When Koopman Meets Hamilton and Jacobi

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***Abstract*— In this paper, we establish a connection between the spectral theory of the Koopman operator and the solution of the Hamilton Jacobi (HJ) equation. The HJ equation occupies a central place in system theory, and its solution is of interest in various control problems, including optimal control, robust control, and input-output analysis. One of the main contributions of this paper is to show that the Lagrangian submanifolds, which are fundamental objects for solving the HJ equation, can be obtained using the spectral analysis of the Koopman operator. We present two different procedures for the approximation of the HJ solution. We utilize the spectral properties of the Koopman operator associated with the uncontrolled dynamical system and Hamiltonian systems that arise from the HJ equation to approximate the HJ solution. We present a convex optimization-based computational framework with convergence analysis for approximating the Koopman eigenfunctions and the Lagrangian submanifolds. Our solution approach to the HJ equation using Koopman theory provides for a natural extension of results from linear systems to nonlinear systems. We demonstrate the application of this work for solving the optimal control problem. Finally, we present simulation results to validate the paper's main findings and compare them against linear quadratic regulator and Taylor series based approximation controllers.**

***Index Terms*— Koopman Operator, Hamilton Jacobi Equation, Optimal Control.**

I. Introduction

Hamilton Jacobi (HJ) equation is at the heart of several problems of interest in systems and control theory. The HJ equation arises in optimal control, robust H_∞ control, dissipativity-based analysis of an input-output system, and control of systems with an adversary or min-max dynamic games [1]. The HJ equation and its discrete-time counterpart, the HJ Bellman (HJB) equation, have attracted renewed attention due to the significance of this equation in data-driven control and Reinforcement learning problems [2], [3]. The HJ equation is a nonlinear partial differential equation (PDE), and given the significance of the HJ equation in system theory, a variety of methods are developed for the approximation of its solution [4].

Literature review: Given the nonlinear nature of the HJ PDE, the analytical solution is impossible, and one has to resort to a numerical scheme for its approximation. In the development of numerical methods for the optimal control problem, the complexity associated with the nonlinear nature of the HJ is broken down by providing an iterative process for solving the HJ equation. The iterative approach involves solving a linear PDE for the value function with a given control input. The value function is then used to update the control input. Finally, the linear PDE is solved approximately for the value function using the Galerkin-type projection scheme [5]. The iterative approach for solving optimal control problems via the HJB equation and the Bellman equation plays a fundamental role in various RL algorithms, including policy iteration, value iteration, and actor-critic method [6]. Another line of research involving viscosity-based approximate solution to the HJ equation is proposed in [7], [8]. The viscosity-based solution is weaker than the classical, differentiable solution of the HJ equation. An approximate suboptimal solution of the HJ equation based on the series expansion of higher-order nonlinear terms is proposed in [9]–[14].

Differential geometric viewpoint of HJ equation and Koopman theory: An alternate approach for analyzing and approximating the HJ equation is based on a differential geometric-based interpretation of its solution. It is well known that a Hamiltonian dynamical system is associated with the HJ equation. The Lagrangian submanifolds of the Hamiltonian dynamical system, which are invariant manifolds, are used to construct the solution of the HJ equation. This differential geometric viewpoint is exploited to solve the optimal control, H_∞ control, and $\mathcal{L}_2$ gain analysis and synthesis problems in [1]. In [15], the authors have exploited this differential geometric approach to develop computational methods for approximating the HJ solution. The methods we discovered in this paper for approximating HJ solution draw parallels to the techniques found in [15]. In particular, our first approach is similar to the approximation procedure developed in [15] relying on decomposing Hamiltonian into integrable and nonintegrable parts. In this paper, we show a strong connection between the differential geometric viewpoint of the HJ equation and the spectral analysis of the Koopman operator. The development of the Koopman operator was originally motivated for studying the ensemble or statistical behavior of conservative dynamical systems [16]. However, the spectral properties of the Koopman operator have an intimate connection to the system geometry [17], [18]. In particular, the invariant manifolds of the dynamical system are obtained as joint zero-level sets of the eigenfunctions. The recent work involving the Koopman operator for dynamical systems with dissipation provides a way of characterizing stable, unstable manifolds of nonlinear dynamical systems in terms of the zero-level sets of Koopman eigenfunctions [19]. The explosion of research activities in Koopman theory provides for systematic data-driven and model-based methods

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for the computation of Koopman eigenfunctions [20]–[23]. On the other hand, there is also extensive literature on the use of Koopman theory for control [24]–[34]. However, one of the fundamental challenges with the current approaches to using Koopman theory for control is the bilinear nature of the Koopman-based lifting of control dynamical system. The bilinear lifting is one of the main hurdles in extending linear system tools as they inhibit the development of convex or linear methods for nonlinear control. This is in contrast to the convex framework for control design using the Perron-Frobenius operator, dual to the Koopman operator discovered in [35]–[38]. In [26], the authors have proposed the Koopman-based lifting of the Hamiltonian dynamical system arising from the Pontryagin maximum principle. One of the main focuses of [26] is to prove the symplectic structure of the lifted Hamiltonian system in the function space for optimal control design. The Hamiltonian system is also the main focus of this paper. However, unlike [26], we discover a relationship between the spectral properties of the Koopman operator and the state space geometry of the Hamiltonian system for optimal control design without explicitly lifting the Hamiltonian system.

