
[\log(g_{i-1}g_i)]_{y_{i-1,2}} &= \frac{1}{\Delta t}\big(\bar{B}\bar{B}^T\big)^{-1}(\theta_i-\theta_{i-1}) - A_2^T(\bar{B}\bar{B}^T)^{-1}\theta_i,\\
[\log(g_{i-1}g_i)]_{y_{i-1,2}} - [\log(g_{i-2}g_{i-1})]_{y_{i-2,2}} &= \frac{1}{\Delta t}\big(\bar{B}\bar{B}^T\big)^{-1}(\theta_i - 2\theta_{i-1}+\theta_{i-2}) - A_2^T(\bar{B}\bar{B}^T)^{-1}(\theta_i-\theta_{i-1}),
\end{aligned}$$

where

$$\theta_i \triangleq y_{i,2} - (I_{q'}-\Delta t A_2)y_{i-1,2} + \Delta t A_1 y_{i-1,1}.$$

Therefore

$$\mathcal{T}_i = \int\zeta\bar{E}_{i-1}(\bar{B}\bar{B}^T)^{-1}\bigg(\frac{\theta_i - 2\theta_{i-1}+\theta_{i-2}}{\Delta t^2}\bigg) - \int\zeta\bar{E}_{i-1}A_2^T(\bar{B}\bar{B}^T)^{-1}\bigg(\frac{\theta_i-\theta_{i-1}}{\Delta t}\bigg) + \int\zeta\bar{E}_{i-1}A_1^T(\bar{B}\bar{B}^T)^{-1}\theta_i. \tag{A3}$$

Collecting all the terms, we obtain

$$\sum_{i=3}^{N_t}\mathcal{T}_i = S_3 + S_2 + S_1,$$

where

$$\begin{aligned}
S_1 &= \sum_{i=3}^{N_t}\int\zeta\bar{E}_{i-1}A_1^T(\bar{B}\bar{B}^T)^{-1}\theta_i,\\
S_2 &= -\sum_{i=3}^{N_t}\int\zeta\bar{E}_{i-1}A_2^T(\bar{B}\bar{B}^T)^{-1}\bigg(\frac{\theta_i-\theta_{i-1}}{\Delta t}\bigg)\\
&= \sum_{i=2}^{N_t-1}\int\zeta\bigg(\frac{\bar{E}_i-\bar{E}_{i-1}}{\Delta t}\bigg)A_2^T(\bar{B}\bar{B}^T)^{-1}\theta_i + \frac{1}{\Delta t}\int\zeta\bar{E}_1A_2^T(\bar{B}\bar{B}^T)^{-1}\theta_2 - \frac{1}{\Delta t}\int\zeta\bar{E}_{N_t-1}A_2^T(\bar{B}\bar{B}^T)^{-1}\theta_{N_t},
\end{aligned}$$

and

$$S_3 = \sum_{i=3}^{N_t} \int \zeta \bar{E}_{i-1} (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_i - 2\theta_{i-1} + \theta_{i-2}}{\Delta t^2} \right)$$
$$= \sum_{i=3}^{N_t-2} \int \zeta \left(\frac{\bar{E}_{i+1} - 2\bar{E}_i + \bar{E}_{i-1}}{\Delta t^2} \right) (\bar{B}\bar{B}^T)^{-1} \theta_i + \int \zeta \bar{E}_{N_t-2} (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_{N_t-1}}{\Delta t^2} \right) + \int \zeta \bar{E}_{N_t-1} (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_{N_t}}{\Delta t^2} \right)$$
$$- 2 \left[\int \zeta \bar{E}_2 (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_2}{\Delta t^2} \right) + \int \zeta \bar{E}_{N_t-1} (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_{N_t-1}}{\Delta t^2} \right) \right] + \int \zeta \bar{E}_2 (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_1}{\Delta t^2} \right) + \int \zeta \bar{E}_3 (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_2}{\Delta t^2} \right).$$

Therefore, we have obtained

$$\sum_{i=3}^{N_t} \mathcal{T}_i = \sum_{i=3}^{N_t} \int \zeta \bar{E}_{i-1} A_1^T (\bar{B}\bar{B}^T)^{-1} \theta_i + \sum_{i=2}^{N_t-1} \int \zeta \left(\frac{\bar{E}_i - \bar{E}_{i-1}}{\Delta t} \right) A_2^T (\bar{B}\bar{B}^T)^{-1} \theta_i$$
$$+ \sum_{i=1}^{N_t-2} \int \zeta \left(\frac{\bar{E}_{i+1} - 2\bar{E}_i + \bar{E}_{i-1}}{\Delta t^2} \right) (\bar{B}\bar{B}^T)^{-1} \theta_i + \mathcal{B}_1 + \mathcal{B}_2, \tag{A4}$$

with

$$\mathcal{B}_1 = \frac{1}{\Delta t} \int \zeta \bar{E}_1 A_2^T (\bar{B}\bar{B}^T)^{-1} \theta_2 - \frac{1}{\Delta t} \int \zeta \bar{E}_{N_t-1} A_2^T (\bar{B}\bar{B}^T)^{-1} \theta_{N_t},$$
$$\mathcal{B}_2 = \int \zeta (\bar{E}_{N_t-2} - 2\bar{E}_{N_t-1}) (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_{N_t-1}}{\Delta t^2} \right) + \int \zeta \bar{E}_{N_t-1} (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_{N_t}}{\Delta t^2} \right) - \int \zeta (-2\bar{E}_1 + \bar{E}_0) (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_1}{\Delta t^2} \right)$$
$$- \int \zeta \bar{E}_1 (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_2}{\Delta t^2} \right).$$

The boundary terms $\mathcal{B}_1$ and $\mathcal{B}_2$ can be reformulated in the following way. First,

$$\Delta t \mathcal{B}_1 = - \int \Phi(x_{N_t}) \hat{\zeta} \left(\sum_{k=3}^{N_t} \bar{E}_{k-1} A_2^T (\bar{B}\bar{B}^T)^{-1} \theta_k \right) + \int \Phi(x_{N_t}) \hat{\zeta} \left(\sum_{k=2}^{N_t-1} \bar{E}_{k-1} A_2^T (\bar{B}\bar{B}^T)^{-1} \theta_k \right)$$
$$= - \int \Phi(x_{N_t-1}) \hat{\zeta} \left(\sum_{k=2}^{N_t-1} \bar{E}_{k-1} A_2^T (\bar{B}\bar{B}^T)^{-1} \theta_k \right) + \int \Phi(x_{N_t}) \hat{\zeta} \left(\sum_{k=2}^{N_t-1} \bar{E}_{k-1} A_2^T (\bar{B}\bar{B}^T)^{-1} \theta_k \right).$$

