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Gianmarco Del Sarto,[1,a)] (ID) Stefano Galatolo,[2,b)] (ID) and Sakshi Jain[3,c)] (ID)

AFFILIATIONS

[1]Class of Science, Scuola Normale Superiore, Pisa, Italy; Department of Science, Technology and Society, University School for Advanced Studies IUSS Pavia, Pavia, Italy; and Department of Mathematics, Technische Universität Darmstadt, Darmstadt, Germany
[2]Dipartimento di Matematica, Centro Interdipartimentale per lo Studio dei Sistemi Complessi Universitá di Pisa, Pisa, Italy
[3]School of Mathematics, Monash University, Melbourne, Australia

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[a)]E-mail: delsarto@mathematik.tu-darmstadt.de
[b)]E-mail: stefano.galatolo@unipi.it
[c)]Author to whom correspondence should be addressed: sakshi.jain@monash.edu

ABSTRACT

We consider a random dynamical system on $\mathbb{R}^d$, whose dynamics is defined by a stochastic differential equation. The annealed transfer operator associated with such systems is a kernel operator. Given a set of feasible infinitesimal perturbations P to this kernel, with support in a certain compact set, and a specified observable function $\phi : \mathbb{R}^d \to \mathbb{R}$, we study which infinitesimal perturbation in P produces the greatest change in expectation of ϕ. We establish conditions under which the optimal perturbation uniquely exists and present a numerical method to approximate the optimal infinitesimal kernel perturbation. Finally, we numerically illustrate our findings with concrete examples.

Linear response theory provides a powerful framework for understanding the impact of perturbations on a given dynamical system. It investigates whether the resulting changes in the system's statistical properties are differentiable with respect to the perturbations. This theory is widely applied in physics, engineering, climate science, and statistical mechanics to analyze how systems evolve under external influences. This article studies an inverse problem related to the linear response, called *optimal response*, in which one searches for the optimal perturbation in order to change the statistical properties of the system in a wanted direction. We study this problem in a class of random dynamical system defined by a stochastic differential equation on a non-compact space, using a functional analytic tool known as the transfer operator. In particular, we consider the problem of finding the optimal response in order to change as much as possible the average of a given observable, showing the existence and uniqueness results for the solutions of this problem. We also show algorithms to approximate the optimal solution. Optimal response finds many applications, including climate sciences, for example, in finding out which initial climatic actions can produce the greatest change in average temperature.

I. INTRODUCTION

The predictive understanding and the control of the statistical properties of a dynamical system is an important topic of study, with applications to many different fields, so is understanding the change in these statistical properties after small changes in the initial dynamical system. The concept of statistical stability of a dynamical system relates to the statistical properties of typical orbits of a dynamical system, which are, in turn, encoded into its invariant or stationary measures, and to how these properties change when the system is perturbed. We say that the system exhibits a linear response to the perturbation when such a change is differentiable (see Theorem 25 for a formalization of this concept). In this case, the long-time average of a given observable changes smoothly during the perturbation.

The linear response for dynamical systems was first studied by Ruelle[1] and then was studied extensively for different classes of systems having some form of hyperbolicity (see Ref. 2 for a general survey). The linear response for stochastic differential equations (SDEs) was studied in Refs. 3–5, where general response results were established. In the context of discrete-time random systems, linear response results have been shown in Refs. 6–8. The study of linear response has great importance in the applications, in particular, to climate sciences (see Refs. 4 and 9).

In the present article, we address a natural inverse problem related to linear response: The optimal response of a given observable. We consider a certain observable, defined on the phase space associated with our system and search for the optimal infinitesimal perturbation to apply to the system in order to maximize the observable's expectation. The understanding of this problem also has evident importance in the applications, as it is a formalization of the natural question of "how to manage the system in such a way that its statistical properties change in a wanted direction," hence an optimal control problem for the statistical properties of the system.[4,6,9–11]

The optimal response problem for a fixed observable as described above was studied for the first time in Ref. 12 for finite-state Markov chains. Then, the case of dynamical systems whose transfer operators are kernel operators (including random dynamical systems that have additive noise) was considered in Ref. 6. The case of one-dimensional deterministic expanding circle maps with deterministic perturbations was studied in Ref. 13. The above articles also consider the problem of optimizing the spectral gap and, hence, the speed of mixing. In Ref. 14, an optimal response problem is considered where optimal coupling is studied in the context of mean-field coupled systems. A problem strictly related to the optimal response is the "linear request problem," which focuses on the search for a perturbation achieving a prescribed response direction.[8,10,11,15,16] All of these studies are in terms of understanding how a system can be modified to control the behavior of its statistical properties.

Stochastic differential equations and random dynamical systems are widely used as models of climate and fluid dynamics related phenomena. This strongly motivates the study of the optimal response for such systems. As mentioned above, the optimal response and the control of the statistical properties for discrete time random dynamical systems whose associated transfer operator is a kernel operator are studied in Refs. 6 and 8. In these papers, the phase space considered was compact. Since the transfer operator associated with a stochastic differential equation is a kernel operator (see Theorem 1 for a precise statement and estimates on the regularity of the kernel). The results of these papers, hence, apply to the case of time discretizations of stochastic differential equations over compact spaces. The extension of these results to non-compact phase space is a non-trivial task, which requires the use of suitable functional spaces, in order to recover the "compact immersion"-like functional analytic properties, which are well known to be important to establish spectral gap for the associated transfer operator. Important stochastic differential models are formulated on noncompact spaces, such as $\mathbb{R}^d$. Thus, such an extension is strongly motivated. An approach to the definition of suitable spaces for the transfer operators associated with stochastic differential equations on $\mathbb{R}^d$

was implemented in Ref. 17 by using a sort of weighted Bounded Variation spaces with the scope of studying extreme events.

In the present paper, motivated by these considerations, we approach the study of optimal linear response for random dynamical systems over $\mathbb{R}^d$ that have a kernel transfer operator. This setting is, in our opinion, a first step in approaching the study of the optimal response for stochastic differential equations.

II. SETTINGS AND RESULTS

Let $T > 0$ and consider the SDE on $\mathbb{R}^d$ given by

$$\begin{cases} dX_s^x = b\left(X_s^x\right) dt + dW_s, & s \in (0, T), \\ X_0^x = x. \end{cases} \tag{1}$$

Here, $(W_s)_s$ is a Brownian motion defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$, and $x \in \mathbb{R}^d$ is the initial condition. We impose the following assumptions on the drift b:

A: (Locally Lipschitz continuity) For each $x_0 \in \mathbb{R}^d$, there exist constants $K > 0$ and $\delta_0 > 0$ such that for all $x \in \mathbb{R}^d$ with $|x_0 - x| < \delta_0$,

$$|b(x_0) - b(x)| \le K|x_0 - x|. \tag{2}$$

B: (Dissipativity) There exist constants $c_1 \in \mathbb{R}$ and $c_2 > 0$ such that for all $x \in \mathbb{R}^d$,

$$\langle b(x), x \rangle \le c_1 - c_2 \|x\|^2. \tag{3}$$

Under assumptions **A** and **B**, SDE (1) admits a unique stationary measure μ (see Ref. 17, Section 4.1 for details).

Now, let θ_s, for $s \ge 0$, be the flow associated with the deterministic part of the above SDE, that is,

$$\begin{cases} \dot{\theta}_s(x) = b(\theta_s(x)), \\ \theta_0(x) = x. \end{cases}$$

For $\lambda \in (0, 1]$, $s > 0$, define the Gaussian density

$$g_\lambda(s, x) := s^{-\frac{d}{2}} e^{\frac{-\lambda |x|^2}{s}}.$$

The following result, due to Ref. 18, provides two-sided estimates and gradient bounds for the density associated with the (unique) solution $(X_s^x)_s$ of SDE (1).

Theorem 1 (Ref. 18, Theorem 1.2 and Remark 1.3). *Fix $T > 0$. For each $t \in (0, T)$ and $x \in \mathbb{R}^d$, the law of X_t^x has a density $\kappa_t(x, y)$ that is continuous in both variables $x, y \in \mathbb{R}^d$. Moreover, κ_t satisfies the following:*

1: *(Two-sided density bounds) There exist constants $\lambda_0 \in (0, 1]$, $C_0 \ge 1$, depending on T, K, d, such that for all $x, y \in \mathbb{R}^d$ and $t < T$,*

$$C_0^{-1} g_{\lambda_0^{-1}}(t, \theta_t(x) - y) \le \kappa_t(x, y) \le C_0 g_{\lambda_0}(t, \theta_t(x) - y).$$

2: *(Gradient estimates) There exist constants $\lambda_1 \in (0, 1]$, $C_1 \ge 1$, depending on T, K, d, such that for all $x, y \in \mathbb{R}^d$, and $t < T$,*

$$|\nabla_x \kappa_t(x, y)| \le C_1 t^{-\frac{1}{2}} g_{\lambda_1}(t, \theta_t(x) - y),$$

$$|\nabla_y \kappa_t(x, y)| \le C_1 t^{-\frac{1}{2}} g_{\lambda_1}(t, \theta_t(x) - y).$$

Remark 2. As stated above, SDE (1) that we consider in this article admits a unique stationary measure μ. In the following, we fix the time $t = 1$ and consider a time discretization of this system. For notational convenience, we drop the subscript t and denote the kernel $\kappa_1(x, y)$ simply by $\kappa(x, y)$.

As discussed in Sec. I, a dynamical system exhibits *linear response* if its invariant measure changes differentiably with respect to the changes in the initial system. One of our main results gives the *explicit characterization for linear response* for system (1), which is suitable for the numerical approximation.

To be able to state the precise result (Theorem 25), we introduce the transfer operator $\mathcal{L} : L^1 \to L^1$ (Definition 4), defined by

$$\mathcal{L}f(y) = \int \kappa(x, y) f(x)\, dx,$$

where κ is the kernel from Theorem 1 (see Remark 2).

To get a spectral gap and other desirable properties, we consider $\mathcal{L}$ as acting on a suitable Banach space $\mathfrak{B}$ of weighted densities [see (16)]. We then consider a class of perturbed systems by applying perturbations directly to the associated transfer operators. We consider a compact domain $D \subset \mathbb{R}^d$ and we introduce a family of *perturbed kernels* κ_δ of the form

$$\kappa_\delta = \kappa + \delta \cdot \dot{\kappa} + r_\delta,$$

where $\dot{\kappa}, r_\delta \in L^2(D \times D)$ and $r_\delta = o(\delta)$ is an higher-order perturbation in $L^2(D \times D)$. This yields a family of perturbed transfer operators,

$$\mathcal{L}_\delta f(y) = \int \kappa_\delta(x, y) f(x)\, dx, \tag{4}$$

with the convention $\mathcal{L}_0 = \mathcal{L}$ (see Sec. IV for more details).

Result A. *Consider the family $\mathcal{L}_\delta : \mathfrak{B} \to \mathfrak{B}$ of transfer operators, with $\delta \in [0, \bar{\delta})$. Then,*

(1) *The operators have invariant densities in $\mathfrak{B}$: for each $\delta \in [0, \bar{\delta})$ there is $f_\delta \neq 0$ such that $\mathcal{L}_\delta f_\delta = f_\delta$ (Propositions 15 and 23).*
(2) *There exists an operator $\dot{\mathcal{L}} : L^1 \to L^1$, defined by $\dot{\mathcal{L}}f(y) = \int \dot{\kappa}(x, y) f(x)\, dx$, such that, restricted to the strong space $\mathfrak{B}$, the following limit holds:*

$$\lim_{\delta \to 0} \left\| \frac{\mathcal{L}_\delta - \mathcal{L}_0}{\delta} f_0 - \dot{\mathcal{L}}f_0 \right\|_s = 0,$$

where $\|\cdot\|_s$ is the norm on the strong space $\mathfrak{B}$ (Lemma 20).
(3) *For δ small enough, we have linear response: that is,*

$$\lim_{\delta \to 0} \left\| \frac{f_\delta - f_0}{\delta} - (Id - \mathcal{L}_0)^{-1} \dot{\mathcal{L}}f_0 \right\|_1 = 0, \tag{5}$$

where $\|\cdot\|_1$ is the L^1 norm (Theorem 25).