Main Contributions: The main contributions of this paper are as follows. We provide two procedures for constructing the Lagrangian submanifold and the HJ solution based on spectral analysis of the Koopman operator. In our first procedure, we show that the Koopman eigenfunctions of the uncontrolled system can be used to decompose the Hamiltonian associated with the HJ equation into integrable and non-integrable parts. The integrable part of the Hamiltonian system can be solved exactly. However, for the non-integrable part, we make certain approximations leading to the approximate solution of the HJ equation. The decomposition of the Hamiltonian dynamical system into integrable and non-integrable parts using the first integral of motion is proposed in [15] for approximating the HJ solution. However, unlike [15], we present a systematic convex optimization-based approach with rigorous results on the convergence analysis for the approximation of Koopman eigenfunctions and Lagrangian submanifold. Furthermore, unlike [15], the approximation of the Lagrangian submanifold and the HJ solution we obtained is time-independent.

Our second procedure for approximating the Lagrangian submanifold and HJ solution uses the Koopman eigenfunctions of the Hamiltonian dynamical system associated with the HJ equation. In particular, the zero-level curves of the Koopman eigenfunctions are used to determine the Lagrangian submanifolds. The second procedure involves computing the Koopman eigenfunction of a higher, $2n$-dimensional Hamiltonian system compared to our first procedure involving n-dimensional uncontrolled system. We show that the Riccatti solution corresponding to the linearized HJ equation is obtained from both methods as a particular case of the approximate HJ solution. This specific case is when only linear basis functions are used to approximate the Koopman eigenfunctions. Hence, the proposed Koopman-based approach for analyzing the HJ equation provides a natural extension of the linear system results to nonlinear systems. Finally, we demonstrate the application of the developed framework to optimal control problems.

This paper is an extended version of [39]. In particular, the first procedure based on the decomposition of Hamiltonian into an integrable and non-integrable part is new to this paper. Similarly, the results presented in this paper for procedure two are stronger than those presented in [39]. Finally, rigorous convergence analysis for approximating the Koopman eigenfunctions is new to this paper.

II. Preliminaries and Notations

In this section, we present some preliminaries on the Hamiltonian dynamical system, the HJ equation, and the spectral theory of the Koopman operator. The preliminaries will also establish a connection between the Hamiltonian dynamics-based symplectic geometry framework and the solution of the HJ equation. We refer the readers to [1], [19], [40], [41] for further details on the preliminaries.

Notations: $\mathbb{R}^n$ denotes the n dimensional Euclidean space. We denote by $\mathcal{L}_\infty(\mathcal{M})$, $\mathcal{C}^k(\mathcal{M})$ the space of all essentially bounded real-valued functions and k-times continuously differentiable functions on n-dimensional manifold $\mathcal{M} \subseteq \mathbb{R}^n$ respectively. $\mathbb{N}$ denotes the set of natural numbers. We denote by $\mathbf{s}_t(\mathbf{z})$ and $\mathbf{s}_t(\mathbf{x})$ the solutions of systems, $\dot{\mathbf{z}} = \mathbf{F}(\mathbf{z})$ and $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$, at time t with initial condition $\mathbf{z}$ and $\mathbf{x}$ respectively.

A. Hamilton Jacobi Solution and Lagrangian Submanifold

We provide a brief overview of some of the existing results on the connection between the solution of the HJ equation and the Lagrangian submanifold. For concreteness, we focus specifically on the HJ equation that arises in the optimal control problem. Consider the infinite-horizon optimal control problem for the control-affine dynamical system.

$$\min_{\mathbf{u}} \int_0^\infty q(\mathbf{x}(t)) + \frac{1}{2}\mathbf{u}^\top(t)\mathbf{D}\mathbf{u}(t)dt \tag{1}$$

$$\text{s.t. } \dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\mathbf{u} =: \mathbf{S}(\mathbf{x}, \mathbf{u}), \tag{2}$$

where $\mathbf{x} \in \mathcal{M} \subseteq \mathbb{R}^n$ and $\mathbf{u} \in \mathbb{R}^q$ are the states and control input respectively. $\mathbf{x}(t)$ is the trajectory of the control system with initial condition $\mathbf{x}$. We make the following assumption on the system dynamics and the cost function applicable for the rest of the paper.

Assumption 1. 1) *We assume that* $\mathbf{f} : \mathcal{M} \to \mathbb{R}^n$ *and* $\mathbf{g}_i : \mathcal{M} \to \mathbb{R}^n$ *for* $i = 1, \ldots, p$ *are* $\mathcal{C}^\infty$ *functions of* $\mathbf{x}$. $\mathbf{x} = 0$ *is an equilibrium point of the uncontrolled system, and the eigenvalues of the linearization, i.e.,* $\mathbf{A} = \frac{\partial \mathbf{f}}{\partial \mathbf{x}}(0)$ *are distinct and not on the imaginary axis. Furthermore, the linearization of system dynamics (2) at the origin i.e., pair* $(\frac{\partial \mathbf{S}}{\partial \mathbf{x}}(0,0), \frac{\partial \mathbf{S}}{\partial \mathbf{u}}(0,0)) = (\mathbf{A}, \mathbf{g}(0))$ *is assumed to be controllable.*