Here we use the stationarity property and the notation

$$\hat{\zeta} = \left(\prod_{j=1}^{N_t} P_j \right) P^{ss}.$$

Therefore

$$\mathcal{B}_1 = \int \hat{\zeta} \left(\frac{\Phi(x_{N_t}) - \Phi(x_{N_t-1})}{\Delta t} \right) \sum_{k=2}^{N_t-1} \bar{E}_{k-1} A_2^T (\bar{B}\bar{B}^T)^{-1} \theta_k. \tag{A5}$$

Next, we focus on $\mathcal{B}_2$. By adding and subtracting $\bar{E}_{N_t}$ and $\bar{E}_2$ in the second and fourth integrals in $\mathcal{B}_2$, we obtain

$$\mathcal{B}_2 = \int \zeta (\bar{E}_{N_t-2} - 2\bar{E}_{N_t-1}) (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_{N_t-1}}{\Delta t^2} \right) + \int \zeta (\bar{E}_{N_t-1} - \bar{E}_{N_t} + \bar{E}_{N_t}) (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_{N_t}}{\Delta t^2} \right)$$
$$- \int \zeta (-2\bar{E}_1 + \bar{E}_0) (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_1}{\Delta t^2} \right) - \int \zeta (\bar{E}_1 - \bar{E}_2 + \bar{E}_2) (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_2}{\Delta t^2} \right).$$

Then we split into two parts $\mathcal{B}_2 = \mathcal{B}_{2,I} + \mathcal{B}_{2,II}$ where

$$\mathcal{B}_{2,I} = - \int \zeta (\bar{E}_{N_t-1} - \bar{E}_{N_t-2}) (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_{N_t-1}}{\Delta t^2} \right) - \int \zeta (\bar{E}_{N_t} - \bar{E}_{N_t-1}) (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_{N_t}}{\Delta t^2} \right)$$
$$+ \int \zeta (\bar{E}_1 - \bar{E}_0) (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_1}{\Delta t^2} \right) + \int \zeta (\bar{E}_2 - \bar{E}_1) (\bar{B}\bar{B}^T)^{-1} \left(\frac{\theta_2}{\Delta t^2} \right)$$

and

$$\mathcal{B}_{2,II} = -\int \zeta \bar{E}_{N_t-1}(\bar{B}\bar{B}^T)^{-1}\left(\frac{\theta_{N_t-1}}{\Delta t^2}\right) + \int \zeta \bar{E}_{N_t}(\bar{B}\bar{B}^T)^{-1}\left(\frac{\theta_{N_t}}{\Delta t^2}\right) + \int \zeta \bar{E}_1(\bar{B}\bar{B}^T)^{-1}\left(\frac{\theta_1}{\Delta t^2}\right) - \int \zeta \bar{E}_2(\bar{B}\bar{B}^T)^{-1}\left(\frac{\theta_2}{\Delta t^2}\right).$$

Next, we reformulate $\mathcal{B}_{2,I}$ and $\mathcal{B}_{2,II}$. For convenience, we use the notation $f_k = (\bar{E}_k - \bar{E}_{k-1})(\bar{B}\bar{B}^T)^{-1}\theta_k \Delta t^{-2}$. We recognize a telescopic sum structure,

$$-\mathcal{B}_{2,I} = \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=2}^{N_t-1} f_k - f_{k-1}\right) + \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=3}^{N_t} f_k - f_{k-1}\right)$$
$$= \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=2}^{N_t-1} f_k\right) - \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=2}^{N_t-1} f_{k-1}\right) + \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=3}^{N_t} f_k\right) - \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=3}^{N_t} f_{k-1}\right).$$

We use the the stationarity property on the left and a simple change of summation in the right:

$$-\mathcal{B}_{2,I} = \int \Phi(x_{N_t-1})\hat{\zeta}\left(\sum_{k=1}^{N_t-2} f_k\right) - \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=1}^{N_t-2} f_k\right) + \int \Phi(x_{N_t-1})\hat{\zeta}\left(\sum_{k=2}^{N_t-1} f_k\right) - \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=2}^{N_t-1} f_k\right).$$

Therefore we obtain

$$\mathcal{B}_{2,I} = \int \hat{\zeta}\left(\frac{\Phi(x_{N_t}) - \Phi(x_{N_t-1})}{\Delta t}\right)\left[\sum_{k=1}^{N_t-2}\left(\frac{\bar{E}_k - \bar{E}_{k-1}}{\Delta t}\right)(\bar{B}\bar{B}^T)^{-1}\theta_k\right] + \int \hat{\zeta}\left(\frac{\Phi(x_{N_t}) - \Phi(x_{N_t-1})}{\Delta t}\right)\left[\sum_{k=2}^{N_t-1}\left(\frac{\bar{E}_k - \bar{E}_{k-1}}{\Delta t}\right)(\bar{B}\bar{B}^T)^{-1}\theta_k\right]. \tag{A6}$$

Now we turn to the boundary term $\mathcal{B}_{2,II}$ and we use the notation $\mathfrak{e}_k = \bar{E}_k(\bar{B}\bar{B}^T)^{-1}\theta_k\Delta t^{-2}$:

$$\mathcal{B}_{2,II} = -\int \zeta \sum_{k=2}^{N_t-1}(\mathfrak{e}_k - \mathfrak{e}_{k-1}) + \int \zeta \sum_{k=3}^{N_t}(\mathfrak{e}_k - \mathfrak{e}_{k-1})$$
$$= -\int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=2}^{N_t-1}\mathfrak{e}_k\right) + \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=2}^{N_t-1}\mathfrak{e}_{k-1}\right) + \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=3}^{N_t}\mathfrak{e}_k\right) - \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=3}^{N_t}\mathfrak{e}_{k-1}\right).$$

We use the stationary property and elementary changes of summation to get

$$\mathcal{B}_{2,II} = -\int \Phi(x_{N_t-1})\hat{\zeta}\left(\sum_{k=1}^{N_t-2}\mathfrak{e}_k\right) + \int \Phi(x_{N_t})\hat{\zeta}\left(\sum_{k=1}^{N_t-2}\mathfrak{e}_k\right) + \int \Phi(x_{N_t-2})\hat{\zeta}\left(\sum_{k=1}^{N_t-2}\mathfrak{e}_k\right) - \int \Phi(x_{N_t-1})\hat{\zeta}\left(\sum_{k=1}^{N_t-2}\mathfrak{e}_k\right).$$

Therefore,

$$\mathcal{B}_{2,II} = \int \hat{\zeta}\left(\frac{\Phi(x_{N_t}) - 2\Phi(x_{N_t-1}) + \Phi(x_{N_t-2})}{\Delta t^2}\right)\left(\sum_{k=1}^{N_t-2}\bar{E}_k(\bar{B}\bar{B}^T)^{-1}\theta_k\right). \tag{A7}$$