While results on the existence of linear response for SDEs on $\mathbb{R}^d$ can be found in the literature (see Refs. 3 and 4), formula (5) is particularly suitable for numerical approximation, within an appropriate numerical scheme that we describe in Sec. V. We exploit this formulation to pursue the main objective of the paper: identifying the optimal perturbation that induces a prescribed response, as outlined in the introduction. Thanks to the explicit characterization that

we derive, we are also able to demonstrate how to approximate such perturbations in concrete examples (see Sec. VI).

This leads to our next main result, which addresses the existence and uniqueness of such an optimal perturbation. To state it, consider a compact neighborhood $D \subset \mathbb{R}^d$ of 0. Formalizing the idea that we mean to perturb the kernel of the transfer operator in a certain direction $\dot{\kappa} \in L^2(D \times D)$, we introduce an operator (see Definition 31),

$$R : L^2(D \times D) \to L^1, \quad R(\dot{\kappa}) = \lim_{\delta \to 0} \frac{f_{\dot{\kappa},\delta} - f_0}{\delta},$$

where $f_{\dot{\kappa},\delta}$ and f_0 are the invariant densities of the perturbed and unperturbed transfer operators $\mathcal{L}_\delta$ and $\mathcal{L}_0$, respectively, acting on the Banach space $\mathfrak{B}$.

Result B. *Let $\phi \in L^\infty$ be an observable, and let $P \subset L^2 (D \times D)$ be a closed, bounded, and strictly convex set whose relative interior contains the zero function. Then, the optimization problem (Proposition 28)*

$$\max\{\mathcal{J}(\dot{\kappa}) : \dot{\kappa} \in P\} \tag{6}$$

admits a unique solution.

The above results are stated more precisely and proved in Sec. IV and V (see the references provided in each statement), where all the necessary definitions and technical details are also introduced.

Finally, in Sec. V B, we present a numerical scheme for approximating the optimal perturbation. This scheme is built upon the constructive nature of our proofs and the explicit formulas derived therein, which are directly implemented in the numerical procedure. A constructive algorithm for computing the optimal perturbation is given. The corresponding numerical experiments are carried out on a concrete example of an SDE in Sec. VI.

We remark that because of the type of perturbations to the system considered in this work [see (4)], the transfer operator obtained after perturbation may no longer be associated with an SDE. Such a perturbation can be interpreted as a "local" change to the initial system (the one arising from an SDE), whose nature is independent of the phenomenon whose model is the SDE. This can be seen as a first step in the study of the optimal response for SDEs, where we apply the simplest possible meaningful perturbations. However, one would like to consider other "non-compact" perturbations as well, such as those arising from perturbations to the drift term b of the SDE [see (1)].

A natural direction for future work is indeed to consider perturbations of the system, to be applied directly on the SDE defining it and, in particular, to the drift term b. We think that this case also would fit our general framework. However, in order to achieve this, the differentiability and the differential of the transfer operator with respect to this perturbation should be obtained, like it is done in Sec. IV for the kind of perturbation we consider. Similar estimates have been achieved in Ref. 5. Unfortunately, the convergence of these estimates in Ref. 5 is in the L^2 topology, which is not sufficient for our purposes (see Remark 18 for an explanation on why L^2 is not a good space in order to consider getting spectral gap for the transfer operator, and, hence, apply our strategy for the optimal response when the phase space is $\mathbb{R}^d$ and, hence, not compact). However, such a result indicates that with some further work, the

goal of fitting this kind of perturbations in our framework for the optimal response is achievable.

A. Overview of the paper

The remainder of this paper is organized as follows. In Sec. III, we introduce the transfer operator associated with the SDE (1) [see (9)]. In particular, it is a kernel operator on the non-compact phase space $\mathbb{R}^d$. Then, we define suitable spaces for this operator. Specifically, we let the transfer operator act on $L^1(\mathbb{R}^d)$ and on a "stronger" space, constructed using a space we denote by $\mathfrak{B}$, which consists of $L^1(\mathbb{R}^d)$ densities that decay at infinity with a prescribed speed and are also in L^2 on the domain D where the perturbations are applied. The choice of the L^2 topology in this domain is motivated by optimization purposes, which are simplified when working on a Hilbert space. The prescribed decay at infinity will be useful in obtaining suitable compactness properties, which will imply that the transfer operator, when considered on the strong space, has a spectral gap (see Lemma 14) and strong mixing properties (see Proposition 17).

In Sec. IV, we define and study the perturbations we intend to apply to our system. We show that the perturbed operators also have a spectral gap, and we prove a linear response statement for these systems and perturbations (see Theorem 25).

In Sec. V, we consider an observable in $L^\infty(\mathbb{R}^d, \mathbb{R})$ and explore the problem of finding the optimal perturbation that maximizes the rate of change of the expectation of the observable. We formalize the optimization problem in Problem 27 and prove that it has a unique solution (see Proposition 28). Moreover, we describe a numerical approach to approximate the unique solution in the case where the set of feasible perturbations is a ball in a suitable Hilbert space.

In Sec. VI, we apply the algorithm to illustrate the optimal perturbation on some examples. In particular, we consider a gradient system SDE with a symmetric double-well potential. Then, via a finite difference method, we numerically approximate the solution of the optimization problem for a smooth observable given by the probability density function (PDF) of a Gaussian random variable.

Finally, there is an Appendix stating some well-known results of convex optimization that we have extensively used in Sec. V.

III. TRANSFER OPERATOR AND BANACH SPACES

A. The Kolmogorov operator and the transfer operator

In this section, we define the transfer operator associated with the evolution of the SDE considered at time $t = 1$ and state/prove some basic properties of these operators. We will extensively use the density $\kappa(x, y)$ (as Remark 2 says, we drop the subscript t) and its properties given by Theorem 1.

Definition 3. The Kolmogorov operator $\mathcal{P} : L^\infty(\mathbb{R}^d) \to C^0(\mathbb{R}^d)$ associated with the system (1) at time $t = 1$ is defined as follows. Let $\phi \in L^\infty(\mathbb{R}^d)$, then for all $x \in \mathbb{R}^d$, we set

$$(\mathcal{P}\phi)(x) := \mathbb{E}[\phi(X_1^x)],$$

where X_1^x is the solution at time $t = 1$ of SDE (1) with initial condition x.

The solution X_1^x, thanks to Theorem 1, has a density $\kappa(x, y)$, and, thus, we have

$$(\mathcal{P}\phi)(x) = \int_{\mathbb{R}^d} \phi(y)\kappa(x, y)dy.$$

By this, we see that

$$\|\mathcal{P}\phi\|_\infty \leq \|\phi\|_\infty. \tag{7}$$

If ν is a Borel signed measure on $\mathbb{R}^d$,

$$\int_{\mathbb{R}^d} (\mathcal{P}\phi)(x)d\nu(x) = \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} \phi(y)\kappa(x, y)dyd\nu(x),$$

supposing that ν has a density with respect to the Lebesgue measure $f \in L^1(\mathbb{R}^d)$, i.e., $d\nu = f(x)dx$. We can, thus, write

$$\int_{\mathbb{R}^d} (\mathcal{P}\phi)(x)d\nu(x) = \int_{\mathbb{R}^d} \phi(y) \left(\int_{\mathbb{R}^d} \kappa(x, y)f(x)dx \right) dy. \tag{8}$$

Now we define the transfer operator $\mathcal{L} : L^1(\mathbb{R}^d) \to L^1(\mathbb{R}^d)$ associated with the evolution of the system at time $t = 1$.

Definition 4 (Transfer operator). Given $f \in L^1(\mathbb{R}^d)$, we define the measurable function $\mathcal{L}f : \mathbb{R}^d \to \mathbb{R}^d$ as follows. For almost each $y \in \mathbb{R}^d$, let

$$[\mathcal{L}f](y) := \int \kappa(x, y)f(x)dx. \tag{9}$$

Remark 5. We will show that this operator has a unique invariant density f_μ, satisfying $f_\mu = \mathcal{L}f_\mu$. This function f_μ is the density of the stationary measure μ associated with SDE (1) (see Proposition 15).

By (8), we now get the duality relation between the Kolmogorov and the transfer operator,

$$\int (P\phi)(x)d\nu(x) = \int \phi(y)[\mathcal{L}f](y)dy. \tag{10}$$

The following are some well-known and basic facts about integral operators with kernels κ in L^p, which will be useful:

- If $\kappa \in L^2$, the operator $\mathcal{L} : L^2 \to L^2$ is bounded and

$$\|\mathcal{L}f\|_2 \leq \|\kappa\|_2 \|f\|_2 \tag{11}$$

(see Proposition 4.7 in II.§ 4[19]).
- If $\kappa \in L^\infty$, then

$$\|\mathcal{L}f\|_\infty \leq \|\kappa\|_\infty \|f\|_1, \tag{12}$$

and the operator $\mathcal{L} : L^1 \to L^\infty$ is bounded.

Now, we discuss the properties of the transfer operator on the space L^1.

Lemma 6. *The operator $\mathcal{L}$ preserves the integral and is a weak contraction with respect to the L^1 norm.*

Proof. The first statement directly follows from (10) setting $\phi = 1$. For the second, we can work similarly using (7) and (10) with $\phi = \frac{[\mathcal{L}f]}{|[\mathcal{L}f]|}$. $\square$

Remark 7. Since $\mathcal{L}$ is a positive operator, we also get that $\mathcal{L}$ is a Markov operator having kernel κ.

Finally, in Sec. III B, we define/construct the strong space that we want to study the operator $\mathcal{L}$ on.

B. Functional spaces

In this section, we construct spaces which are suitable to obtain spectral gap on non-compact domains for the action of the transfer operator associated with the system.

The spaces we consider consist of densities whose behavior far away from the origin is controlled using certain weight functions going to ∞ at infinity, following the approach of Ref. 17.

Let $\alpha > 0$ and define the weight function

$$\rho_\alpha(|x|) = \left(1 + |x|^2\right)^{\alpha/2}. \tag{13}$$

Let $L_\alpha^1(\mathbb{R}^d)$ be the space of Lebesgue measurable $f: \mathbb{R}^d \to \mathbb{R}$ such that

$$\|f\|_{L_\alpha^1(\mathbb{R}^d)} := \int_{\mathbb{R}^d} \rho_\alpha(|x|)\, |f(x)|\, dx < \infty.$$

Note that, $L_\alpha^1 \subset L^1$ and for $f \in L_\alpha^1$, $\|f\|_1 \le \|f\|_{L_\alpha^1}$. Moreover, for $\alpha = 0$, $L_0^1 = L^1$.

Remark 8. Throughout the article, we denote the L^1, L^2, and L^∞ norms by $\|\cdot\|_1, \|\cdot\|_2$, and $\|\cdot\|_\infty$, respectively.

For a Borel subset $S \subseteq \mathbb{R}^d$, let us define

$$\mathrm{osc}(f, S) = ess\, sup_{x \in S} f - ess\, inf_{x \in S} f.$$

Let ψ be a Radon probability measure on $\mathbb{R}^d$ and assume that:

$(A_\psi 1)$ ψ is absolutely continuous with respect to the Lebesgue measure, having a continuous bounded density ψ' such that $\psi' > 0$ everywhere.

With such a probability measure satisfying $(A_\psi 1)$, define a norm $\|\cdot\|_{BV_\alpha}$ for $f \in L_\alpha^1(\mathbb{R}^d)$ by setting

$$\|f\|_{BV_\alpha} := \|f\|_{L_\alpha^1(\mathbb{R}^d)} + \sup_{\epsilon \in (0,1]} \epsilon^{-1} \int_{\mathbb{R}^d} \mathrm{osc}\left(f, B_\epsilon(x)\right) d\psi(x), \tag{14}$$

where $B_\epsilon(x)$ denotes the ball in $\mathbb{R}^d$ with center x and radius ϵ. Being the sum of a norm and a seminorm, $\|\cdot\|_{BV_\alpha}$ indeed defines a norm and the following space is a Banach space see Ref. 21, Proposition 3.3 (In Refs. 20 and 21, these spaces have been studied extensively and in more general form as well.):

$$BV_\alpha(\mathbb{R}^d) = \left\{ f \in L_\alpha^1 : \|f\|_{BV_\alpha} < \infty \right\}.$$

The presence of the measure ψ in the definition of the oscillatory seminorm is necessary to treat the case when we have a non-compact domain, which in this case is $\mathbb{R}^d$. Instead, if the domain was compact, one could simply take $\psi = 1$.