2) *The state cost function* $q(\mathbf{x})$ *is* $\mathcal{C}^\infty$ *function of* $\mathbf{x}$ *with* $q(0) = \frac{\partial q}{\partial \mathbf{x}}(0) = 0$, *and* $\frac{\partial^2 q}{\partial \mathbf{x}^2} = \mathbf{Q}$ *is a symmetric, positive definite matrix. The pair* $(\mathbf{A}, \sqrt{\mathbf{Q}})$ *is detectable, and the matrix* $\mathbf{D}$ *is symmetric and positive definite.*

Similarly, the pair $(\mathbf{f}(\mathbf{x}), q(\mathbf{x}))$ *is zero-state detectable i.e.,* $q(\mathbf{x}(t)) = 0$ *for all* $t \geq 0$ *then* $\mathbf{x}(t) \to 0$ *as* $t \to \infty$.

3) *We assume that the optimal control exists and that the optimal cost function is finite.*

The hyperbolicity assumption of the equilibrium point ensures that the spectrum of the Koopman operator (as defined later) is discrete and well-defined. The controllability and detectability assumptions on the linearization of system dynamics and cost function ensure that the solution of the Riccatti equation for the linearized system is well-defined.

The connection between the HJ solution and the Lagrangian submanifold can be understood based on the two approaches available for solving the optimal control problem. The first approach is based on solving the optimal control problem in the state space leading to the HJ equation, and the second approach is in the time domain based on the Pontryagin maximum principle. Let $V^\star(\mathbf{x})$ be the optimal value function assumed to be atleast $\mathcal{C}^2$ function of $\mathbf{x}$ i.e.,

$$V^\star(\mathbf{x}) = \min_{\mathbf{u}} \int_0^\infty q(\mathbf{x}(t)) + \frac{1}{2}\mathbf{u}^\top(t)\mathbf{D}\mathbf{u}(t)dt, \tag{3}$$

where $\mathbf{x}(t)$ is the trajectory of the control system starting from initial condition $\mathbf{x}$. The optimal cost function is independent of time since the cost is evaluated over an infinite time horizon. It is well known that the optimal cost function $V^\star(\mathbf{x})$ satisfy following HJ equation [1]

$$\frac{\partial V}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) - \frac{1}{2}\frac{\partial V}{\partial \mathbf{x}}\mathbf{g}(\mathbf{x})\mathbf{D}^{-1}\mathbf{g}(\mathbf{x})^\top \frac{\partial V}{\partial \mathbf{x}}^\top + q(\mathbf{x}) = 0, \tag{4}$$

and the optimal control input is expressed using the $V^\star(\mathbf{x})$ as

$$u^\star(\mathbf{x}) = -\mathbf{D}^{-1}\mathbf{g}(\mathbf{x})^\top \frac{\partial V}{\partial \mathbf{x}}^\top. \tag{5}$$

The HJ equation is a nonlinear partial differential equation, and it has to be solved for the unknown function $V : \mathcal{M} \to \mathbb{R}$.

An alternate approach for solving the optimal control problem is via the Pontryagin maximum principle. The optimal control problem is an infinite-dimensional optimization problem with the cost function given by (1) and system dynamics (2) as constraints. For solving this optimization problem, an auxiliary function or Hamiltonian is introduced using a Lagrangian multiplier or co-state variable $\mathbf{p} \in \mathbb{R}^n$ as follows.

$$\bar{H}(\mathbf{x}, \mathbf{p}, \mathbf{u}) = (\mathbf{f}(\mathbf{x}) + \mathbf{g}(\mathbf{x})\mathbf{u})^\top \mathbf{p} + q(\mathbf{x}) + \frac{1}{2}\mathbf{u}^\top\mathbf{D}\mathbf{u}. \tag{6}$$

The optimal $\mathbf{u}^\star$ is obtained by the extremum of the Hamiltonian w.r.t. $\mathbf{u}$ as

$$\frac{\partial \bar{H}}{\partial \mathbf{u}} = \mathbf{g}(\mathbf{x})^\top\mathbf{p} + \mathbf{D}\mathbf{u} = 0 \implies \mathbf{u} = -\mathbf{D}^{-1}\mathbf{g}(\mathbf{x})^\top\mathbf{p}. \tag{7}$$

Substituting the optimal value of $\mathbf{u}$ from (7) in (6), we obtain

$$\begin{aligned} H(\mathbf{x}, \mathbf{p}) &:= \bar{H}(\mathbf{x}, \mathbf{p}, \mathbf{u}(\mathbf{x}, \mathbf{p})) \\ &= \mathbf{f}(\mathbf{x})^\top\mathbf{p} - \frac{1}{2}\mathbf{p}^\top\mathbf{g}(\mathbf{x})\mathbf{D}^{-1}\mathbf{g}(\mathbf{x})^\top\mathbf{p} + q(\mathbf{x}). \end{aligned} \tag{8}$$