Now we collect all our results for the boundary terms (A5)–(A7) and substitute them into the right-hand side of (A4) before passing to the limit. We obtain

$$\sum_{i=3}^{N_t}\mathcal{T}_i = \sum_{i=3}^{N_t}\int \hat{\zeta}\Phi(x_{N_t})\bar{E}_{i-1}A_1^T(\bar{B}\bar{B}^T)^{-1}\theta_i + \sum_{i=2}^{N_t-1}\int \hat{\zeta}\Phi(x_{N_t})\left(\frac{\bar{E}_i - \bar{E}_{i-1}}{\Delta t}\right)A_2^T(\bar{B}\bar{B}^T)^{-1}\theta_i$$
$$+ \sum_{i=1}^{N_t-2}\int \hat{\zeta}\Phi(x_{N_t})\left(\frac{\bar{E}_{i+1} - 2\bar{E}_i + \bar{E}_{i-1}}{\Delta t^2}\right)(\bar{B}\bar{B}^T)^{-1}\theta_i + \int \hat{\zeta}\left(\frac{\Phi(x_{N_t}) - \Phi(x_{N_t-1})}{\Delta t}\right)\sum_{k=2}^{N_t-1}\bar{E}_{k-1}A_2^T(\bar{B}\bar{B}^T)^{-1}\theta_k$$
$$+ \int \hat{\zeta}\left(\frac{\Phi(x_{N_t}) - \Phi(x_{N_t-1})}{\Delta t}\right)\left[\sum_{k=1}^{N_t-2}\left(\frac{\bar{E}_k - \bar{E}_{k-1}}{\Delta t}\right)(\bar{B}\bar{B}^T)^{-1}\theta_k\right]$$
$$+ \int \hat{\zeta}\left(\frac{\Phi(x_{N_t}) - \Phi(x_{N_t-1})}{\Delta t}\right)\left[\sum_{k=2}^{N_t-1}\left(\frac{\bar{E}_k - \bar{E}_{k-1}}{\Delta t}\right)(\bar{B}\bar{B}^T)^{-1}\theta_k\right]$$
$$+ \int \hat{\zeta}\left(\frac{\Phi(x_{N_t}) - 2\Phi(x_{N_t-1}) + \Phi(x_{N_t-2})}{\Delta t^2}\right)\left(\sum_{k=1}^{N_t-2}\bar{E}_k(\bar{B}\bar{B}^T)^{-1}\theta_k\right). \tag{A8}$$

Again assuming we can take the limit as $N_t \to \infty$, we obtain our second main result when $n' = 2$,

$$\frac{\mathrm{d}}{\mathrm{d}\lambda}\langle\Phi[(x(t)]\rangle_\lambda\bigg|_{\lambda=0} = \langle\Phi[x(t)][p_{00}(t)+p_{10}(t)+p_{20}(t)]\rangle + \langle\dot{\Phi}[x(t)][p_{11}(t)+2p_{21}(t)]\rangle + \langle\ddot{\Phi}[(x(t)]\ p_{22}(t)\rangle,$$

where

$$\dot{p}_{0,0}(t) = \bar{E}[x(t)]A_1^T(\bar{B}\bar{B}^T)^{-1}B\dot{w}(t), \quad p_{1,0}(t) = \frac{\mathrm{d}}{\mathrm{d}t}(\bar{E}[x(t)])A_2^T(\bar{B}\bar{B}^T)^{-1}B\dot{w}(t),$$

$$\dot{p}_{2,0}(t) = \frac{\mathrm{d}^2}{\mathrm{d}t^2}(\bar{E}[x(t)])(\bar{B}\bar{B}^T)^{-1}B\dot{w}(t), \quad \dot{p}_{1,1}(t) = \bar{E}[x(t)]A_2^T(\bar{B}\bar{B}^T)^{-1}B\dot{w}(t),$$

$$\dot{p}_{2,1}(t) = \frac{\mathrm{d}}{\mathrm{d}t}(\bar{E}[x(t)])(\bar{B}\bar{B}^T)^{-1}B\dot{w}(t), \text{ and } \dot{p}_{2,2}(t) = \bar{E}[x(t)](\bar{B}\bar{B}^T)^{-1}B\dot{w}(t).$$

b. Case $n' \geqslant 1$ *: Key steps*

Now we turn to the general case $n' \geqslant 1$.

Step 3. The counterpart of formula (A3) becomes

$$\sum_{i=n'+1}^{N_t}\mathcal{T}_i = \sum_{k=0}^{n'}\underbrace{\frac{(-1)^k}{(\Delta t)^k}\left(\sum_{i=n'+1}^{N_t}\int \bar{E}(x_{i-1})A_{k+1}^T(\bar{B}\bar{B}^T)^{-1}(D_k\theta)_i\Phi(x_{N_t})\hat{\zeta}\right)}_{S_k:=}. \tag{A9}$$

The finite difference at the order $k \geqslant 0$ is defined as follows: $(D_0\theta)_i = \theta_i$ and $(D_k\theta)_i = (D_{k-1}\theta)_i - (D_{k-1}\theta)_{i-1}$ for $k \geqslant 1$. We recall that the matrices A_k for $1 \leqslant k \leqslant n'$ are defined in (9) and $A_{n'+1} = I_{q'}$.

Next we use a summation by part formula shown in Lemma 4 to reformulate each of the S_k, that is swapping the finite difference on θ to a finite difference on $\bar{E}$ and obtaining boundary terms.

Step 4. Below, we use the notation $h_{i,k} = A_k^T(\bar{B}\bar{B}^T)^{-1}\theta_i$. In the rhs of (A9), we consider each of the $n'+1$ sums individually. For $k = 0$, we can rewrite the sum as

$$S_0 = \sum_{i=n'+1}^{N_t}\int \hat{\zeta}\,\Phi(x_{N_t})\bar{E}_{i-1}h_{i,1},$$

and for $k \geqslant 1$, we apply Lemma 4 (summation by part below) to obtain $S_k = M_0 + B_0$ where

$$M_0 = \sum_{i=n'+1}^{N_t}\int \hat{\zeta}\,\Phi(x_{N_t})\left(\frac{D_k\bar{E}_{i-1}}{(\Delta t)^k}\right)h_{i-k,k+1},$$

$$B_0 = \frac{1}{(\Delta t)^k}\sum_{j_1=1}^{k}(-1)^{k+j_1}\int \zeta(D_{j_1-1}\bar{E}_{i-1})(D_{k-j_1}h_{i-j_1+1,k+1})\bigg|_{n'}^{N_t}.$$

Then, we use the stationarity property to transform B_0 into

$$B_0 = \frac{1}{(\Delta t)^k}\sum_{j_1=1}^{k}(-1)^{k+j_1}\sum_{i=n'}^{N_t-1}\int \hat{\zeta}(D_1\Phi_{N_t})(D_{j_1-1}\bar{E}_{i-1})(D_{k-j_1}h_{i-j_1+1,k+1}).$$