Finally, to define the strong space, let D be a compact set in $\mathbb{R}^d$. In what follows, D is the set where we allow perturbations in our system. Accordingly, we define a suitable norm, adapted to such perturbations, as follows:

$$\|f\|_s := \|f\|_{L_2^1} + \|1_D f\|_2. \tag{15}$$

We define the strong space of densities as follows, equipped with the norm $\|\cdot\|_s$:

$$\mathfrak{B} := \left\{ f \in L_2^1(\mathbb{R}^d), \|f\|_s < \infty \right\}. \tag{16}$$

The following results from Ref. 17 will be useful to prove the compact inclusion of the strong space $\mathfrak{B}$ in L^1 and, ultimately, the spectral gap.

Proposition 9. $BV_\alpha(\mathbb{R}^d) \hookrightarrow L^1(\mathbb{R}^d)$ is a compact embedding.

Lemma 10. There exist constants $A, B > 0$ and $\lambda \in (0, 1)$ such that

$$\left\|\mathcal{L}^n f\right\|_{L_2^1} \le A\lambda^n \|f\|_{L_2^1} + B \|f\|_1 \tag{17}$$

for every $f \in L_2^1$ and every $n \in \mathbb{N}$.

Lemma 11. For every $t > 0$, $\mathcal{L}$ is bounded linear from L^1 to C^1; in particular, there exists $C > 0$ such that

$$\left\|\mathcal{L}f\right\|_{C^1} \le C \|f\|_1. \tag{18}$$

Moreover, if $f \in L_2^1$, then

$$\left\|\mathcal{L}f\right\|_{BV_2} \le C \|f\|_{L_2^1}. \tag{19}$$

The proofs of Proposition 9, Lemma 10, and Lemma 11 can be found in Theorem 16, Lemma 19, and Lemma 20 of Ref. 17, respectively.

Now, we proceed to prove that the transfer operator $\mathcal{L}$ has spectral gap when acting on $\mathfrak{B}$, for which we need some preliminary results like compact inclusion (Proposition 12) and Lasota–Yorke inequality (Lemma 13) etc.

By Proposition 9 and Lemma 11, we have the following:

Proposition 12. Let B be the closed unit ball in $\mathfrak{B}$. Then, $\mathcal{L}(B)$ is a compact set in L^1.

Proof. Using Proposition 9, which states that BV_2 is compactly embedded in L^1, it suffices to prove that $\mathcal{L}(B)$ is a closed and bounded set in the space BV_2. By Lemma 11, for every $f \in B$, there exists $C > 0$ such that $\left\|\mathcal{L}f\right\|_{BV_2} \le C \|f\|_{L_2^1} \le C \|f\|_s \le C$, which implies $\mathcal{L}(B)$ is a bounded set in BV_2.

To prove that $\mathcal{L}(B)$ is closed, let $(x_n)_{n \in \mathbb{N}}$ be a Cauchy sequence in $\mathcal{L}(B)$. Since $\mathcal{L}(B) \subset BV_2$ and BV_2 is a Banach space, there exists $x \in BV_2 \subset L^1$ such that $\|x_n - x\|_{BV_2} \to 0$. We want to show that $x \in \mathcal{L}(B)$. Since $x_n \in \mathcal{L}(B)$, there exists a sequence $(y_n)_{n \in \mathbb{N}} \in B$ such that, for all $n \in \mathbb{N}$, $\|y_n\|_s \le 1$ and $\mathcal{L}(y_n) = x_n$. As the unit ball B is closed, there exists $y \in B$ such that $\|y_n - y\|_s \to 0$. By continuity, we have $\mathcal{L}(y) = x$, which implies $x \in \mathcal{L}(B)$, completing the proof. $\square$

Lemma 13. There exist constants $A, B > 0$ and $\lambda \in (0, 1)$ such that

$$\left\|\mathcal{L}^n f\right\|_s \le A\lambda^n \|f\|_s + B \|f\|_{L^1} \tag{20}$$

for every $f \in \mathfrak{B}$ and every $n \in \mathbb{N}$.

Proof. By Lemma 10, $\exists\, A_1, B_1 \ge 0, \lambda \in (0, 1)$ such that

$$\left\|\mathcal{L}^n f\right\|_s = \left\|\mathcal{L}^n f\right\|_{L_2^1} + \left\|1_D \mathcal{L}^n f\right\|_2 \le A_1 \lambda^n \|f\|_{L_2^1} + B_1 \|f\|_1 + \left\|1_D \mathcal{L}^n f\right\|_2.$$

Furthermore, by (12) and Lemma 6,

$$\left\|1_D \mathcal{L}^n f\right\|_2 \le \sqrt{m(D)} \left\|\mathcal{L}^n f\right\|_\infty$$

$$\le \sqrt{m(D)} \|\kappa\|_\infty \left\|\mathcal{L}^{n-1} f\right\|_1$$

$$\le \sqrt{m(D)} \|\kappa\|_\infty \|f\|_1,$$

which leads to (20) [$m(D)$ denotes the d-dimensional Lebesgue measure of D]. $\square$

Let us define the spaces of zero-average functions in $\mathfrak{B}$ and L^1, respectively, as

$$V_{\mathfrak{B}} = \left\{ f \in \mathfrak{B} : \int f dm = 0 \right\} \qquad (21)$$

and

$$V_{L^1} = \left\{ f \in L^1 : \int f dm = 0 \right\}. \qquad (22)$$

In the rest of this section, we prove results on the functional analytic properties of the operator $\mathcal{L}$, namely, the existence of eigenvalues on the unit circle, the spectral gap, and the boundedness of the resolvent. These results, along with other inferences, give us the uniqueness of the invariant measure of the system in the strong space and its convergence to equilibrium. To prove these results, we extensively use the positivity of the kernel k associated with the operator $\mathcal{L}$.

Lemma 14. *The transfer operator $\mathcal{L}$ has spectral gap on $\mathfrak{B}$ and it has 1 as its simple and only eigenvalue on the unit circle.*

Proof. By Lemma 6, the operator $\mathcal{L}$ is integral preserving, which implies that 1 lies in the spectrum of $\mathcal{L}$.

Recall that, by Lemmas 6 and 13, the operator $\mathcal{L}$ satisfies the hypothesis of Hennion theorem (see Ref. 22, Theorem B.14), which implies that the operator is quasi-compact, which, in turn, implies that it has spectral gap on $\mathfrak{B}$. Consequently, 1 is an eigenvalue of $\mathcal{L}$.

Now, we want to prove that 1 is the unique eigenvalue of $\mathcal{L}$ on the unit circle. Let us suppose, to the contrary, that there exists an eigenvalue $\theta \neq 1$ such that $|\theta| = 1$. Accordingly, there exists a corresponding eigenvector $f_\theta \in \mathfrak{B}$, that is,

$$\mathcal{L}f_\theta = \theta f_\theta.$$

Then, for any $n \in \mathbb{N}$,

$$\left\| \mathcal{L}^{n+1} f_\theta - \mathcal{L}^n f_\theta \right\|_1 = \left\| \theta^n \mathcal{L} f_\theta - \theta^n f_\theta \right\|_1$$
$$= \left\| \mathcal{L} f_\theta - f_\theta \right\|_1.$$

Since $\mathcal{L}$ preserves the integral (Lemma 6), we have

$$\int (\mathcal{L}f_\theta - f_\theta) = \int \mathcal{L}f_\theta - \int f_\theta = \int f_\theta - \int f_\theta = 0.$$

This implies $\mathcal{L}f_\theta - f_\theta (\neq 0) \in V_{\mathfrak{B}}$. Then, since the kernel k is positive (by Theorem 1), we get

$$\left\| \mathcal{L}^n (\mathcal{L}f_\theta - f_\theta) \right\|_1 < \left\| \mathcal{L}^{n-1}(\mathcal{L}f_\theta - f_\theta) \right\|_1 < \left\| \mathcal{L}f_\theta - f_\theta \right\|_1.$$

This contradicts the earlier calculation. Hence, 1 is the only eigenvalue of $\mathcal{L}$ on the unit circle.

Now, to show that 1 is a simple eigenvalue, let $u, v \in \mathfrak{B}$ be two distinct eigenvectors corresponding to the eigenvalue 1. Then,

$$\mathcal{L}u = u, \ \mathcal{L}v = v.$$

Since u and v are fixed points of $\mathcal{L}$, $u - v$ is also a fixed point of $\mathcal{L}$ and, hence, an invariant measure. Notice that $\int u - v = \int u - \int v = 0$, which implies $u - v \in V_{\mathfrak{B}}$. Again, since k is positive, we have $\|\mathcal{L}(u-v)\|_s < \|u-v\|_s$, which contradicts the fact that $u - v$ is a fixed point. Consequently, 1 is a simple eigenvalue of $\mathcal{L}$ on $\mathfrak{B}$. $\square$

A first direct consequence of Lemma 14 is the uniqueness of the invariant probability measure of $\mathcal{L}$.

Proposition 15. *The operator has a unique invariant probability density $f \in \mathfrak{B}$, hence satisfying $\int f = 1$ and $\mathcal{L}f = f$.*

Remark 16. We remark that the unique stationary measure μ of SDE (1) must be also invariant for $\mathcal{L}$, and this must be the unique invariant probability measure found above. This also implies that μ has a density in the strong space $\mathfrak{B}$ (see Remark 2). We conclude that the unique stationary measure of the SDE is indeed equal to the invariant measure of the transfer operator.

The spectral gap and the uniqueness of the invariant probability measure for $\mathcal{L}$ imply the following two classical consequences, which will be used later.

Proposition 17. *For each $f \in V_{\mathfrak{B}}$,*

$$\lim_{n \to +\infty} \left\| \mathcal{L}^n(f) \right\|_s = 0,$$

and the resolvent operator $(Id - \mathcal{L})^{-1} : V_{\mathfrak{B}} \to V_{\mathfrak{B}}$ is a bounded operator.

Proof. By Lemma 14 and the fact that the operator is positive and integral preserving, we get that $\mathcal{L} : \mathfrak{B} \to \mathfrak{B}$ has spectral gap, which implies it can be decomposed as

$$\mathcal{L} = \Pi + \mathcal{Q},$$

where Π is the projection operator onto the one-dimensional eigenspace corresponding to the eigenvalue 1, and the spectral radius of $\mathcal{Q}$ is strictly less than 1, that is $\|\mathcal{Q}\|_s < 1$.

Furthermore, for $f \in V_{\mathfrak{B}}$ we have $\mathcal{L}^n f = \mathcal{Q}^n f$, and

$$\left\| \mathcal{Q}^n f \right\|_s \leq \|\mathcal{Q}^n\|_s \left\| f \right\|_s \leq C e^{-\lambda n} \left\| f \right\|_s$$

for some $C \geq 0$ and $\lambda \in (0, 1)$. The first claim follows directly by this estimate. The second claim also follows from the estimate, since the resolvent operator $(Id - \mathcal{L})^{-1} : V_{\mathfrak{B}} \to V_{\mathfrak{B}}$ can be written as $(Id - \mathcal{L})^{-1} = \sum_{n=0}^{\infty} \mathcal{L}|_{V_{\mathfrak{B}}}^n$. $\square$

Remark 18. We have seen that the transfer operator is quasi-compact when acting on L_2^1. In this remark, we discuss the optimality of the result and the importance of L_2^1 to obtain such a result, showing that the transfer operator neither always have a spectral gap on L^2, nor is always a compact operator on L_2^1 and hence we cannot rely on a simple spectral perturbation theory for such operators.

For simplicity let us illustrate this in the particularly simple, but meaningful case where $d = 1$ and $b(x) = -x$.

We, hence, have the following SDE on the real line:

$$dX_t = -X_t \, dt + dW_t.$$

We will exploit the fact that for such an SDE there are explicit formulas for the evolution of densities through the transfer operator (see, e.g., Ref. 23) when the initial condition is distributed as a Gaussian.