Associated with the Hamiltonian (8) is a Hamiltonian dynamical system written as

$$\begin{aligned} \dot{\mathbf{x}} &= \frac{\partial H(\mathbf{x}, \mathbf{p})}{\partial \mathbf{p}} = \mathbf{f} - \mathbf{g}\mathbf{D}^{-1}\mathbf{g}^\top\mathbf{p} \\ \dot{\mathbf{p}} &= -\frac{\partial H(\mathbf{x}, \mathbf{p})}{\partial \mathbf{x}} = -\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^\top \mathbf{p} + \frac{1}{2}\frac{\partial(\mathbf{p}^\top\mathbf{g}\mathbf{D}^{-1}\mathbf{g}^\top\mathbf{p})}{\partial \mathbf{x}} - \frac{\partial q}{\partial \mathbf{x}}^\top. \end{aligned} \tag{9}$$

Remark 1. *The Hamiltonian dynamical system is of* $2n$*-dimensions and evolves on the co-tangent bundle* $T^\star\mathcal{M}$*, i.e.,* $(\mathbf{x}, \mathbf{p}) \in T^\star\mathcal{M}$ *[41]. Following Assumption 1, it is clear that the origin* $(\mathbf{x}, \mathbf{p}) = (0, 0)$ *is also the equilibrium point of the Hamiltonian system. An equilibrium point of any Hamiltonian system will be either elliptic (i.e., all the eigenvalues of the linearization on the imaginary axis) or saddle-type (with eigenvalues forming a mirror image along the imaginary axis). In the Hamiltonian dynamical system that arises in the context of the HJ equation, the equilibrium point at the origin is of saddle type. This fact is significant regarding the existence and well-defined discrete spectrum of the Koopman operator associated with the Hamiltonian system.*

The solutions of the HJ equation (4) and the Hamiltonian system (9) are closely connected. Note the similarity between the HJ equation (4) and the Hamiltonian (8), where (8) can be obtained from (4) by replacing $\frac{\partial V}{\partial \mathbf{x}}^\top$ by $\mathbf{p}$. The Lagrangian submanifold is the connecting link between the two approaches for solving the optimal control problem.

1) Lagrangian Submanifold: Later in this section, we will provide a formal definition of the Lagrangian submanifold. However, in the following discussion, we first provide an informal description of the Lagrangian submanifold and its connection to the HJ solution. The $2n$-dimensional Hamiltonian system (9) has n-dimensional stable (unstable), $\mathcal{M}_{s(u)}$ manifold associated with the saddle-type equilibrium point at the origin. The Lagrangian submanifolds, $\mathcal{L}$, are subsets of these invariant manifolds, which can be written as $\mathcal{L} = \{(\mathbf{x}, \mathbf{p}) \in \mathcal{M}_{u(s)} : (\mathbf{x}, \mathbf{p} = \frac{\partial V}{\partial \mathbf{x}}^\top)\}$ for some scalar-valued function $V : \mathcal{M} \to \mathbb{R}$ i.e., these manifolds can be parameterized in terms of $\mathbf{x}$ variable only. The scalar-valued function, V, used in this parameterization will qualify as the solution of the HJ equation.

For a more formal definition of the Lagrangian submanifold, it is necessary to involve concepts from differential geometry. The state space of the Hamiltonian system (9) i.e., $T^\star\mathcal{M}$ is a symplectic manifold with symplectic 2-form given by $\omega = \sum_i^n dp_i \wedge x_i$ (Refer to [41], [42]) for more details on symplectic manifolds, definition of 2-form, and the wedge product $\wedge$.

Definition 1 (Lagrangian submanifold)**.** *An n-dimensional submanifold* $\mathcal{L}$ *of* $T^\star\mathcal{M}$ *is Lagrangian if* ω *restricted to* $\mathcal{L}$ *is zero.*

Now consider any $\mathcal{C}^2$ function $V : \mathcal{M} \to \mathbb{R}$, and the n-dimensional submanifold $\mathcal{L}_V \subset T^\star\mathcal{M}$, in local coordinates

given as

$$\mathcal{L}_V = \left\{ (\mathbf{x}, \mathbf{p}) \in T^\star\mathcal{M} : \quad \mathbf{p} - \frac{\partial V}{\partial x}^\top = 0 \right\}. \tag{10}$$

It follows that $\mathcal{L}_V$ is a Lagrangian submanifold as the 2-form ω restricted to $\mathcal{L}_V$ is zero. Note that Lagrangian submanifold $\mathcal{L}_V$ in (10) is parameterized by $\mathbf{x}$ coordinates only. The converse of the above statement is also true [1, Proposition 11.1.2]. The Lagrangian submanifold can be obtained as an invariant manifold of the Hamiltonian system (9). A submanifold $\mathcal{N} \subset T^\star\mathcal{M}$ is invariant manifold of (9) if solutions starting on $\mathcal{N}$ remains in $\mathcal{N}$. We have the following Proposition from [1].

Proposition 1. *Let $S : \mathcal{M} \to \mathbb{R}$ and consider the submanifold $\mathcal{L}_S \subset T^\star\mathcal{M}$ of the form (10). Then*

$$H\left(\mathbf{x}, \frac{\partial S}{\partial \mathbf{x}}^\top\right) = \text{constant}, \quad \forall \mathbf{x} \in \mathcal{M}, \tag{11}$$

if and only if $\mathcal{L}_S$ is an invariant submanifold of the Hamiltonian system (9).