Step 5. We decompose $B_0 = M_{1,1} + M_{1,2} + B_1$ by separating the sum into two parts ($k - j_1 = 0$ and $k - j_1 \neq 0$):

$$M_{1,1} = \sum_{\substack{j_1=1,\\ j_1=k}}^{k}\sum_{i=n'}^{N_t-1}\int \hat{\zeta}\left(\frac{D_1\Phi_{N_t}}{(\Delta t)^1}\right)\left(\frac{D_{k-1}\bar{E}_{i-1}}{(\Delta t)^{k-1}}\right)h_{i-k+1,k+1},$$

$$M_{1,2} = \sum_{\substack{j_1=1,\\ j_1\neq k}}^{k}\sum_{i=n'}^{N_t-1}\int \hat{\zeta}\left(\frac{D_1\Phi_{N_t}}{(\Delta t)^1}\right)\left(\frac{D_{k-1}\bar{E}_{i-1}}{(\Delta t)^{k-1}}\right)h_{i-k+1,k+1},$$

$$B_1 = \frac{1}{(\Delta t)^k}\sum_{j_1=1}^{k-1}\sum_{j_2=1}^{k-j_1}(-1)^{k+j_1+j_2}\int \hat{\zeta}(D_1\Phi_{N_t})(D_{j_1-j_2-2}\bar{E}_{i-1})(D_{k-j_1-j_2}h_{i-j_1-j_2+2,k+1})\bigg|_{n'-1}^{N_t-1}.$$

Notice that

$$M_{1,1}+M_{1,2}=\sum_{j_1=1}^{k}\sum_{i=n'}^{N_t-1}\int\hat{\zeta}\left(\frac{D_1\Phi_{N_t}}{(\Delta t)^1}\right)\left(\frac{D_{k-1}\bar{E}_{i-1}}{(\Delta t)^{k-1}}\right)h_{i-k+1,k+1}.$$

Step 6. We repeat the steps above to the boundary term (B_1) and the subsequent boundary terms that appear at each iteration. The result obtained after repeating these a total of $k-1$ times is

$$\sum_{m=1}^{k-1}\binom{k}{m}\sum_{i=n'-(m-1)}^{N_t-m}\int\hat{\zeta}\left(\frac{D_m\Phi_{N_t}}{(\Delta t)^k}\right)\left(\frac{D_{k-m}\bar{E}_{i-1}}{(\Delta t)^k}\right)h_{i-k+m,k+1}$$
$$+\sum_{j_1=1}^{1}\sum_{j_2=1}^{2-j_1}\cdots\sum_{j_k=1}^{k-\mathcal{J}_{m-1}}(-1)^{k+\mathcal{J}_m}\int\hat{\zeta}(D_{k-1}\Phi_{N_t})(D_{\mathcal{J}_k-k}\bar{E}_{i-1})(D_{k-\mathcal{J}_k}h_{i-\mathcal{J}_k+k,k+1})\Big|_{n'-(l-1)}^{N_t-(l-1)}.$$

Here, $\mathcal{J}_k=j_1+j_2+\cdots+j_k$.

Step 7. By applying the stationarity property to the boundary term, collecting terms, and rearranging, we arrive at the desired result:

$$\sum_{i=n'+1}^{N_t}\mathcal{T}_i=\sum_{k=0}^{n'}\sum_{m=0}^{k}\binom{k}{m}\sum_{i=n'+1-k}^{N_t-k}\int\hat{\zeta}\left(\frac{D_m\Phi_{N_t}}{(\Delta t)^m}\right)\left(\frac{D_{k-m}\bar{E}_{i-1+(k-m)}}{(\Delta t)^{k-m}}\right)A_{k+1}^T(\bar{B}\bar{B}^T)^{-1}\theta_i. \tag{A10}$$

Step 8. Taking limits as $N_t\to\infty$ and rearranging further, we then have the formula (21) and (22).

c. Technical lemmata

Lemma 3. $\mathcal{T}_i$ defined by (A1) satisfies (A2).

Proof. We start from (A1) with $n'=2$,

$$\mathcal{T}_i=\int\Phi(x_{N_t})P'_{\lambda=0,i}\left(\prod_{j=1,j\neq i}^{N_t}P_j\right)P^{ss}$$
$$=\int\Phi(x_{N_t})\bar{E}_{i-1}\cdot(\delta\mathcal{X}_i)_{y_{i-1,1}}(\delta\mathcal{Y}_{i-1,1}\delta\mathcal{Y}_{i,1}g_i)\left(\prod_{j=1,j\notin\{i-1,i\}}^{N_t}P_j\right)\delta\mathcal{X}_{i-1}g_{i-1}P^{ss}.$$

An integration by part gives $\mathcal{T}_i=-\mathcal{T}_{i,1}-\mathcal{T}_{i,2}-\mathcal{T}_{i,3}$ where

$$\mathcal{T}_{i,1}=\int\Phi(x_{N_t})\bar{E}_{i-1}\cdot(\delta\mathcal{Y}_{i-1,1})_{y_{i-1,1}}\left(\prod_{j=1,j\neq i-1}^{N_t}P_j\right)\delta\mathcal{X}_{i-1}g_{i-1}P^{ss},$$

$$\mathcal{T}_{i,2}=\int\Phi(x_{N_t})\bar{E}_{i-1}\cdot(\delta\mathcal{Y}_{i,1})_{y_{i-1,1}}\delta\mathcal{X}_ig_i\left(\prod_{j=1,j\neq i}^{N_t}P_j\right)P^{ss},$$

$$\mathcal{T}_{i,3}=\int\Phi(x_{N_t})\bar{E}_{i-1}\cdot(g_i)_{y_{i-1,1}}\delta\mathcal{Y}_{i,1}\delta\mathcal{X}_i\left(\prod_{j=1,j\neq i}^{N_t}P_j\right)P^{ss}.$$

Using $(\delta\mathcal{Y}_{i-1,1})_{y_{i-1,1}}=-(\Delta t)^{-1}(\delta\mathcal{Y}_{i-1,1})_{y_{i-2,2}}$, we reformulate $\mathcal{T}_{i,1}$ as follows

$$\mathcal{T}_{i,1}=-\frac{1}{\Delta t}\int\Phi(x_{N_t})\bar{E}_{i-1}\cdot(\delta\mathcal{Y}_{i-1,1})_{y_{i-2,2}}\left(\prod_{j=1,j\neq i-1}^{N_t}P_j\right)\delta\mathcal{X}_{i-1}g_{i-1}P^{ss}$$
$$=\frac{1}{\Delta t}\int\zeta\bar{E}_{i-1}\cdot(\log[g_{i-2}g_{i-1})]_{y_{i-2,2}}\text{ (by integration by parts)},$$

where we reuse the notation

$$\zeta=\Phi(x_{N_t})\left(\prod_{j=1}^{N_t}P_j\right)P^{ss}.$$

Next, using $(\delta y_{i,1})_{y_{i-1,1}} = (\Delta t)^{-1}(\delta y_{i-1,1})_{y_{i-1,2}}$, we reformulate $\mathcal{T}_{i,2}$ as follows:

$$\mathcal{T}_{i,2} = \frac{1}{\Delta t}\int \Phi\big(x_{N_t}\big)\bar{E}_{i-1}\cdot\big(\delta y_{i,1}\big)_{y_{i-1,2}}\left(\prod_{j=1,\,j\neq i}^{N_t} P_j\right)\delta_{\mathcal{X}_i} g_i P^{ss}$$
$$= -\frac{1}{\Delta t}\int \zeta \bar{E}_{i-1}\cdot[\log(g_{i-1}g_i)]_{y_{i-1,2}} \text{ (by integration by parts).}$$