It is well known, in fact, that if for such an SDE, the initial condition is

$$X_0 \sim \mathcal{N}(\mu_0, \sigma_0^2),$$

then X_t has Gaussian distribution for all $t \geq 0$, i.e.,

$$X_t \sim \mathcal{N}\left(\mu(t), \sigma^2(t) \right),$$

where the average is

$$\mu(t) = \mathbb{E}[X_t] = \mu_0 e^{-t},$$

and the variance is

$$\sigma^2(t) = \text{Var}(X_t) = \sigma_0^2 e^{-2t} + \frac{1}{2}\left(1 - e^{-2t}\right).$$

Let $V_{L^2} = \{f \in L^2 : \int f dm = 0\}$. By a reasoning similar to the one done in the proof of Lemma 14 and Proposition 17, if the transfer operator $\mathcal{L}$ had a spectral gap on L^2, there was an iterate $\mathcal{L}^{n_0}$ with n_0 big enough such that $||\mathcal{L}^{n_0}|_{V_{L^2}}||_2 \leq \frac{1}{2}$. Let $x_n \in \mathbb{R}$ be a sequence of points of the type $x_n = 2e^n$, and let us consider a sequence of L^2 distributions in the unit sphere $f_n = \frac{\mathcal{N}(x_n,1) - \mathcal{N}(-x_n,1)}{||\mathcal{N}(x_n,1) - \mathcal{N}(-x_n,1)||_2}$. Now, n_0 big enough corresponds to t large enough in the Fokker–Planck equation, leading to the fact that $L^{n_0}(f_n)$ is the difference of two Gaussian distributions with variance which is smaller than 1 while the two averages diverge as $n \to \infty$. We have then that $\lim_{n\to\infty} \frac{||L^{n_0}(f_n)||_2}{||f_n||_2} \geq 1$, contradicting spectral gap.

Similarly, we can remark that $\mathcal{L}$ is not, in general, a compact operator when acting on L_2^1 by noting that the sequence $g_n = \frac{\mathcal{N}(x_n,1)}{||\mathcal{N}(x_n,1)||_{L_2^1}}$ is a bounded sequence such that $\mathcal{L}g_n$ has no converging subsequences.

IV. PERTURBATIONS AND LINEAR RESPONSE

From now on, we denote the original transfer operator $\mathcal{L}$ defined above by $\mathcal{L}_0$.

As mentioned in Sec. I, to perturb the initial stochastic differential equation (1) that we began with, we perturb the associated transfer operator $\mathcal{L}_0$ (defined in Sec. III). Since the transfer operator $\mathcal{L}_0$ associated with a time discretization t of the system is a kernel operator [see Theorem 1 and Eq. (9)], we perturb the operator by perturbing the associated kernel. We would like to emphasize the fact that this method of perturbation has the limitation that the perturbed system may not correspond to a SDE. Rather, it signifies a "local" change in the initial SDE, whose nature is independent of the SDE model.

The local kernel perturbations are conducted in the following way:

Let $D \subset \mathbb{R}^d$ be a compact set, and let $\bar{\delta} > 0$ be given, then for every $\delta \in [0, \bar{\delta})$, define the family $\kappa_\delta \in L^2(D \times D)$ of kernels as

$$\kappa_\delta = \kappa_0 + \delta \cdot \dot{\kappa} + r_\delta, \tag{23}$$

where $\dot{\kappa}, r_\delta \in L^2(D \times D)$ with $||r_\delta||_2 = o(\delta)$.

Finally, define the linear operators (Hilbert–Schmidt integral operators) $\dot{\mathcal{L}}, \mathcal{L}_\delta : L^1 \to L^1$ by

$$\dot{\mathcal{L}}f(y) := \int \dot{\kappa}(x,y)f(x)dx, \tag{24}$$

$$\mathcal{L}_\delta f(y) := \int \kappa_\delta(x,y)f(x)dx. \tag{25}$$

Let us assume that the operators $\mathcal{L}_\delta$ are integral preserving for every $\delta \in [0, \bar{\delta})$, that is, for each $g \in L^1$,

$$\int \mathcal{L}_\delta g \, dm = \int g \, dm,$$

where m is the Lebesgue measure.

Lemma 19. *For $\delta \in [0, \bar{\delta})$, the operator $\mathcal{L}_\delta$ is integral preserving if and only if both $\dot{\kappa}$ and r_δ are zero average in y direction, that is, for almost each x, $\int \dot{\kappa}(x,y)dy = \int r_\delta(x,y)dy = 0$.*

Proof. The converse part is straightforward; therefore, we prove the forward implication. $\mathcal{L}_\delta$ is integral preserving if and only if, for every $g \in L^1$,

$$\int g \, dm = \int \mathcal{L}_\delta g \, dm$$

$$= \int \int \kappa_\delta(x,y)g(x) \, dxdy$$

$$= \int \int (\kappa_0 + \delta\dot{\kappa} + r_\delta)(x,y)g(x) \, dxdy$$

$$= \int \int \kappa_0(x,y)g(x) \, dxdy + \int \int (\delta\dot{\kappa} + r_\delta)(x,y)g(x) \, dxdy$$

$$= \int \int g(x) \, dxdy + \int \int (\delta\dot{\kappa} + r_\delta)(x,y)g(x) \, dxdy.$$

Thus, the above equality reduces to, for every $g \in L^1$,

$$\int \int (\delta\dot{\kappa} + r_\delta)(x,y)g(x) \, dxdy = 0 = \int \int (\delta\dot{\kappa} + r_\delta)(x,y)g(x) \, dydx.$$

Hence, for almost every $x \in \mathbb{R}^d$,

$$0 = \int (\delta\dot{\kappa} + r_\delta)(x,y)g(x) \, dy = \int \delta\dot{\kappa}(x,y)g(x) \, dy + \int r_\delta(x,y)g(x) \, dy.$$

That is,

$$\int \dot{\kappa}(x,y)g(x) \, dy = -\int \frac{r_\delta}{\delta}(x,y)g(x) \, dy.$$

Taking limit $\delta \to 0$ both sides, we get

$$\lim_{\delta\to 0} \int \dot{\kappa}(x,y)g(x) \, dy = -\lim_{\delta\to 0} \int \frac{r_\delta}{\delta}(x,y)g(x). \, dy = 0.$$

Since so is true for all $g \in L^1$, we get that for almost all $x \in \mathbb{R}^d$, $\int \dot{\kappa}(x,y)dy = 0$, which implies $\int r_\delta(x,y) \, dy = 0$. □

Now recall that by Proposition 15, there exists an invariant density $f_0 \in \mathfrak{B}$ (the eigenvector corresponding to the eigenvalue 1) of the operator $\mathcal{L}_0$. Consequently, we have the following lemma.

Lemma 20. *The operators $\dot{\mathcal{L}}$ and $\mathcal{L}_\delta$ restricted to the strong space $\mathfrak{B}$ satisfy the following limit:*

$$\lim_{\delta\to 0} \left\| \frac{\mathcal{L}_\delta - \mathcal{L}_0}{\delta}f_0 - \dot{\mathcal{L}}f_0 \right\|_s = 0,$$

where f_0 is the invariant density for the operator $\mathcal{L}_0$.

Proof. By definition,

$$\left\| \frac{\mathcal{L}_\delta - \mathcal{L}_0}{\delta} f_0 - \dot{\mathcal{L}} f_0 \right\|_s$$

$$= \left\| \int \frac{\kappa_\delta(x,y) - \kappa_0(x,y)}{\delta} f_0(x)\, dx - \int \dot{\kappa}(x,y) f_0(x)\, dx \right\|_s$$

$$= \left\| \int \frac{r_\delta(x,y)}{\delta} f_0(x)\, dx \right\|_s$$

$$= \left\| \int \frac{r_\delta(x,y)}{\delta} f_0(x)\, dx \right\|_{L_2^1} + \left\| 1_D \int \frac{r_\delta(x,y)}{\delta} f_0(x)\, dx \right\|_2.$$

Now using Holder's inequality and the fact that r_δ has compact support, there exists $C > 0$ such that

$$\left\| \frac{\mathcal{L}_\delta - \mathcal{L}_0}{\delta} f_0 - \dot{\mathcal{L}} f_0 \right\|_s$$

$$\leq \|1_D \rho_2\|_2 \left\| \int \frac{r_\delta(x,y)}{\delta} f_0(x)\, dx \right\|_2 + \left\| \int \frac{r_\delta(x,y)}{\delta} f_0(x)\, dx \right\|_2$$

$$\leq (\|1_D \rho_2\|_2 + 1) \left\| \int \frac{r_\delta(x,y)}{\delta} f_0(x)\, dx \right\|_2$$

$$\leq (\|1_D \rho_2\|_2 + 1) \|1_D f_0\|_2 \left\| \frac{r_\delta}{\delta} \right\|_2$$

$$\leq \frac{C}{\delta} \|1_D f_0\|_2 \to 0,$$

where ρ_2 is as described in (13), $C > 0$ is some constant, and the second last inequality comes from (11). $\square$

The above lemma implies that the operator $\dot{\mathcal{L}}$ can be thought of as the derivative, with respect to δ, of the operator $\mathcal{L}_\delta$. Now, we are interested to consider the linear response of our systems to such perturbations. However, first, let us understand how close the perturbed operators $\mathcal{L}_\delta$ are to the initial operator $\mathcal{L}_0$.

Lemma 21. *Let $\mathcal{L}_\delta$ be a family of transfer operators associated with the kernels κ_δ as before. Then, there exist constants $\bar{\delta}, C \geq 0$ such that for each $\delta \in [0, \bar{\delta})$,*

$$\|\mathcal{L}_0 - \mathcal{L}_\delta\|_{\mathfrak{B} \to L^1} \leq C\delta. \tag{26}$$

Proof. Let $f \in \mathfrak{B}$ be such that $\|f\|_s \leq 1$. Since $\delta\dot{\kappa} + r_\delta$ is compactly supported on $D \times D$, it implies that $(\delta\dot{\kappa} + r_\delta)f$ is also compactly supported in D. Using the fact that inside set D, by Cauchy–Schwartz inequality, the norms satisfy $\|\cdot\|_1 \leq C_1 \|\cdot\|_2$, for some $C_1 > 0$, we have

$$\|(\mathcal{L}_\delta - \mathcal{L}_0)f\|_1 = \left\| \int (\delta\dot{\kappa} + r_\delta)(x,y) f(x) dx \right\|_1$$

$$\leq C_1 \left\| \int (\delta\dot{\kappa} + r_\delta)(x,y) f(x) dx \right\|_2$$

$$= C_1 \left\| \delta\dot{\mathcal{L}} f + \int r_\delta(x,y) f(x) dx \right\|_2$$

$$\leq \delta C_1 \|\dot{\kappa}\|_2 \|f_D\|_2 + C_1 \|r_\delta\|_2 \|f_D\|_2,$$

where we have used that $\dot{\kappa}, r_\delta \in L^2(D \times D)$ and in the last inequality, we used (11). Since $\|r_\delta\|_2 = o(\delta)$, there exists $C > 0$ such that

$\|\delta C_1 \dot{\kappa} + C_1 r_\delta\|_2 \leq C\delta$. Finally, using $\|f_D\|_2 \leq \|f\|_s \leq 1$, we have the result. $\square$

To obtain a result on linear response, we need the perturbed operators to possess certain properties, such as the Lasota–Yorke inequality, the existence of an invariant density, and a bounded resolvent. We prove these properties in the following lemmas.