Adding a constant to the Hamiltonian (8) does not change the vector field (9) and hence (11) reduces to (4), thereby providing a link between the Lagrangian submanifold, HJ solution, and Hamiltonian dynamics. So, the Lagrangian submanifold can be constructed as an invariant manifold of the Hamiltonian system, but not every invariant manifold is Lagrangian. However, stable and unstable invariant manifolds of the Hamiltonian system are Lagrangian [1, Proposition 11.1.4].

Remark 2. 1) *There are various notions of solution to the HJ equation: classical, weak, and generalized or viscosity solution. All these solutions can be connected to the Lagrangian submanifold. Refer to [43] on the connection between Lagrangian submanifold and different notions of solutions. The classical and weak solutions differ by their differentiability properties; the viscosity solution is non-smooth.*

2) *In this paper, we restrict to approximating the classical solution of the HJ equation. Hence, there is an implicit assumption that the classical solution exists to the HJ equation.*

2) Riccatti Equation: The Riccatti equation can be viewed as the linearization of the nonlinear HJ equation. In particular, following Assumption 1 the HJ equation is replaced by its linearization with the Lagrangian submanifold given by $\mathbf{p} = \frac{1}{2}\frac{\partial \mathbf{x}^\top \mathbf{P}\mathbf{x}}{\partial \mathbf{x}} = \mathbf{P}\mathbf{x}$ for some symmetric positive matrix $\mathbf{P}$, where $\mathbf{P}$ satisfies

$$\mathbf{A}^\top\mathbf{P} + \mathbf{P}\mathbf{A} - \mathbf{P}\mathbf{R}\mathbf{P} + \mathbf{Q} = 0, \tag{12}$$

with $\mathbf{R} := \mathbf{g}(0)\mathbf{D}^{-1}\mathbf{g}(0)^\top$ and $\mathbf{Q} = \frac{\partial^2 q}{\partial \mathbf{x}^2}(0)$. Just like we associate Hamiltonian system (9) with the HJ equation (4), we can associate linear Hamiltonian system with Hamiltonian matrix $\mathcal{H}$ as follows,

$$\mathcal{H} := \begin{pmatrix} \mathbf{A} & -\mathbf{R} \\ -\mathbf{Q} & -\mathbf{A}^\top \end{pmatrix} \in \mathbb{R}^{2n \times 2n}. \tag{13}$$

The Hamiltonian matrix corresponds to linearizing the nonlinear Hamiltonian system at the origin. The necessary and sufficient conditions for the existence of a positive definite solution to the Riccatti equation (12) is that the Hamiltonian matrix has no eigenvalues on the imaginary axis, and the generalized stable eigenspace $\mathbb{E}_s$ corresponding to stable eigenvalues of $\mathcal{H}$ satisfies the following condition [44]

$$\mathbb{E}_s \oplus \begin{pmatrix} 0^\top & I^\top \end{pmatrix}^\top = \mathbb{R}^{2n}. \tag{14}$$

We now make following assumption on the Hamiltonian matrix $\mathcal{H}$ in (13).

Assumption 2. *We assume that the Hamiltonian matrix $\mathcal{H}$ in (13) satisfy (14) and has all its eigenvalues distinct with none of them on the imaginary axis.*

The part of the assumption that none of the eigenvalues of the Hamiltonian are on the imaginary axis is necessary and sufficient for the existence of local and hence global solution to the HJ equation [44]. The assumption that eigenvalues are distinct is a generic assumption made to simplify the presentation of proofs and the computational framework.

B. Spectral theory of Koopman operator

In this section, we provide a brief overview of existing results on the spectral theory of the Koopman operator. For more details on this topic, refer to [18], [19]. Consider an autonomous dynamical system of the form

$$\dot{\mathbf{z}} = \mathbf{F}(\mathbf{z}), \quad \mathbf{z} \in \mathcal{Z} \subseteq \mathbb{R}^p, \tag{15}$$

where $\mathcal{Z}$ is an open set containing the origin.

Remark 3. *The main contribution of this paper is in providing two different procedures for approximating the Lagrangian submanifold and the HJ solution. These two approaches relies on the spectral properties of Koopman operator associated with uncontrolled system $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ (refer to Eq. (2)) and the Hamiltonian system (9). Hence, we describe the spectral theory of Koopman in the context of system (15) so that the state $\mathbf{z}$ could either correspond to state $\mathbf{x}$ i.e., $\mathcal{Z} = \mathcal{M}$ or $\mathbf{z} = (\mathbf{x}^\top, \mathbf{p}^\top)^\top$ i.e., $\mathcal{Z} = T^\star\mathcal{M}$ depending upon the procedure used in the approximation.*

Remark 4. *From Assumptions 1 and 2 it follows that the vector field $\mathbf{F}$ is also $\mathcal{C}^\infty$ function with the origin as the hyperbolic equilibrium point and $\mathbf{E} := \frac{\partial \mathbf{F}}{\partial \mathbf{z}}(0)$ having all eigenvalues distinct.*

We have the following definitions for the Koopman operator and its spectrum.