Finally, we reformulate $\mathcal{T}_{i,3}$ as follows:

$$\mathcal{T}_{i,3} = \int \zeta \bar{E}_{i-1}\cdot[\log(g_i)]_{y_{i-1,1}}.$$

We can collect the results above to obtain (A2). ■

Lemma 4. Summation by parts formula for $1 \leqslant k \leqslant n$:

$$\sum_{i=n+1}^{N}\phi_{i-1}D_k\psi_i = (-1)^k\sum_{i=n+1}^{N} D_k\phi_{i-1}\psi_{i-k} + \sum_{j=1}^{k}(-1)^{j-1}(D_{j-1}\phi_{i-1}D_{k-j}\psi_{i-j+1})\Big|_n^N.$$

Proof. We have that

$$\sum_{i=n+1}^{N}\phi_{i-1}D^k\psi_i = -\left(\sum_{i=n+1}^{N}\phi_{i-1}D^{k-1}\psi_{i-1} - \sum_{i=n+1}^{N}\phi_{i-2}D^{k-1}\psi_{i-1}\right) + \left(\sum_{i=n+1}^{N}\phi_{i-1}D^{k-1}\psi_i - \sum_{i=n+1}^{N}\phi_{i-2}D^{k-1}\psi_{i-1}\right)$$
$$= -\sum_{i=n+1}^{N} D^1\phi_{i-1}D^{k-1}\psi_{i-1} + (\phi_{i-1}D^{k-1}\psi_i)\Big|_n^N.$$

By inductively applying the above identity to $\sum_{i=n+1}^{N} D^l\phi_{i-1}D^{k-l}\psi_{i-l}$, it can be shown that the following holds for $l = 1, \ldots, k$:

$$\sum_{i=n+1}^{N}\phi_{i-1}D^k\psi_i = (-1)^l\sum_{i=n+1}^{N} D^l\phi_{i-1}D^{k-l}\psi_{i-l} + \sum_{j=1}^{l}(-1)^{j-1}(D^{j-1}\phi_{i-1}D^{k-j}\psi_{i-j+1})\Big|_n^N.$$

In particular, the case $l = k$ holds and concludes the proof. ■

3. Details of weight formulas

Calculations yield the following formulas. In the rest of this section, let $\alpha = k/\xi_0 + \ell$ and $\beta = k/\xi_0 - \ell$. Furthermore, when the average, $\langle\cdots\rangle$, appears without the dependence on t, we implicitly mean to take the average with respect to the steady state.

a. Weight formulas associated with (25)

$$\langle x(t)p^1_{0,0}(t)\rangle = \frac{1 - e^{-\frac{k}{\xi_0}t}}{k} - \frac{e\sigma}{\xi_0}c(t), \quad \text{and} \quad \langle \dot{x}(t)p^1_{1,1}(t)\rangle = \frac{e\sigma}{\xi_0}c(t),$$

where

$$c(t) = \frac{e^{-\ell t}[\beta\cos(\omega t) + \omega\sin(\omega t)] - \beta e^{-\frac{k}{\xi_0}t}}{\beta^2 + \omega^2}.$$

b. Weight formulas associated with (26)

$$\big\langle x^2(t)p^2_{0,0}(t)\big\rangle = \frac{\sigma^2}{\xi_0^2}e^{-2\ell t}\left(\frac{\cos(2\omega t)\mathcal{A}_1 + \sin(2\omega t)\mathcal{B}_1 + \mathcal{C}_1}{2\beta(\beta^2+\omega^2)^2}\right) + \frac{2\sigma}{\xi_0}e^{-\alpha t}\left(\frac{\cos(\omega t)\mathcal{D}_1 + \sin(\omega t)\mathcal{E}_1}{\beta^2+\omega^2}\right) + \frac{\sigma}{k}(e^{-2k/\xi_0 t} - 1)a_{1,1},$$

$$\big\langle x^2(t)p^2_{1,0}(t)\big\rangle = \frac{\sigma^2}{\xi_0^2}e^{-2\ell t}\left(\frac{\cos(2\omega t)\mathcal{A}_2 + \sin(2\omega t)\mathcal{B}_2 + \mathcal{C}_2}{2\big(\frac{k}{\xi_0}-\ell\big)\big[\big(\frac{k}{\xi_0}-\ell\big)^2+\omega^2\big]^2}\right) + \frac{2\sigma}{\xi_0}e^{-(k/\xi_0+\ell)t}\left(\frac{\cos(\omega t)\mathcal{D}_2 + \sin(\omega t)\mathcal{E}_2}{\big(\frac{k}{\xi_0}-\ell\big)^2+\omega^2}\right) + \frac{\sigma}{k}(e^{-2k/\xi_0 t} - 1)a_{1,2},$$

and

$$\langle \dot{x^2}(t) p_{1,1}^2(t)\rangle = \frac{-2k\sigma^2}{\xi_0^3} e^{-2\ell t}\left(\frac{\cos(2\omega t)\mathcal{A}_3 + \sin(2\omega t)\mathcal{B}_3 + \mathcal{C}_3}{2\left(\frac{k}{\xi_0}-\ell\right)\left[\left(\frac{k}{\xi_0}-\ell\right)^2+\omega^2\right]^2}\right) + \frac{-4k\sigma}{\xi_0^2} e^{-(k/\xi_0+\ell)t}\left(\frac{\cos(\omega t)\mathcal{D}_3 + \sin(\omega t)\mathcal{E}_3}{\left(\frac{k}{\xi_0}-\ell\right)^2+\omega^2}\right)$$
$$+ \frac{-2\sigma}{\xi_0}(e^{-2k/\xi_0 t}-1)a_{1,3} + \frac{\sigma}{\xi_0}e^{-2\ell t}\left(\frac{\cos^2(\omega t)\mathcal{F} + \cos(\omega t)\sin(\omega t)\mathcal{G} + \sin^2(\omega t)\mathcal{H}}{\alpha^2+\omega^2}\right)$$
$$+ e^{-(k/\xi_0+\ell)t}[\cos(\omega t)a_{1,3} + \sin(\omega t)a_{2,3}] - a_{1,3},$$

where we use the following constant:

$$\begin{aligned}
\mathcal{A}_i &= c_{1,i}\beta^3 - c_{2,i}\beta\omega^2 - (2b_{2,i})\beta^2\omega,\\
\mathcal{B}_i &= c_{1,i}\beta^2\omega + c_{2,i}\beta^2\omega + (2b_{2,i})\beta^3,\\
\mathcal{C}_i &= c_{2,i}\beta(\beta^2+\omega^2) + (2b_{2,i})\omega(\beta^2+\omega^2),\\
\mathcal{D}_i &= a_{1,i}\beta - a_{2,i}\omega,\\
\mathcal{E}_i &= a_{1,i}\omega + a_{2,i}\beta,\\
\mathcal{F} &= (b_{1,3}a + b_{2,3}\omega),\\
\mathcal{G} &= (b_{1,3}\omega + 2b_{2,3}a + b_{3,3}\omega),\\
\mathcal{H} &= (b_{2,3}\omega + b_{3,3}a),
\end{aligned}$$

and

$$\begin{aligned}
c_{1,i} &= \frac{4\ell^2\langle y_1F_{1,i}\rangle + 4\omega\ell\langle y_2F_{1,i}\rangle + 4\omega\ell\langle y_1F_{2,i}\rangle - 4\ell^2\langle y_2F_{2,i}\rangle}{-4(\ell^2+\omega^2)},\\
c_{2,i} &= -(\langle y_1F_{1,i}\rangle + \langle y_2F_{2,i}\rangle),\\
b_{1,i} &= \frac{2(2\ell^2+\omega^2)\langle y_1F_{1,i}\rangle + 2\omega\ell\langle y_2F_{1,i}\rangle + 2\omega\ell\langle y_1F_{2,i}\rangle + 2\omega^2\langle y_2F_{2,i}\rangle}{-4(\ell^2+\omega^2)},\\
b_{2,i} &= \frac{-2\omega\ell\langle y_1F_{1,i}\rangle + 2\ell^2\langle y_2F_{1,i}\rangle + 2\ell^2\langle y_1F_{2,i}\rangle + 2\omega\ell\langle y_2F_{2,i}\rangle}{-4(\ell^2+\omega^2)},\\
b_{3,i} &= \frac{\omega^2 2\langle y_1F_{1,i}\rangle + -2\ell\omega(\langle y_2F_{1,i}\rangle + \langle y_1F_{2,i}\rangle) + (2\ell^2+\omega^2)2\langle y_2F_{2,i}\rangle}{-4(\ell^2+\omega^2)},\\
a_{1,i} &= \frac{-\alpha(\ell\langle xF_{1,i}\rangle - b_{1,i}) + \omega(\ell\langle xF_{2,i}\rangle - b_{2,i})}{\alpha^2+\omega^2},\\
a_{2,i} &= \frac{\omega(\ell\langle xF_{1,i}\rangle - b_{1,i}) - \alpha(\ell\langle xF_{2,i}\rangle - b_{2,i})}{\alpha^2+\omega^2},
\end{aligned}$$

with $F_{1,1} = ex,\ F_{2,1} = e\omega\ell^{-1}x,\ F_{1,2} = e\ell^{-1}\dot{x},\ F_{2,2} = 0,\ F_{1,3} = e\ell^{-1}x,\ F_{2,3} = 0.$

c. Weight formulas associated with (27)

$$\langle x(t)p_{00}^3(t)\rangle = e\gamma\alpha_0\left(\frac{1-e^{-k/\xi_0 t}}{k} - \ell\frac{te^{-\ell t}}{k-\ell\xi_0} - (k-2\ell\xi_0)\frac{e^{-\ell t}-e^{-k/\xi_0 t}}{(k-\ell\xi_0)^2}\right),$$
$$\langle \dot{x}(t)p_{11}^3(t)\rangle = e\gamma\alpha_1\left(\ell\frac{te^{-\ell t}}{k-\ell\xi_0} - \ell\xi_0\frac{e^{-\ell t}-e^{-k/\xi_0 t}}{(k-\ell\xi_0)^2}\right),$$

and

$$\langle \ddot{x}(t)p_{22}^3(t)\rangle = e\gamma\left(-\ell\frac{te^{-\ell t}}{k-\ell\xi_0} + k\frac{e^{-\ell t}-e^{-k/\xi_0 t}}{(k-\ell\xi_0)^2}\right).$$

d. Weight formulas associated with (28)

$$\langle x^2(t)p^4_{0,0}(t)\rangle = \mathcal{A}_1(t^2e^{-2\ell t}) + \mathcal{B}_1(te^{-2\ell t}) + \mathcal{C}_1(te^{-\ell t}) + \mathcal{D}_1(te^{-\alpha t}) + \mathcal{E}_1(e^{-2\ell t} - e^{-2k/\xi_0 t}) + \mathcal{F}_1(e^{-\ell t} - e^{-2k/\xi_0 t}) + \mathcal{G}_1(e^{-\alpha t} - e^{-2k/\xi_0 t}) + \frac{\gamma}{k}b_{1,1}(1 - e^{-2k/\xi_0 t}),$$

$$\langle x^2(t)p^4_{1,0}(t)\rangle = \mathcal{A}_2(t^2e^{-2\ell t}) + \mathcal{B}_2(te^{-2\ell t}) + \mathcal{C}_2(te^{-\ell t}) + \mathcal{D}_2(te^{-\alpha t}) + \mathcal{E}_2(e^{-2\ell t} - e^{-2k/\xi_0 t}) + \mathcal{F}_2(e^{-\ell t} - e^{-2k/\xi_0 t}) + \mathcal{G}_2(e^{-\alpha t} - e^{-2k/\xi_0 t}) + \frac{\gamma}{k}b_{1,2}(1 - e^{-2k/\xi_0 t}),$$

$$\langle x^2(t)p^4_{1,0}(t)\rangle = \mathcal{A}_3(t^2e^{-2\ell t}) + \mathcal{B}_3(te^{-2\ell t}) + \mathcal{C}_3(te^{-\ell t}) + \mathcal{D}_3(te^{-\alpha t}) + \mathcal{E}_3(e^{-2\ell t} - e^{-2k/\xi_0 t}) + \mathcal{F}_3(e^{-\ell t} - e^{-2k/\xi_0 t}) + \mathcal{G}_3(e^{-\alpha t} - e^{-2k/\xi_0 t}) + \frac{\gamma}{k}b_{1,3}(1 - e^{-2k/\xi_0 t}),$$