Lemma 22. *Let $\mathcal{L}_\delta$ be the family of transfer operators associated with the kernels κ_δ as above. Then, there exist constants $A, B, \bar{\delta} > 0$, $\lambda < 1$ such that for each $\delta \in [0, \bar{\delta})$, $n \geq 0$,*

$$\|\mathcal{L}_\delta^n f\|_s \leq A\lambda^n \|f\|_s + B \|f\|_1. \tag{27}$$

Proof. We have that

$$\|\mathcal{L}_\delta f - \mathcal{L}_0 f\|_s$$

$$= \left\| \mathcal{L}_0 f + \delta \int \dot{\kappa}(x,y) f(x) dx + \int r_\delta(x,y) f(x)\, dx - \mathcal{L}_0 f \right\|_s$$

$$= \left\| \int (\delta\dot{\kappa}(x,y) + r_\delta(x,y)) f(x) dx \right\|_s$$

$$\leq \left\| \int (\delta\dot{\kappa} + r_\delta) f(x) dx \right\|_{L_2^1} + \left\| 1_D \int (\delta\dot{\kappa} + r_\delta) f(x) dx \right\|_2$$

$$\leq (\|1_D \rho_2\|_2 + 1) \left\| \int (\delta\dot{\kappa} + r_\delta) f(x) dx \right\|_2,$$

where in the last inequality, we have used Holder's inequality and the fact that $\dot{\kappa}(x,y)$ and $r_\delta(x,y)$ are supported only in D. Now, using (11) and the fact that $\|r_\delta\|_2 = o(\delta)$, there exists $C_1 > 0$ such that

$$\|\mathcal{L}_\delta f - \mathcal{L}_0 f\|_s \leq \delta C_1 \|1_D f\|_2 \leq \delta C_1 \|f\|_s. \tag{28}$$

Hence, there exists $C(n) \geq 0$ (depending on n) such that

$$\|\mathcal{L}_\delta^n f - \mathcal{L}_0^n f\|_s \leq \delta C(n) \|f\|_s.$$

By Theorem 13,

$$\|\mathcal{L}_\delta^n f\|_s \leq \|\mathcal{L}_\delta^n f - \mathcal{L}_0^n f\|_s + \|\mathcal{L}_0^n f\|_s$$

$$\leq \|\mathcal{L}_0^n f\|_s + \delta C(n) \|f\|_s$$

$$\leq A\lambda^n \|f\|_s + B \|f\|_1 + \delta C(n) \|f\|_s$$

$$\leq (A\lambda^n + \delta C(n)) \|f\|_s + B \|f\|_1.$$

Taking n_1 large enough, so that $A\lambda^{n_1} \leq \frac{1}{3}$ and $\delta \in [0, \bar{\delta})$ so small such that $\delta C(n_1) \leq \frac{1}{3}$, we get

$$\|\mathcal{L}_\delta^{n_1} f\|_s \leq \frac{2}{3} \|f\|_s + B \|f\|_1.$$

Then, for every $m \in \mathbb{N}$, we get

$$\|\mathcal{L}_\delta^{mn_1} f\|_s \leq \left(\frac{2}{3} \right)^m \|f\|_s + (B+2) \|f\|_1.$$

Similarly, for any $n < n_1$, $\|\mathcal{L}_\delta^{n_1+n} f\|_s \leq \frac{2}{3}(3\delta C_1 + A\lambda)^n \|f\|_s + C_2 \|f\|_1$, proving a uniform Lasota–Yorke inequality for $\mathcal{L}_\delta$. $\square$

Proposition 23. *For operators $\mathcal{L}_\delta$, and for δ small enough, there exists a unique invariant density $f_\delta \in \mathfrak{B}$ with $\int f_\delta = 1$, that is, $L_\delta f_\delta = f_\delta$.*

Proof. First, recall that for all $\delta \in [0, \bar{\delta})$, the operators $\mathcal{L}_\delta$ are integral preserving, which implies that 1 lies in the spectrum of $\mathcal{L}_\delta$. Indeed, consider the dual operators $\mathcal{L}_\delta^*$; the fact that the operators are integral preserving implies that the Lebesgue measure is invariant for the dual operator $\mathcal{L}_\delta^*$. Accordingly, $\mathcal{L}_\delta^* 1 = 1$, that is, 1 is in the spectrum of the dual operators and, hence, in the spectrum of operators $\mathcal{L}_\delta$ for all $\delta \geq 0$.

Now, recall that by Lemma 14, 1 is the only eigenvalue of $\mathcal{L}_0$ on the unit circle. Observe that for every $\delta \in [0, \bar{\delta})$, the operator $\mathcal{L}_\delta$ is a weak contraction on L_1 and satisfies Lasota–Yorke inequality (by Lemma 22). Further, using Lemma 21, and the fact that $\mathfrak{B}$ is compactly immersed inside L^1 (Lemma 12), we get, using Ref. 24, Theorem 1 that the isolated eigenvalues of $\mathcal{L}_\delta$ are arbitrarily close to that of $\mathcal{L}_0$, that is, the leading eigenvalue λ_δ of $\mathcal{L}_\delta$ is also simple and satisfies that

$$\lim_{\delta \to 0} \lambda_\delta = 1,$$

which, in turn, implies that $\lambda_\delta = 1$ for small enough $\delta \in [0, \bar{\delta})$. Accordingly, there exists $f_\delta \in \mathfrak{B}$ such that $\mathcal{L}_\delta f_\delta = f_\delta$ satisfying $\int f_\delta = 1$ being a probability density. Note that such an invariant density is unique. Indeed, if there exists another invariant density $g_\delta \in \mathfrak{B}$, then note that $\int (f_\delta - g_\delta) = \int f_\delta - \int g_\delta = 1 - 1 = 0$, which implies

$$\int |f_\delta - g_\delta| = 0 = \|f_\delta - g_\delta\|_1 .$$

Accordingly, using (12),

$$\begin{aligned}
\|f_\delta - g_\delta\|_\infty = \|\mathcal{L}_\delta f_\delta - \mathcal{L}_\delta g_\delta\|_\infty &= \|\mathcal{L}_\delta (f_\delta - g_\delta)\|_\infty \\
&\leq \|\kappa_\delta\|_\infty \|f_\delta - g_\delta\|_1 \\
&\leq \|\kappa_\delta\|_\infty \|f_\delta - g_\delta\|_1 \\
&= 0,
\end{aligned}$$

hence the uniqueness. $\square$

To be able to state the linear response result, the last ingredient we need is the bounds on the resolvent of perturbed operators and, hence, the following lemma. Recall the definition of $V_\mathfrak{B}$ and V_{L^1} given by (21) and (22), respectively.

Lemma 24. *For $\delta > 0$ small enough, the resolvent operators of the perturbed operators $\mathcal{L}_\delta$, given by $(Id - \mathcal{L}_\delta)^{-1}$, are well-defined and satisfy*

$$\left\| (Id - \mathcal{L}_\delta)^{-1} \right\|_{V_\mathfrak{B} \to V_{L^1}} < +\infty$$

and

$$\lim_{\delta \to 0} \left\| (Id - \mathcal{L}_\delta)^{-1} - (Id - \mathcal{L}_\delta)^{-1} \right\|_{V_\mathfrak{B} \to V_{L^1}} = 0.$$

Proof. Note that operators $\mathcal{L}_\delta$ are weak contractions on L_1, satisfy Lasota–Yorke inequality (by Lemma 22), and, by the fact that $\|\mathcal{L}_0 - \mathcal{L}_\delta\|_{\mathfrak{B} \to L^1} \leq C\delta$ (by Lemma 21), we can use Ref. 24, Theorem 1 to get the result. $\square$

Finally, we can state a response result adapted to our kind of systems and perturbations.

Theorem 25. *For the operators $\mathcal{L}_\delta$, for $\delta > 0$ small enough, we have linear response, that is,*

$$\lim_{\delta \to 0} \left\| \frac{f_\delta - f_0}{\delta} - (Id - \mathcal{L}_0)^{-1} \dot{\mathcal{L}} f_0 \right\|_1 = 0.$$

Though, in this work, we consider operators that are not necessarily positive, the proof of the above statement is similar to many other linear response results (see, e.g., Ref. 13, Theorem 12, Appendix A). We include it for completeness.

Proof. By Proposition 23, we know that for each $\delta \in [0, \bar{\delta})$, the operator $\mathcal{L}_\delta$ has a fixed point f_δ. Accordingly, we get

$$\begin{aligned}
(Id - \mathcal{L}_\delta) \frac{f_\delta - f_0}{\delta} &= \frac{f_\delta - f_0}{\delta} - \frac{\mathcal{L}_\delta f_\delta - \mathcal{L}_\delta f_0}{\delta} \\
&= \frac{-f_0 + \mathcal{L}_\delta f_0}{\delta} \\
&= \frac{1}{\delta} (\mathcal{L}_\delta - \mathcal{L}_0) f_0 .
\end{aligned}$$

By the preservation of integral, for each δ, L_δ preserves $V_\mathfrak{B}$. Since for all $\delta > 0$, $\frac{L_\delta - L_0}{\delta} f_0 \in V_\mathfrak{B}$ and by Lemma 24, for δ small enough, $(Id - L_\delta)^{-1} : V_\mathfrak{B} \to V_{L^1}$ is a uniformly bounded operator. Accordingly, we can apply the resolvent to both sides of the expression above to get

$$(Id - \mathcal{L}_\delta)^{-1} (Id - \mathcal{L}_\delta) \frac{f_\delta - f_0}{\delta}$$

$$= (Id - \mathcal{L}_\delta)^{-1} \frac{\mathcal{L}_\delta - \mathcal{L}_0}{\delta} f_0 \qquad (29)$$

$$= \left[(Id - \mathcal{L}_\delta)^{-1} - (Id - \mathcal{L}_0)^{-1} + (Id - \mathcal{L}_0)^{-1} \right] \frac{\mathcal{L}_\delta - \mathcal{L}_0}{\delta} f_0 . \qquad (30)$$

Since, by Lemma 24, $\left\| (Id - \mathcal{L}_\delta)^{-1} - (Id - \mathcal{L}_0)^{-1} \right\|_{V_\mathfrak{B} \to V_{L^1}} \to 0$, we have

$$\left\| [(Id - \mathcal{L}_\delta)^{-1} - (Id - \mathcal{L}_0)^{-1}] \frac{\mathcal{L}_\delta - \mathcal{L}_0}{\delta} f_0 \right\|_{L^1}$$

$$\leq \left\| (Id - \mathcal{L}_\delta)^{-1} - (Id - \mathcal{L}_0)^{-1} \right\|_{V_\mathfrak{B} \to V_{L^1}} \left\| \frac{\mathcal{L}_\delta - \mathcal{L}_0}{\delta} f_0 \right\|_s$$

$$\to 0.$$

Further, Lemma 20 implies that $\lim_{\delta \to 0} \frac{\mathcal{L}_\delta - \mathcal{L}_0}{\delta} f_0$ converges in $V_\mathfrak{B}$; then, (29) implies that

$$\begin{aligned}
0 &= \lim_{\delta \to 0} \left\| \frac{f_\delta - f_0}{\delta} - (Id - \mathcal{L}_0)^{-1} \frac{\mathcal{L}_\delta - \mathcal{L}_0}{\delta} f_0 \right\|_{L^1} \\
&= \lim_{\delta \to 0} \left\| \frac{f_\delta - f_0}{\delta} - (Id - \mathcal{L}_0)^{-1} (\dot{\mathcal{L}} f_0) \right\|_{L^1} .
\end{aligned}$$

$\square$

V. OPTIMIZATION OF RESPONSE

A. Optimization of the expectation of an observable

Consider the set $P \subset L^2(D \times D)$ of allowed infinitesimal perturbations $\dot{\kappa}$ (as described in Sec. IV) to the kernel κ_0. Fix an observable $\phi \in L^\infty$; we are interested in finding, from the set of allowed perturbations, an *optimal* perturbation $\dot{\kappa}_{opt}$ that maximizes the rate of change of the expectation of ϕ. To perform the optimization, we assume that P is a bounded, closed, and convex subset of the Hilbert space $L^2(D \times D)$.

We believe that the above hypotheses on P are natural; convexity is so because if two different perturbations of a system are possible, then their convex combination—applying the two perturbations with different intensities—should also be possible.

Let $\phi \in L^\infty(\mathbb{R}^d, \mathbb{R})$ be an observable. If ϕ were the indicator function of a certain set, for example, one could control the invariant density toward the support of ϕ.

Given a family of kernels $\kappa_\delta = \kappa_0 + \delta \dot{\kappa} + r_\delta$ (as in Lemma 20) with associated transfer operators $\mathcal{L}_\delta$ and invariant densities $f_{\kappa,\delta}$, we denote the response of the system to $\dot{\kappa}$ by

$$R(\dot{\kappa}) = \lim_{\delta \to 0} \frac{f_{\dot{\kappa},\delta} - f_0}{\delta}. \tag{31}$$

This limit converges in L^1 as proved in Theorem 25.