Definition 2 (Koopman Operator)**.** *$\mathbb{U}_t : \mathcal{L}_\infty(\mathcal{Z}) \to \mathcal{L}_\infty(\mathcal{Z})$ for dynamical system* (15) *is defined as*

$$[\mathbb{U}_t\psi](\mathbf{z}) = \psi(\mathbf{s}_t(\mathbf{z})), \quad \psi(\mathbf{z}) \in \mathcal{L}_\infty(\mathcal{Z}). \tag{16}$$

The infinitesimal generator of the Koopman operator is given by

$$\lim_{t\to 0} \frac{(\mathbb{U}_t - I)\psi}{t} = \frac{\partial \psi}{\partial \mathbf{z}}\mathbf{F}(\mathbf{z}) =: \mathcal{K}_{\mathbf{F}}\psi, \quad t \geq 0. \tag{17}$$

Definition 3. *[Eigenvalues and Eigenfunctions of Koopman] A function $\phi_\lambda(\mathbf{z}) \in \mathcal{C}^1(\mathcal{Z})$ is said to be an eigenfunction of the Koopman operator associated with eigenvalue λ if*

$$[\mathbb{U}_t \phi_\lambda](\mathbf{z}) = e^{\lambda t}\phi_\lambda(\mathbf{z}). \tag{18}$$

Using the Koopman generator, the (18) can be written as

$$\frac{\partial \phi_\lambda}{\partial \mathbf{z}}\mathbf{F}(\mathbf{z}) = \lambda \phi_\lambda(\mathbf{z}). \tag{19}$$

The eigenfunctions and eigenvalues of the Koopman operator enjoy the following property [19], [45].

Property 1. *Let ϕ_{λ_1} and ϕ_{λ_2} are the eigenfunctions of the Koopman generator associated with eigenvalues λ_1 and λ_2 respectively. If $\phi_{\lambda_1}^{k_1}\phi_{\lambda_2}^{k_2} \in \mathcal{C}^1(\mathcal{Z})$, for $k_1, k_2 \in \mathbb{R}^+$, then it is an eigenfunctions of Koopman generator with eigenvalue $k_1\lambda_1 + k_2\lambda_2$.*

Definition 4 (Koopman mode decomposition)**.** *Consider a scalar-valued function $g : \mathcal{Z} \to \mathbb{R}$, and assume that the function g can be expanded in terms of Koopman eigenfunctions as follows.*

$$g(\mathbf{z}) = \sum_{\mathbf{k}\in\mathbb{N}^n}^{N} \bar{g}_{\mathbf{k}} \prod_{i=1}^{n} \phi_i^{k_i}(\mathbf{z}), \tag{20}$$

where $\mathbf{k} = (k_1, \ldots, k_n)$ and $\bar{g}_{\mathbf{k}}$ are the Koopman modes and correspond to the projection of function $g(\mathbf{z})$ on the eigenfunctions, $\phi_{\lambda_1}^{k_1}(\mathbf{z}), \ldots, \phi_{\lambda_n}^{k_n}(\mathbf{z})$. The scalar-valued function will propagate under system dynamics as follows

$$g(\mathbf{s}_t(\mathbf{z})) = [\mathbb{U}_t g](\mathbf{z}) = \sum_{\mathbf{k}\in\mathbb{N}^n}^{N} \bar{g}_{\mathbf{k}} \prod_{i=1}^{n} \phi_{\lambda_i}^{k_i}(\mathbf{z}) e^{k_i\lambda_i t}. \tag{21}$$

The spectrum of the Koopman operator, in general, is very complex and could consist of discrete and continuous parts. Furthermore, the spectrum depends on the underlying functional space used in the approximation [19]. In this paper, we are interested in approximating the eigenfunctions of the Koopman operator with associated eigenvalues, the same as that of the linearization of the nonlinear system at the equilibrium point. With the hyperbolicity assumption on the equilibrium point of the system (15), this part of the spectrum of interest to us is known to be discrete and well-defined. In the following discussion, we summarize the results from [19] relevant to this paper and justify some of the claims made above on the spectrum of the Koopman operator.

Equations (18) and (19) provide a general definition of the Koopman spectrum. However, the spectrum can be defined over finite time or over a subset of the state space. The spectrum of interest to us in this paper could be well-defined over the subset of the state space.

Definition 5 (Open Eigenfunction [19])**.** *Let $\phi_\lambda : \boldsymbol{\mathcal{C}} \to \mathbb{C}$, where $\boldsymbol{\mathcal{C}} \subset \mathcal{Z}$ is not an invariant set. Let $\mathbf{z} \in \boldsymbol{\mathcal{C}}$, and $\tau \in (\tau^-(\mathbf{z}), \tau^+(\mathbf{z})) = I_{\mathbf{z}}$, a connected open interval such that $\tau(\mathbf{x}) \in \boldsymbol{\mathcal{C}}$ for all $\tau \in I_{\mathbf{z}}$. If*

$$[\mathbb{U}_\tau \phi_\lambda](\mathbf{z}) = \phi_\lambda(\mathbf{s}_\tau(\mathbf{z})) = e^{\lambda\tau}\phi_\lambda(\mathbf{z}), \quad \forall \tau \in I_{\mathbf{z}}.$$

Then $\phi_\lambda(\mathbf{z})$ is called the open eigenfunction of the Koopman operator family $\mathbb{U}_t$, for $t \in \mathbb{R}$ with eigenvalue λ.