$$\langle \dot{x^2}(t)p^4_{1,1}(t)\rangle = \left(\frac{-2k}{\xi_0}\mathcal{A}_4 + \frac{2\gamma}{\xi_0}\mathcal{I}_4\right)(t^2e^{-2\ell t}) + \left(\frac{-2k}{\xi_0}\mathcal{B}_4 + \frac{2\gamma}{\xi_0}\mathcal{J}_4\right)(te^{-2\ell t}) + \frac{-2k}{\xi_0}\mathcal{C}_4(te^{-\ell t}) + \left(\frac{-2k}{\xi_0}\mathcal{D}_4 + \frac{2\gamma}{\xi_0}\mathcal{L}_4\right)(te^{-\alpha t}) + \frac{-2k}{\xi_0}\mathcal{E}_4(e^{-2\ell t} - e^{-2k/\xi_0 t}) + \frac{-2k}{\xi_0}\mathcal{F}_4(e^{-\ell t} - e^{-2k/\xi_0 t}) + \frac{-2k}{\xi_0}\mathcal{G}_4(e^{-\alpha t} - e^{-2k/\xi_0 t}) + \frac{2\gamma}{\xi_0}b_{1,4}(e^{-2k/\xi_0 t}) + \frac{2\gamma}{\xi_0}\mathcal{K}_4(e^{-2\ell t}) + \frac{2\gamma}{\xi_0}\mathcal{M}_4(e^{-\alpha t}),$$

$$\langle \dot{x^2}(t)p^4_{2,1}(t)\rangle = \left(\frac{-2k}{\xi_0}\mathcal{A}_5 + \frac{2\gamma}{\xi_0}\mathcal{I}_5\right)(t^2e^{-2\ell t}) + \left(\frac{-2k}{\xi_0}\mathcal{B}_5 + \frac{2\gamma}{\xi_0}\mathcal{J}_5\right)(te^{-2\ell t}) + \frac{-2k}{\xi_0}\mathcal{C}_5(te^{-\ell t}) + \left(\frac{-2k}{\xi_0}\mathcal{D}_5 + \frac{2\gamma}{\xi_0}\mathcal{L}_5\right)(te^{-\alpha t}) + \frac{-2k}{\xi_0}\mathcal{E}_5(e^{-2\ell t} - e^{-2k/\xi_0 t}) + \frac{-2k}{\xi_0}\mathcal{F}_5(e^{-\ell t} - e^{-2k/\xi_0 t}) + \frac{-2k}{\xi_0}\mathcal{G}_5(e^{-\alpha t} - e^{-2k/\xi_0 t}) + \frac{2\gamma}{\xi_0}b_{1,5}(e^{-2k/\xi_0 t}) + \frac{2\gamma}{\xi_0}\mathcal{K}_5(e^{-2\ell t}) + \frac{2\gamma}{\xi_0}\mathcal{M}_5(e^{-\alpha t}),$$

and

$$\langle \ddot{x^2}(t)p^4_{2,2}(t)\rangle = \left(\frac{4k^2}{\xi_0^2}\mathcal{A}_6 - \frac{6k\sigma}{\xi_0^2}\mathcal{I}_6 + \frac{2\sigma^2}{\xi_0^2}\mathcal{N}_6 - \frac{2\sigma}{\xi_0}\mathcal{I}_6\right)(t^2e^{-2\ell t}) + \left(\frac{4k^2}{\xi_0^2}\mathcal{B}_6 - \frac{6k\sigma}{\xi_0^2}\mathcal{J}_6 + \frac{2\sigma^2}{\xi_0^2}\mathcal{O}_6 + \frac{2\sigma}{\xi_0}\mathcal{R}_6\right)(te^{-2\ell t}) + \frac{4k^2}{\xi_0^2}\mathcal{C}_6(te^{-\ell t}) + \left(\frac{4k^2}{\xi_0^2}\mathcal{D}_6 - \frac{6k\sigma}{\xi_0^2}\mathcal{L}_6 - \frac{2\sigma}{\xi_0}\mathcal{L}_6\right)(te^{-\alpha t}) + \frac{4k^2}{\xi_0^2}\mathcal{E}_6(e^{-2\ell t} - e^{-2k/\xi_0 t}) + \frac{4k^2}{\xi_0^2}\mathcal{F}_6(e^{-\ell t} - e^{-2k/\xi_0 t}) + \frac{4k^2}{\xi_0^2}\mathcal{G}_6(e^{-\alpha t} - e^{-2k/\xi_0 t}) + \frac{4k^2}{\xi_0^2}\frac{\gamma}{k}b_{1,i}(1 - e^{-2k/\xi_0 t}) + \left(-\frac{6k\sigma}{\xi_0^2}\mathcal{K}_6 - \frac{2\sigma}{\xi_0}\frac{1}{2}\mathcal{K}_6\right)(e^{-2\ell t}) + \left(-\frac{6k\sigma}{\xi_0^2}\mathcal{M}_6 + \frac{2\sigma}{\xi_0}\mathcal{U}_6\right)(e^{-\alpha t}) + \left(-\frac{6k\sigma}{\xi_0^2}b_{1,6} + \frac{2\sigma^2}{\xi_0^2}\mathcal{P}_6 + \frac{2\sigma}{\xi_0}b_{2,6}\right),$$

where we use the following constants:

$$\mathcal{A}_i = \frac{\sigma}{\xi_0}A_i(-1/\beta^2),$$

$$\mathcal{B}_i = \frac{\sigma}{\xi_0}A_i[1/\beta^3 - 2/(\ell\beta^2)],$$

$$\mathcal{C}_i = \frac{\sigma}{\xi_0}A_i(1/\beta^3),$$

$$\mathcal{D}_i = \left[\frac{\sigma}{\xi_0}A_i(-2/\beta^3) + 2\gamma/\xi_0\ell(b_{1,i} + b_{2,i})/\beta\right],$$

$$\mathcal{E}_i = \frac{\sigma}{\xi_0}A_i[-1/(2\beta^4) + 1/(\ell\beta^3)],$$

$$\mathcal{F}_i = \frac{\sigma}{\xi_0}A_i[-1/(2\beta^4) + 2/(\ell\beta^3)],$$
$$\mathcal{G}_i = \left\{\frac{\sigma}{\xi_0}A_i[2/\beta^4 - 4/(\ell\beta^3)] + 2\gamma/\xi_0[-\ell(b_{1,i} + b_{2,i})/\beta^2 + b_{1,i}\beta]\right\},$$
$$\mathcal{I}_i = -A_i(\ell^2/\beta),$$
$$\mathcal{J}_i = A_i(\ell^2/\beta^2 - 2\ell/\beta),$$
$$\mathcal{K}_i = 2A_i\ell/\beta^2,$$
$$\mathcal{L}_i = [-A_i\ell^2/\beta^2 + \ell(b_{1,i} + b_{2,i})],$$
$$\mathcal{M}_i = (2A_i\ell/\beta^2 + b_{1,i}),$$
$$\mathcal{N}_i = -(\langle y_1F_i\rangle + \langle y_2F_i\rangle)\ell^2,$$
$$\mathcal{O}_i = -(2\langle y_1F_i\rangle + \langle y_2F_i\rangle)\ell,$$
$$\mathcal{P}_i = \left(\langle y_1F_i\rangle + \tfrac{1}{2}\langle y_2F_i\rangle\right),$$
$$\mathcal{R}_i = A_i(-\ell^2/\beta^2 + \ell/\beta),$$
$$\mathcal{U}_i = (A_i\ell/\beta^2 + b_{2,i}),$$
$$A_i = \gamma/\xi_0\langle y_1F_i\rangle,$$
$$b_{1,i} = 1/\alpha^2[-(\alpha + \ell)\gamma/\xi_0(\langle y_1F_i\rangle + (1/2)\langle y_2F_i\rangle) - \ell^2\langle xF_i\rangle],$$
$$b_{2,i} = 1/\alpha^2(\ell\gamma/\xi_0(\langle y_1F_i\rangle + (1/2)\langle y_2F_i\rangle) - (k/\xi_0)\ell\langle xF_i\rangle),$$