Lemma 26. *The operator $R : L^2(D \times D) \to L^1$ defined in (31) is continuous.*

Proof. Using Theorem 25, we have

$$R(\dot{\kappa}) = \lim_{\delta \to 0} \frac{f_{\dot{\kappa},\delta} - f_0}{\delta} = (Id - \mathcal{L}_0)^{-1} \dot{\mathcal{L}} f_0,$$

which implies that

$$\|R(\dot{\kappa})\|_1 \leq \|R(\dot{\kappa})\|_s \leq \left\| (Id - \mathcal{L}_0)^{-1} \right\|_s \left\| \dot{\mathcal{L}} f_0 \right\|_s.$$

Thanks to Proposition 17, operator $(Id - \mathcal{L}_0)^{-1}$ is bounded, and, thus, $\left\| (Id - \mathcal{L}_0)^{-1} \right\|_s$ is finite. Consider the following:

$$\left\| \dot{\mathcal{L}} f_0 \right\|_s = \left\| \int \dot{\kappa}(x,y) f_0(x) dx \right\|_s$$

$$= \left\| \int \dot{\kappa}(x,y) f_0(x) dx \right\|_{L_2^1} + \left\| 1_D \int \dot{\kappa}(x,y) f_0(x) dx \right\|_2.$$

Using Holder's inequality and the fact that $\dot{\kappa}$ has compact support, we get

$$\left\| \int \dot{\kappa}(x,y) f_0(x) dx \right\|_{L_2^1} \leq \|1_D \rho_2\|_2 \left\| \int \dot{\kappa}(x,y) f_0(x) dx \right\|_2,$$

where ρ_2 is the same as given in (13). Finally, using (12) and again the fact that $\dot{\kappa}$ has compact support, there exists $C \geq 0$ such that

$$\left\| \dot{\mathcal{L}} f_0 \right\|_s \leq (\|1_D \rho_2\|_2 + 1) \left\| \int \dot{\kappa}(x,y) f_0(x) dx \right\|_2$$

$$\leq (\|1_D \rho_2\|_2 + 1) \|1_D f_0\|_2 \|\dot{\kappa}\|_2$$

$$\leq C \|1_D f_0\|_2$$

$$\leq C \|f_0\|_s.$$

The above calculation implies the operator R is bounded and, hence, continuous. □

Under our assumptions, since $\phi \in L^\infty$, we easily get

$$\lim_{\delta \to 0} \frac{\int \phi(x) f_\delta(x) \, dx - \int \phi(x) f_0(x) \, dx}{\delta} = \int \phi(x) R(\dot{\kappa})(x) \, dx. \tag{32}$$

Hence, the rate of change of the expectation of ϕ with respect to δ is given by the linear response of the system under the given perturbation. To take advantage of the general results of the Appendix,

we perform the optimization of $\dot{\kappa}$ over the closed, bounded, and convex subset P of the Hilbert space $\mathfrak{H} = L^2(D \times D)$ containing the zero perturbation. To maximize the RHS of (32), we set

$$\mathcal{J}(\dot{\kappa}) := -\int \phi(x) \cdot R(\dot{\kappa})(x) \, dx$$

and consider the following problem:

Problem 27. *Find the solution $\dot{\kappa}_{opt}$ to*

$$\max \left\{ \mathcal{J}(\dot{\kappa}) \ : \ \dot{\kappa} \in L^2(D \times D), \ \|\dot{\kappa}\|_2 \leq 1 \right\}. \tag{33}$$

To answer the above problem, we state a rather general following result:

Proposition 28. *Let $P \subset L^2$ be a closed, bounded, and strictly convex set such that its relative interior contains the zero vector. If $\mathcal{J}$ is not uniformly vanishing on P, then the problem*

$$\max \{ \mathcal{J}(\dot{\kappa}) \ : \ \dot{\kappa} \in P \}$$

has a unique solution.

Proof. The linearity of R from Lemma 26 implies that the function $\dot{\kappa} \mapsto \int \phi(x) R(\dot{\kappa})(x) dx$ is continuous. Since P satisfies the hypothesis, we can apply Propositions 30 and 31 to get the result. □

Finally, to address Problem 27, note that the perturbations $\dot{\kappa}$ lie in the closed unit ball of $L^2(D \times D)$, which is a closed, bounded, and a strictly convex set having the zero vector in its interior. Thus, we get the unique kernel perturbation $\dot{\kappa}_{opt}$ using Proposition 28.

B. Numerical scheme for the approximation of the optimal perturbation

In this section, we present a simple numerical recipe to obtain a Fourier approximation of the optimal perturbation $\dot{\kappa}_{opt}$ in Problem 27. Similar methods based on Fourier approximation on suitable Hilbert spaces were used in Refs. 13 and 25.

By Lemma 26, and the fact that $\phi \in L^\infty$, we obtained in the proof of Proposition 28 that $\mathcal{J} : L^2(D \times D) \to \mathbb{R}$ is continuous. Thus, $L^2(D \times D)$ being a Hilbert space, by using Riesz's representation theorem, there exists $g \in L^2$ such that

$$\mathcal{J}(\dot{\kappa}) = \langle g, \dot{\kappa} \rangle,$$

which implies that

$$\dot{\kappa}_{opt} = \frac{g}{\|g\|_2}.$$

Now we state how to approximate g by computing its Fourier coefficients. Consider an orthonormal basis $\{h_i\}_{i \in \mathbb{N}}$ of $L^2(D \times D)$ (One can consider the basis consisting of indicator functions, or that of Hermite polynomials, etc.) and define

$$G_i = \langle g, h_i \rangle = \mathcal{J}(h_i) = \int \phi \, dR(h_i).$$

We have then that the sequence $\Sigma_{i=0}^n G_i h_i$ converges to g as $n \to \infty$.

VI. NUMERICAL EXPERIMENTS

In this section, we present numerical experiments related to Problem 27.

We find the optimal infinitesimal perturbation that maximizes the expected value of an observable, as discussed in Sec. V A. We will consider a suitable SDE on the real line and on this simple example, we search for the optimal perturbation in order to maximize the increase of a certain observable.

Specifically, in Sec. VI A, we present and describe the details of the gradient SDE that will express the dynamics of each of our experiments. Section VI B is aimed at describing a classical finite difference method used to solve the partial derivative equation of the parabolic type that identifies the solution law of the SDE. Section VI C presents how to numerically find the solution to the problem presented in Sec. V B. Finally, Sec. VI D presents and explains the results of our experiments. They consist of taking observables as probability density functions of Gaussian variables: symmetric with respect to the domain in the first case and asymmetric in the second.

A. Gradient system and Fokker–Planck equation

We consider, for a noise intensity, $\varepsilon > 0$ and a final time $T > 0$, the SDE given by

$$dY_t^x = -V'\left(Y_t^x\right)dt + \varepsilon dW_t, \quad t \in (0, T),$$
$$Y_0^x = x, \tag{34}$$

where $V(y) = \frac{y^4}{4} - \frac{y^2}{2}$ is a symmetric double-well potential. $(W_t)_t$ denotes a Brownian Motion (BM) and $x \in \mathbb{R}$ is a deterministic initial condition. The final time $T > 0$ will be the time in which we investigate the optimal response in Sec. VI C. In other words, we will numerically investigate the properties of the transfer operator associated with the evolution of the SDE from time $t = 0$ to time $t = T$.

This SDE, which belongs to the class of gradient systems, is often used to describe bistability in many applications, such as phase separation in physics or abrupt climate shifts in paleoclimate studies. If $\varepsilon = 0$, the dynamical system given by (34) presents three fixed points: ± 1 and 0. The former are asymptotically stable and correspond to the minimum points of V; the latter is unstable, since it corresponds to a local maximum point of V.

Considering the case $\varepsilon > 0$, the existence and uniqueness of a solution is classical. Indeed, since the drift term $y \mapsto y - y^3$ is locally Lipschitz, SDE (34) admits, locally in time, an almost everywhere (a.e.) continuous strong solution (see Ref. 26 for more details). Further, since the potential V is coercive, finite time explosion of the solution can be ruled out (Ref. 27, Theorem 3.5), resulting in the existence and uniqueness of a strong solution $(Y_t^x)_{0 \le t \le T}$, for any $T > 0$. Furthermore, since the potential V is regular and coercive, Hormander's theorem assures that the law $\mathcal{L}_{Y_t^x}$ of Y_t^x has a C^∞ density $y \mapsto p^x(y, t)$ with respect to the Lebesgue measure on $\mathbb{R}$ (see Refs. 28 and 29, Section 7). It satisfies, in the weak sense, the Fokker–Planck equation (FPE) (Refs. 30–32)

$$\begin{cases} \partial_t p^x - \dfrac{\varepsilon^2}{2}\Delta_y p^x + \partial_y\left(pb\right) = 0, & x \quad (y, t) \in \mathbb{R} \times (0, T), \\ p(0, y) = \delta_x(y), & y \in \mathbb{R}, \end{cases} \tag{35}$$

where $b(y) = -V'(y) = y - y^3$ is the drift term of SDE (34) and δ_x denotes the Dirac delta concentrated in x. Note that, given the final time $T > 0$, which is the same time at which we investigate the linear response, the kernel $\kappa(x, y)$ defining the transfer operator $\mathcal{L}_0$ is given by

$$\kappa(x, y) := p^x(y, T).$$

A numerical approximation of the kernel is represented in Fig. 1(a), obtained for $T = 1$ and $\varepsilon = 0.25$. Given an initial condition x, the probability density function (PDF) p is concentrated around either 1

(A) Kernel $(x, y) \mapsto \kappa(x, y)$

(B) Invariant density for $\mathcal{L}_0$
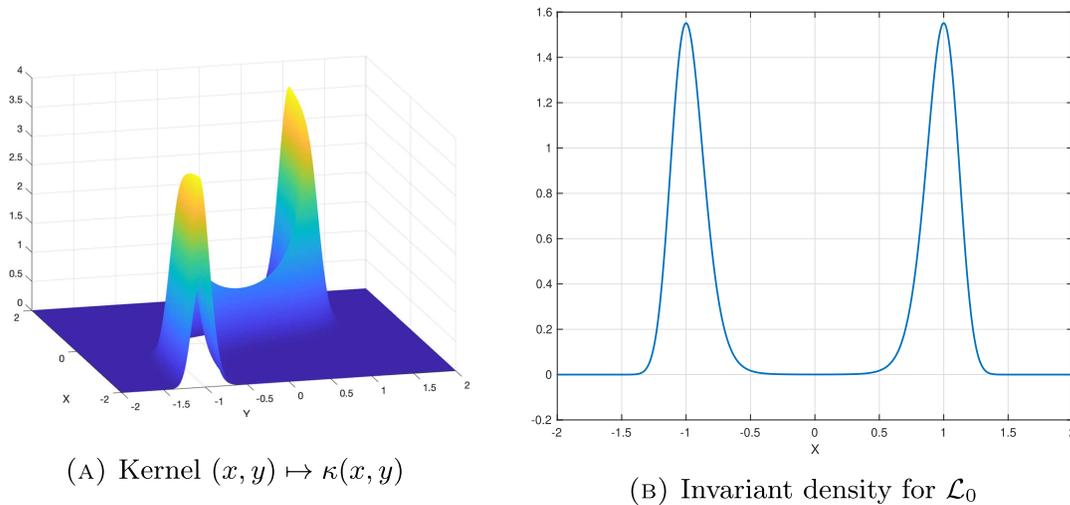
FIG. 1. Numerical approximation for (a) kernel $\kappa(x, y) = p^x(y, T)$, where p is a solution of the FPE (36), and (b) invariant density for the transfer operator $\mathcal{L}_0$. The final time is $T = 1$, the noise intensity is $\varepsilon = 0.25$, and the domain is $\Omega = (-2, 2)$, while the mesh sizes are $\Delta x = \Delta x = 2 \times 10^{-3}$. (a) Kernel $(x, y) \mapsto \kappa(x, y)$. (b) Invariant density for $\mathcal{L}_0$.

or -1, depending on the sign of the initial condition. This bistability is clear also in Fig. 1(b), which depicts the invariant density f_0 for $\mathcal{L}_0$. In fact, it is symmetric, with two maximum points in ± 1. In Sec. VI B, we are going to describe our numerical approximation for the solution of the FPE and how to use it to study the linear response problem.