1) If $\boldsymbol{\mathcal{C}}$ is a proper invariant subset of $\mathcal{Z}$ in which case $I_{\mathbf{z}} = \mathbb{R}$ for every $\mathbf{z} \in \boldsymbol{\mathcal{C}}$, then ϕ_λ is called the subdomain eigenfunction. If $\boldsymbol{\mathcal{C}} = \mathcal{Z}$ then ϕ_λ will be the ordinary eigenfunction associated with eigenvalue λ as defined in (18).

2) The open eigenfunctions as defined above can be extended from $\boldsymbol{\mathcal{C}}$ to a larger reachable set when $\boldsymbol{\mathcal{C}}$ is open based on the construction procedure outlined in [19, Definition 5.2, Lemma 5.1]. Let $\mathcal{P}_z$ be that larger domain.

3) The eigenvalues of the linearization of the system dynamics at the origin, i.e., $\mathbf{E}$, will form the eigenvalues of the Koopman operator [19, Proposition 5.8]. Our interest will be in constructing the corresponding eigenfunctions, defined over the domain $\mathcal{P}_z$. We will refer to these eigenfunctions as *principal eigenfunctions*.

4) The principal eigenfunctions can be used as a change of coordinates in the linear representation of a nonlinear system and draw a connection to the famous Hartman-Grobman theorem on linearization and Poincare normal form [42]. The principal eigenfunctions will be defined over a proper subset $\mathcal{P}_z$ of the state space $\mathcal{Z}$ (called subdomain eigenfunctions) or over the entire $\mathcal{Z}$ [19, Lemma 5.1, Corollary 5.1, 5.2, and 5.8].

5) The conjugacy between the linear and nonlinear system provided by the principal eigenfunction through the Hartman-Grobman theorem is exploited in this paper to compute these eigenfunctions. The spectrum of the Koopman operator reveals essential information about the state space geometry of the dynamical system [18], [19]. In particular, we have the following results.

Corollary 1. *[19, Corollary 5.10] Let the origin be the hyperbolic equilibrium point of the system (15) with $\lambda_1, \ldots, \lambda_p$ the eigenvalues of the linearization of the system (15) at the origin. Let $\lambda_1, \ldots, \lambda_u$ be eigenvalues with positive real part with associated open eigenfunctions $\Phi_u = \{\phi_{\lambda_1}, \ldots, \phi_{\lambda_u}\}$ and $\lambda_{u+1}, \ldots, \lambda_p$ be eigenvalues with negative real part with associated open eigenfunctions $\Phi_s = \{\phi_{\lambda_{u+1}}, \ldots, \phi_{\lambda_p}\}$ defined over the set $\mathcal{P}_z$. Then, the joint level set of the eigenfunctions*

$$\mathcal{M}_{\mathcal{P}}^s = \{\mathbf{z} \in \mathcal{Z} : \phi_{\lambda_1}(\mathbf{z}) = \ldots = \phi_{\lambda_u}(\mathbf{z}) = 0\}, \tag{22}$$

forms the stable manifold on $\mathcal{P}_z$ and the joint level set of the eigenfunctions

$$\mathcal{M}_{\mathcal{P}}^u = \{\mathbf{z} \in \mathcal{Z} : \phi_{\lambda_{u+1}}(\mathbf{z}) = \ldots = \phi_{\lambda_p}(\mathbf{z}) = 0\}, \tag{23}$$

is the unstable manifold on $\mathcal{P}_z$ of origin equilibrium point.

For the stable and unstable manifolds to be well-defined it is assumed that the Jacobian matrix of unstable and stable eigenfunctions satisfy the rank conditions i.e., $\operatorname{rank}\left(\frac{\partial \Phi_u(\mathbf{z})}{\partial \mathbf{z}}\right) = u$ and $\operatorname{rank}\left(\frac{\partial \Phi_s(\mathbf{z})}{\partial \mathbf{z}}\right) = p - u$ for all $\mathbf{z} \in \Phi_u^{-1}(0)$ and $\mathbf{z} \in \Phi_s^{-1}(0)$ respectively. The following remark on the eigenfunctions of the Koopman operator for a linear system is easy to prove.

Remark 5. *The Koopman eigenfunctions corresponding to the eigenvalue λ_j of the linear dynamical system, $\dot{\mathbf{z}} = \mathbf{E}\mathbf{z}$, are given by $\phi_{\lambda_j}(\mathbf{z}) = \mathbf{v}_j^\top \mathbf{z}$, where $\mathbf{v}_j^\top$ is the left eigenvector of $\mathbf{E}$ with eigenvalue λ_j i.e., $\mathbf{v}_j^\top \mathbf{E} = \lambda_j \mathbf{v}_j^\top$.*

III. Main Results

We provide two different procedures for the approximation of the Lagrangian submanifold and the HJ solution based on the spectral properties of the Koopman operator associated with dynamical system $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ and the Hamiltonian system (9). Our first procedure for approximating the Lagrangian submanifold and, hence, the HJ solution follows the approximation procedure outlined in [15] with the fundamental difference that the spectral theory of the Koopman operator forms the foundation of our approximation procedure.