and $F_1 = ex,\ F_2 = \frac{2e}{\ell}\dot{x},\ F_3 = \frac{e}{\ell^2}\ddot{x},\ F_4 = \frac{2e}{\ell}x,\ F_5 = \frac{e}{\ell^2}\dot{x},\ F_6 = \frac{e}{\ell^2}x.$

APPENDIX B: FURTHER DETAILS ON MONTE CARLO SIMULATIONS

1. The harmonic case

We provide details on the implementation of the Monte Carlo (MC) method in calculating the sensitivity indices. For pedagogical purposes, we consider (25) where the underlying unperturbed dynamics is $\dot{x} = \xi_0^{-1}(-kx + \sigma y_1)$, $\dot{y}_1 = -\ell_1 y_1 + \frac{\ell_1}{2}y_2 + \ell_1\dot{w}_1$, $\dot{y}_2 = -\frac{\ell_1}{2}y_1 - \ell_1 y_2 + \ell_1\dot{w}_2$. Other cases follow the same method. The time discretization and the MC estimation work as follows: Let $T > 0$. Let N_T be the number of time steps and $\mathfrak{h} = T/N_T$ be the time step. We discretize the time interval $[0, T]$ with $\{i\mathfrak{h},\ 0 \leqslant i \leqslant N_T\}$. Let N be the number of MC samples. Consider two independent sequences of i.i.d. standard Gaussian variables $\{\Delta W_{1,i}^n,\ \Delta W_{2,i}^n\ 1 \leqslant i \leqslant N_T, 1 \leqslant n \leqslant N\}$. For each $1 \leqslant n \leqslant N$, the discretization of the unperturbed dynamics and the corresponding Malliavin weights lead to the following sequences for $0 \leqslant i \leqslant N_T - 1$:

$$x_{i+1}^{\mathfrak{h},n} = x_i^{\mathfrak{h},n} + \mathfrak{h}\xi_0^{-1}\left(-kx_i^{\mathfrak{h},n} + \sigma_1 y_{1,i}^{\mathfrak{h},n}\right),$$
$$y_{1,i+1}^{\mathfrak{h},n} = y_{1,i}^{\mathfrak{h},n} - \mathfrak{h}\ell_1\left(y_{1,i}^{\mathfrak{h},n} - y_{2,i}^{\mathfrak{h},n}/2\right) + \sqrt{\mathfrak{h}}\Delta W_{1,i}^n,$$
$$y_{2,i+1}^{\mathfrak{h},n} = y_{2,i}^{\mathfrak{h},n} - \mathfrak{h}\ell_1\left(y_{1,i}^{\mathfrak{h},n}/2 + y_{2,i}^{\mathfrak{h},n}\right) + \sqrt{\mathfrak{h}}\Delta W_{2,i}^n,$$
$$p_{00,i+1}^{1,\mathfrak{h},n} = p_{00,i}^{1,\mathfrak{h},n} + \sigma_1^{-1}\sqrt{\mathfrak{h}}\left(\Delta W_{1,i}^n + \Delta W_{2,i}^n/2\right),$$
$$p_{11,i+1}^{1,\mathfrak{h},n} = p_{11,i}^{1,\mathfrak{h},n} + \sigma_1^{-1}\ell_1^{-1}\sqrt{\mathfrak{h}}\Delta W_{1,i}^n.$$

Here for each n, $p_{00,0}^{1,\mathfrak{h},n} = p_{11,0}^{1,\mathfrak{h},n} = 0$ and $(x_0^{\mathfrak{h},n}, y_{1,0}^{\mathfrak{h},n}, y_{2,0}^{\mathfrak{h},n})$ is distributed according to the steady state of the unperturbed process (x, y_1, y_2). The latter is Gaussian, its mean and variance covariance can be easily identified as a fixed point solution for the differential equations governing the time-dependent mean and variance covariance. Then we can build the MC estimator $I_{N,i}$ for $\mathrm{d}\langle x(i\mathfrak{h})\rangle_{\lambda_1}/\mathrm{d}\lambda_1$ at $\lambda_1 = 0$, for any $1 \leqslant i \leqslant N_T$, with

$$I_{N,i} = \frac{1}{N}\sum_{n=1}^{N} x_i^{\mathfrak{h},n} p_{00,i}^{1,\mathfrak{h},n} + \xi_0^{-1}\left(-kx_i^{\mathfrak{h},n} + \sigma_1 y_{1,i}^{\mathfrak{h},n}\right)p_{11,i}^{1,\mathfrak{h},n}.$$

In our simulations, we use $N = 10^6$ and $\mathfrak{h} = 10^{-3}$ with $T = 10$. It is worth mentioning that in our setting the stationary measure of (x, y_1, y_2) is known. However, as pointed out in [27], the detailed balance (equilibrium system) does not hold for systems with persistence time, which is the case here.

2. The screened Coulomb case

We discuss the practical aspects of the simulation of the particle system when the interaction force is given by the repulsive screened Coulomb potential $V(r) = A_V \exp[-\kappa(r - \sigma_V)]/r$, and we use the same parameters as in [3]: $N = 1372$, $A_V = 475T_{\text{eff}}^{\text{sp}}\sigma_V$, $\kappa\sigma_V = 24$. We take $\sigma_V = 1$ without loss of generality. We consider a periodic domain which is a cube of length $L = (1372/0.51)^{1/3}$ so that we keep $N = 1372$ particles with a concentration $N/L^3 = 0.51$ and the system admits a stationary state. The initial condition is a realization of the steady state. We obtain it in the following way: we simulate the system from an arbitrary condition over a sufficiently long period of time (the burn-in phase) to reach the steady state. We follow an important statistic of the system, $\mathrm{MSD}(t)/t$, where $\mathrm{MSD}(t)$ is defined in Eq. (30). When this statistic stabilizes around a constant value, we consider that the steady state is reached. The MC method and the discretization of the dynamics and the Malliavin weights are very similar to what was presented in the previous section. It will be noted that due to the stiffness of the potential we have used an adaptive time step, this is very useful in the burn-in phase until the system reaches its steady state. We can also see that the time step becomes constant from this point onwards.

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