B. Finite difference method for the Fokker–Planck equation

We apply an implicit finite difference (FD) method[33,34] to approximate the solution of the parabolic problem (35) in the finite domain $\Omega \times (0, T) = (-a, a) \times (0, T)$, with the constraint to choose a sufficiently large $a > 0$ such that p, which describes a PDF, is negligible on Ω^c. FPE (35) is a second-order parabolic PDE, and to consider a solution, we need to complete it with boundary conditions at the end of the domain Ω. We choose reflecting boundary conditions, which means that no probability mass can escape the domain $\Omega = (-a, a)$.[30] This leads to

$$
\begin{cases}
\partial_t p^x - \dfrac{\varepsilon^2}{2} \Delta_y p^x + \partial_y (pb) = 0, & (y, t) \in \Omega \times (0, T), \\[2mm]
\dfrac{\varepsilon^2}{2} \partial_y p(-a, t) - p(-a, t) b(-y) = 0, & t > 0, \\[2mm]
\dfrac{\varepsilon^2}{2} \partial_y p(a, t) - p(a, t) b(y) = 0, & t > 0, \\[2mm]
p(0, y) = \delta_x(y), & y \in \Omega.
\end{cases}
\tag{36}
$$

First, we consider a uniform mesh of the space and time domain, i.e., we fix

$$
y_i := -a + i \Delta y, \quad i = 0, \ldots, m, \quad \Delta y = \frac{2a}{n}
$$

and

$$
t_j := j \Delta t, \quad j = 0, \ldots, m, \quad \Delta t = \frac{T}{m},
$$

where $n, m > 0$ determine the number of points in the meshes. We denote by

$$
p_{ij} := u(y_i, t_j), \quad i = 0, \ldots, n, \ j = 0, \ldots, m,
$$

the numerical approximation for the solution of (36). Similarly, we set

$$
b_i = b(x_i), \quad i = 0, \ldots, n.
$$

Second, we use the centered formula to approximate the second derivative, i.e.,

$$
\Delta_y p_{|(y,t)=(y_i, t_j)} \approx \frac{p_{i-1,j+1} - 2 p_{i,j+1} + p_{i+1,j+1}}{\Delta x^2},
$$

and a centered difference for the first derivative

$$
\partial_y (pb)_{|(y,t)=(y_i, t_j)} \approx \frac{p_{i+1,j+1} b_{i+1} - p_{i-1,j+1} b_{i-1}}{2\Delta x}.
$$

Note that in the previous equations, when we are at the boundary of Ω, there appear the terms $p_{-1,j}, p_{n+1,j}, b_{-1}$, and b_{n+1}. The former are just auxiliary unknowns, since the solution p of the FPE is not defined outside $\Omega \times (0, T)$; the latter are defined as

$$
b_{-1} = b(y_{-1}), \quad b_{n+1} = b(y_{n+1}).
$$

In addition to this, to approximate the Dirac Delta, we consider the same mesh for the initial condition domain, i.e., we set

$$
x_l = y_l, \quad l = 0, \ldots, n.
$$

Furthermore, for each $l = 0, \ldots, n$ we approximate the Dirac Delta δ_{x_i} with the PDF f_{μ_l, σ^2} of a Gaussian random variable with mean $\mu_l = x_l$ and standard deviation $\sigma = 10^2 \cdot \Delta x$.

In conclusion, for each $l > 0$, the implicit FD that we apply can be written as

$$
\begin{cases}
\dfrac{p_{i,j+1} - p_{i,j}}{\Delta t} = \dfrac{\varepsilon}{2\Delta x^2} \left(p_{i-1,j+1} - 2 p_{i,j+1} + p_{i+1,j+1} \right) - \dfrac{p_{i+1,j+1} b_{i+1} - p_{i-1,j+1} b_{i-1}}{2\Delta x}, & i = 0, \ldots, n, \ j = 1, \ldots, m, \\[2mm]
0 = \dfrac{\varepsilon^2}{2} \left(\dfrac{p_{1,j} - p_{-1,j}}{2\Delta x} \right) - p_0 b_0, & j = 1, \ldots, m, \\[2mm]
0 = \dfrac{\varepsilon^2}{2} \left(\dfrac{p_{n+1,j} - p_{n-1,j}}{2\Delta x} \right) - p_n b_n, & j = 1, \ldots, m, \\[2mm]
p_{i,0} = f_{\mu_l, \sigma}(y_i), & i = 0, \ldots, n.
\end{cases}
\tag{37}
$$

C. Numerical scheme for the optimal response problem

In this section, we describe how to numerically approximate the solution of

$$
\min \left\{ \mathcal{J}(\dot{\kappa}) \ \middle| \ \dot{\kappa} \in L^2(D), \ \|\dot{\kappa}\|_{L^2(D)} \leq 1 \right\},
\tag{38}
$$

where $D = [-d, d] \subsetneq \Omega$. We know that, given an observable $\phi \in L^\infty$, the optimal perturbation is given by

$$
g = \frac{\sum_{r=0}^{+\infty} G_r h_r}{\left(\sum_{r=0}^{+\infty} G_r^2 \right)^{1/2}},
$$

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where $(h_r)_r$ denotes an orthonormal basis of $L^2(D \times D)$ and

$$G_r = \int_D \phi(y)(Id - \mathcal{L}_0)^{-1} \int_D h_r(x,y)f_0(x)dxdy.$$

Further, f_0 denotes the invariant density for $\mathcal{L}_0$. In particular, we consider as basis of $L^2(D \times D)$ the sine-cosine wavelets $\mathcal{B}$ defined as

$$\mathcal{B} = \bigcup_{i \geq 1, j \geq 0} \left\{ \frac{1}{\sqrt{2d}} \cos\left(i\frac{\pi}{d}x\right) \cdot \cos\left(j\frac{\pi}{d}y\right), \frac{1}{\sqrt{2d}} \cos\left(i\frac{\pi}{d}x\right) \right.$$
$$\cdot \sin\left(j\frac{\pi}{d}y\right), \frac{1}{\sqrt{2d}} \sin\left(i\frac{\pi}{d}x\right) \cdot \cos\left(j\frac{\pi}{d}y\right), \frac{1}{\sqrt{2d}} \sin\left(i\frac{\pi}{d}x\right)$$
$$\left. \cdot \sin\left(j\frac{\pi}{d}y\right) \right\}.$$

Note that we avoid inserting the wavelets with index $i = 0$ in the basis $\mathcal{B}$ defining the vector space of the allowed perturbation, since we impose that any perturbation $\dot{\kappa}$ needs to satisfy $\int_D \dot{\kappa}(x,y)dx = 0$. Then, for each r, we approximate the coefficient G_r as follows.

Let $I_1 = \{x_i \mid x_i \in D\} = \{x_i'\}_{i=0,\ldots,n_1}$ and $|I_1| = n_1 + 1$. We adopt the same notation for $I_2 = \{y_j \mid y_j \in D\} = \{y_j'\}_{j=0,\ldots,n_1}$. First, the definite integral defining G_r is approximated by using the composite Simpson's 1/3 rule,[35] which leads to

$$\int_{-d}^{d} \eta_1(x)dx \approx S_{1/3}(\vec{\eta}_1) =: \frac{\Delta x}{3}\left(\eta_1(y_0') + 4\eta_1(y_1') + 2\eta_1(y_2')\right.$$
$$+ 4\eta_1(y_3') + 2\eta_1(y_4') + \cdots$$
$$\left. + 2\eta_1(y_{n-2}') + 4\eta_1(y_{n-1}') + \eta_1(y_{n_1}')\right),$$
$$(39)$$
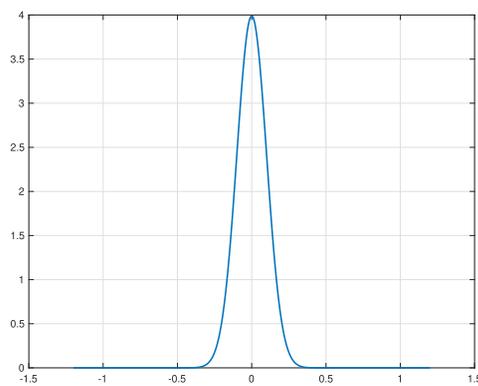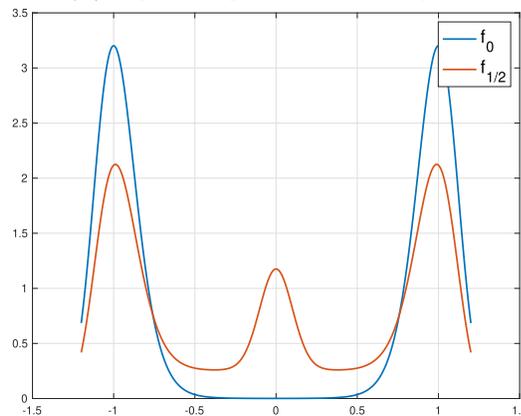

(A) Observable.
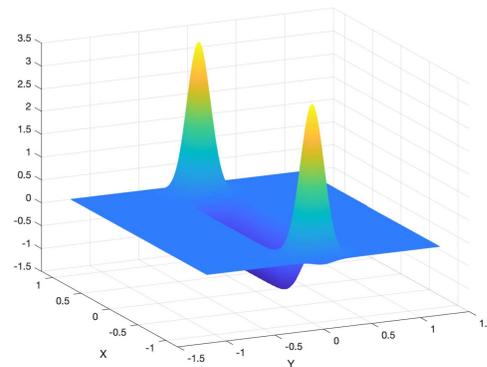
(B) Optimal perturbation $g_{I,J}$.
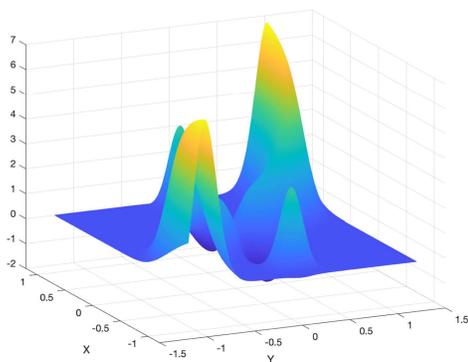
(C) Perturbed kernel $\kappa_{1/2} = \kappa + \frac{1}{2}g_{I,J}$.

(D) Invariant densities f_0 and $f_{1/2}$.

FIG. 2. Symmetric experiment, $\Delta x = \Delta t = 2 \times 10^{-3}$, $T = 1$, $D = [-1.2, 1.2]$, $I = 35$, and $J = 35$. (a) Symmetric observable $y \mapsto \phi(y)$. (b) Optimal perturbation $g_{I,J} = \frac{\sum_{r:h_r \in \mathcal{B}_{I,J}} G_r h_r}{\left(\sum_{r:h_r \in \mathcal{B}_{I,J}} G_r^2\right)^{1/2}}$. (c) Perturbed kernel $k_{1/2} = \kappa + \frac{1}{2}g_{I,J}$. (d) Invariant densities f_0 and $f_{1/2}$ for $\mathcal{L}_0$ and $\mathcal{L}_{1/2}$, respectively. (a) Observable. (b) Optimal perturbation $g_{I,J}$. (c) Perturbed kernel $\kappa_{1/2} = \kappa + \frac{1}{2}g_{I,J}$. (d) Invariant densities f_0 and $f_{1/2}$.
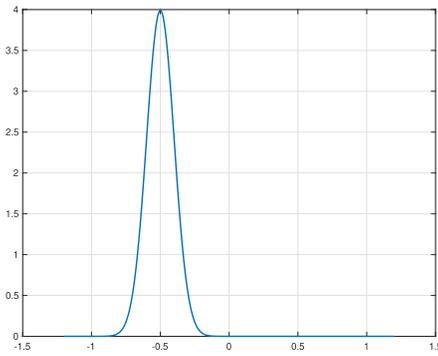
with

$$\eta_1(y_j') = \phi(y_j') \cdot (Id - \mathcal{L}_0)^{-1} \int_D h_r(x, y_j') f_0(x) dx := \phi(y_j') \cdot \eta_2(y_j').$$

Second, the vector $\vec{\eta}_2 = (\eta_2(y_j'))_j \in \mathbb{R}^{n_1+1}$ is the solution of the linear system

$$\left(Id_{n_1+1} - L_0^T\right) \vec{\eta}_2 = \vec{d}.$$

The matrix $L_0 = (l_{ij})_{ij} \in \mathbb{R}^{(n_1+1)\times(n_1+1)}$ represents the numerical approximation, via the same Simpson rule recalled before, of the operator $\mathcal{L}_0$. Its elements are given by

$$l_{ij} = \begin{cases} \dfrac{\Delta x}{3} \kappa(x_i', y_j') & \text{if } i = 0, j \geq 0, \\[2mm] 4\dfrac{\Delta x}{3} \kappa(x_i', y_j') & \text{if } i \text{ is odd}, j \geq 0, \\[2mm] 2\dfrac{\Delta x}{3} \kappa(x_i', y_j') & \text{if } i \text{ is even}, j \geq 0. \end{cases}$$

Further, the constant term vector $\vec{d} = (d_j)_j \in \mathbb{R}^{n_1+1}$ is obtained by approximating the innermost integral of G_r as follows:

$$d_j = \int_D h_r(x, y_j) f_0(x) dx \approx S_{1/3}(\vec{\eta}_3),$$

with $\vec{\eta}_3^{(j)} = (\eta_3^{(j)}(x_i))_i \in \mathbb{R}^{n_1+1}$ and $\eta_3^{(j)}(x_i) = h_r(x_i', y_j') \cdot f_0(x_i').$

Third, the invariant density f_0 is obtained by computing the left eigenvector $\vec{f}_0 = (f_{0,i})_{i=0,\dots,n}$ corresponding to eigenvalue 1 of the matrix
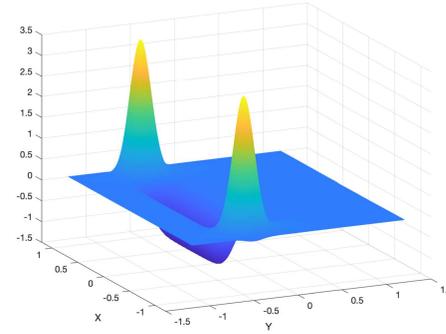
$$K \cdot dx,$$

where the entries of the matrix $K = (\kappa_{ij})_{ij} \in \mathbb{R}^{(n+1)\times(n+1)}$ are given by
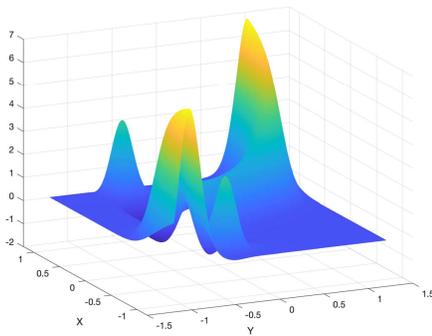
$$\kappa_{ij} = \kappa(x_i, y_j).$$

Indeed, this is equivalent to find a vector $\vec{f}_0 \in \mathbb{R}^{n+1}$ such that

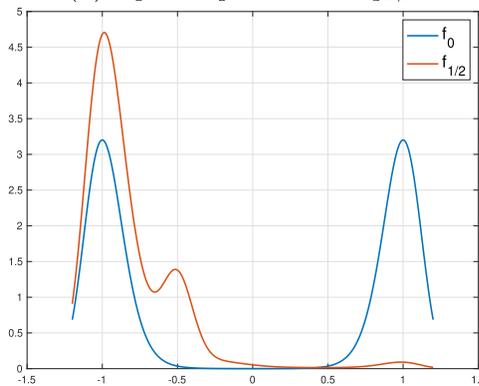$$\vec{f}_0 \cdot K \cdot dx = \vec{f}.$$

Note that the left-hand side is an approximation of the transfer operator $\mathcal{L}_0$ evaluated on f_0. In fact, the previous equation,

(A) Observable.

(B) Optimal perturbation $g_{I,J}$.

(C) Perturbed kernel $\kappa_{1/2} = \kappa + \frac{1}{2} g_{I,J}$.

(D) Invariant densities f_0 and $f_{1/2}$.

FIG. 3. Asymmetric experiment, $\Delta x = \Delta t = 2 \times 10^{-3}$, $T = 1$, $D = [-1.2, 1.2]$, $I = 35$, and $J = 35$. (a) Asymmetric observable $y \mapsto \phi(y)$. (b) Optimal perturbation $g_{I,J} = \dfrac{\sum_{r:h_r \in \mathcal{B}_{I,J}} G_r h_r}{\left(\sum_{r:h_r \in \mathcal{B}_{I,J}} G_r^2\right)^{1/2}}$. (c) Perturbed kernel $\kappa_{1/2} = \kappa + \frac{1}{2} g_{I,J}$. (d) Invariant densities f_0 and $f_{1/2}$ for $\mathcal{L}_0$ and $\mathcal{L}_{1/2}$, respectively. (a) Observable. (b) Optimal perturbation $g_{I,J}$. (c) Perturbed kernel $\kappa_{1/2} = \kappa + \frac{1}{2} g_{I,J}$. (d) Invariant densities f_0 and $f_{1/2}$.

component-wise, reads as

$$dx \cdot \sum_i \kappa(x_i', y_j') f_{0,i} = f_j, \quad \forall j = 0, \ldots, n,$$

with the left side being an approximation of $\mathcal{L}_0 f$. The existence of a such eigenvector for eigenvalue 1 is a consequence of the Perron–Frobenius theorem for row stochastic matrices (see Ref. 36).

Last, the sum defining g is truncated, and we consider the approximation of g given by the elements in the truncated basis $B_{I,J}$ defined as

$$\mathcal{B}_{I,J} = \bigcup_{i=1,\ldots,I} \bigcup_{j=0,\ldots,J} \left\{ \frac{1}{\sqrt{2d}} \cos\left(i\frac{\pi}{d}x\right) \cdot \cos\left(j\frac{\pi}{d}y\right), \frac{1}{\sqrt{2d}} \cos\left(i\frac{\pi}{d}x\right) \right.$$
$$\cdot \sin\left(j\frac{\pi}{d}y\right), \frac{1}{\sqrt{2d}} \sin\left(i\frac{\pi}{d}x\right) \cdot \cos\left(j\frac{\pi}{d}y\right), \frac{1}{\sqrt{2d}} \sin\left(i\frac{\pi}{d}x\right)$$
$$\left. \cdot \sin\left(j\frac{\pi}{d}y\right) \right\}.$$

Thus, our approximation of the solution g is given by

$$g_{I,J} = \frac{\sum_{r:h_r \in \mathcal{B}_{I,J}} G_r h_r}{\left(\sum_{r:h_r \in \mathcal{B}_{I,J}} G_r^2\right)^{1/2}}.$$

D. Results

In this section, we present our numerical experiments to approximate the solution of the optimal control problem (38) using two different observables, ϕ. Both observables are selected from the class of PDFs f_{μ,σ^2} of Gaussian random variables with mean μ and variance σ^2.

In the first experiment, we use a symmetric observable with $\mu = 0$ and $\sigma = 0.1$. In the second experiment, we use an asymmetric observable with $\mu = -0.5$ and $\sigma = 0.1$. Similar results can be achieved by varying μ, σ, and the class of the observable (such as continuous bump functions or polynomials). However, using non-continuous observables (like indicator functions) may introduce minor numerical errors due to the finite selection of basis elements. We will discuss the results of the symmetric experiment, shown in Fig. 2, in detail. The results for the asymmetric case, shown in Fig. 3, follow the same explanation and are not repeated here.

First, Fig. 2(a) depicts the symmetric observable used in the first experiment. Figure 2(b) represents the approximation $g_{I,J}$ of the optimal perturbation g that solves the problem (38). This optimal perturbation, $g_{I,J}$, provides the infinitesimal adjustment to the kernel needed to maximize $\int_D \phi(y) f_\delta(y) \, dy$. It is worth pointing out that the perturbation $g_{I,J}$ is significant (i.e., far from zero) only where the observable is significant. Furthermore, for any given value y where $g_{I,J}$ is significant, for example, $y = 0$, the restriction of the perturbation $x \mapsto g_{I,J}(x,y)$ redistributes mass from areas where the invariant density f_0 is small (away from $x = \pm 1$) to areas where the invariant density is large (around $x = \pm 1$). Additionally, due to the choice of basis $\mathcal{B}_{I,J}$, it can be numerically verified that $\int_D g_{I,J}(x,y) \, dx = 0$ for any $y > 0$.

Figure 2(c) visually represents the perturbed kernel $\kappa_\delta = \kappa + \delta \cdot g_{I,J} + r_\delta$ with $\delta = \frac{1}{2}$ and $r_\delta = 0$.

Last, Fig. 2(d) compares the invariant densities f_0 and $f_{1/2}$ for the transfer operators $\mathcal{L}_0$ and $\mathcal{L}_{1/2}$, respectively. These two symmetric densities, both normalized to satisfy $\|f_0\|_{L^1(D)} = \|f_{1/2}\|_{L^1(D)}$, weight the points in D differently. Specifically, f_0 is concentrated around ± 1, whereas $f_{1/2}$, while preserving the same maximum points as f_0, also shows a third local maximum at $x = 0$, where the observable is concentrated.

CODE AVAILABILITY

All material in the text and figures was produced by the authors using standard mathematical and numerical analysis tools. The only externally supplied code of this work consists of the implementation of Simpson's rule for numerical integration by Damien Garcia (link), which we acknowledge.

The code for the numerical simulations performed in Sec. VI is available at Zenodo (https://doi.org/10.5281/zenodo.13820212). (The code available on Zenodo performs the numerical experiments described in this work using $\Delta x = 8 \times 10^{-3}$ and $\Delta t = 2 \times 10^{-3}$. To reproduce the results of this work, i.e., with $\Delta x = 2 \times 10^{-3}$, the reader should modify the number of points in the spatial mesh at line 16 of the code.)

AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Gianmarco Del Sarto: Conceptualization (equal); Formal analysis (equal); Methodology (equal); Software (equal); Writing – original draft (equal). **Stefano Galatolo:** Conceptualization (equal); Formal analysis (equal); Methodology (equal); Software (equal); Writing – original draft (equal). **Sakshi Jain:** Conceptualization (equal); Formal analysis (equal); Methodology (equal); Software (equal); Writing – original draft (equal).

DATA AVAILABILITY

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

APPENDIX: RECAP OF CONVEX OPTIMIZATION

In this section, we recall some general results on the optimization of linear functions in convex sets adapted for our needs (see Ref. 6 for the proofs and other details). Let P be a bounded and convex subset of a Hilbert space $\mathfrak{H}$.

Definition 29. We say that a convex closed set $P \subseteq \mathfrak{H}$ is *strictly convex* if for each pair $x, y \in P$ and for all $\gamma \in (0, 1)$, the points $\gamma x + (1 - \gamma)y \in \text{int}(P)$, where $\text{int}(P)$ is the relative interior (The relative interior of a closed convex set C is the interior of C relative to the closed affine hull of C.) of P.

Let us briefly recall some relevant results from convex optimization.

Suppose $\mathfrak{H}$ is a separable Hilbert space and $P \subset \mathfrak{H}$. Let $\mathcal{J} : \mathfrak{H} \to \mathbb{R}$ be a continuous linear function. Consider the abstract problem to find $p_* \in P$ such that

$$\mathcal{J}(p_*) = \max_{p \in P} \mathcal{J}(p). \tag{A1}$$

The existence and uniqueness of an optimal perturbation follows from the properties of P as stated in the following two propositions.

Proposition 30 (Existence of the optimal solution). *Let P be bounded, convex, and closed in $\mathfrak{H}$. Then, problem (A1) has at least one solution.*

Upgrading the convexity of the feasible set P to strict convexity provides the uniqueness of the optimal solution.

Proposition 31 (Uniqueness of the optimal solution). *Suppose P is closed, bounded, and strictly convex subset of $\mathfrak{H}$ and that P contains the zero vector in its relative interior. If $\mathcal{J}$ is not uniformly vanishing on P, then the optimal solution to (A1) is unique.*

Note that in the case when $\mathcal{J}$ is uniformly vanishing, all the elements of P are solutions of the problem (A1).

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