Following the discussion in Section II-A.1, we know that the scalar-valued function, V, which is used for expressing the Lagrangian submanifolds of the Hamiltonian system (9), i.e., $\mathbf{p} = \frac{\partial V}{\partial \mathbf{x}}^\top$ constitute the solution of the HJ equation. For the optimal control problem, if we are only interested in determining the optimal control, then it suffices to determine the Lagrangian submanifold as the optimal input only requires knowledge of $\frac{\partial V}{\partial \mathbf{x}}$ (Eq. (5)). However, in the HJ equation that arises in other applications, such as dissipativity theory, we are interested in determining the function $V(\mathbf{x})$, which acts as a storage function. We write the HJ equation (4) and Hamiltonian function (8) in the following form

$$\frac{\partial V}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) - \frac{1}{2}\frac{\partial V}{\partial \mathbf{x}}\mathbf{R}(\mathbf{x})\frac{\partial V}{\partial \mathbf{x}}^\top + q(\mathbf{x}) = 0, \tag{24}$$

$$H(\mathbf{x},\mathbf{p}) = \mathbf{f}(\mathbf{x})^\top \mathbf{p} - \frac{1}{2}\mathbf{p}^\top \mathbf{R}(\mathbf{x})\mathbf{p} + q(\mathbf{x}). \tag{25}$$

Note that for the optimal control problem

$$\mathbf{R}(\mathbf{x}) = \mathbf{g}(\mathbf{x})\mathbf{D}^{-1}\mathbf{g}(\mathbf{x})^\top. \tag{26}$$

The definition of $\mathbf{R}(\mathbf{x})$ and $q(\mathbf{x})$ will differ based on the problem and the HJ equation under consideration, such as $\mathcal{L}_2$-gain analysis or robust control problem. It is important to emphasize that the HJ equation and the Hamiltonian are nonlinear functions of $\frac{\partial V}{\partial \mathbf{x}}$ and $\mathbf{p}$, respectively. Hence, using equations (24) and (25) directly to solve for the Lagrangian submanifold is impossible. One of the main contributions of this paper is to show that the problem of solving the nonlinear HJ equation can be converted to a convex problem using the spectral theory of the Koopman operator. We now assume the following on the Koopman operator eigenfunctions and the HJ solution.

Assumption 3. *We will assume that the Koopman generator for the dynamical system (15) admits p principal Koopman eigenfunctions $\{\phi_{\lambda_1}(\mathbf{z}), \ldots, \phi_{\lambda_p}(\mathbf{z})\}$ associated with the eigenvalues $\{\lambda_1, \ldots, \lambda_p\}$ of the linearization $\mathbf{E} = \frac{\partial \mathbf{F}}{\partial \mathbf{z}}(0)$. The eigenfunctions are assumed to be defined over domain $\mathcal{P}_z$ and atleast $\mathcal{C}^2$ function of $\mathbf{z}$. Following the results of Corollary 1, the stable and unstable manifolds of the equilibrium point are well-defined in domain $\mathcal{P}_z$. The HJ solution (24) admits a classical solution $V(\mathbf{x}) \in \mathcal{C}^2$ on the domain $\mathcal{Q} \subseteq \mathcal{P}_z$.*

Our next two subsections discuss two procedures developed for the approximation of the Lagrangian manifolds and the HJ solution.

A. Integrable Hamiltonian System and Koopman Eigenfunctions: Procedure One

Our first approach for approximating the Lagrangian submanifold and the HJ solution uses the Koopman operator's principal eigenfunctions corresponding to the dynamical system $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$. Hence following Remark 3, the discussion and Assumptions from Section II-B applies with $\mathbf{F}(\mathbf{z}) = \mathbf{f}(\mathbf{x})$. The procedure relies on decomposing the Hamiltonian in Eq. (25) into integrable (i.e., the part that can be resolved exactly) and non-integrable parts. This approximation procedure closely follows procedure one developed in [15]. The fundamental difference is that we use Koopman eigenfunctions instead of *integral of motions* to decompose the Hamiltonian into integrable and non-integrable parts. We write the Hamiltonian function, $H(\mathbf{x},\mathbf{p})$, as the sum of the nominal Hamiltonian, H_0, and its perturbation, H_1.

$$H(\mathbf{x},\mathbf{p}) = H_0(\mathbf{x},\mathbf{p}) + H_1(\mathbf{x},\mathbf{p}), \tag{27}$$

where

$$H_0(\mathbf{x},\mathbf{p}) = \mathbf{p}^\top \mathbf{f}(\mathbf{x}), \quad H_1(\mathbf{x},\mathbf{p}) = -\frac{1}{2}\mathbf{p}^\top \mathbf{R}(\mathbf{x})\mathbf{p} + q(\mathbf{x}).$$

Consider the Hamiltonian system constructed using the nominal Hamiltonian $H_0(\mathbf{x},\mathbf{p}) = \mathbf{p}^\top \mathbf{f}(\mathbf{x})$ and denoted by $\mathcal{X}_{H_0}$

$$\begin{aligned} \dot{\mathbf{x}} &= \frac{\partial H_0(\mathbf{x},\mathbf{p})}{\partial \mathbf{p}} = \mathbf{f}(\mathbf{x}) \\ \dot{\mathbf{p}} &= -\frac{\partial H_0(\mathbf{x},\mathbf{p})}{\partial \mathbf{x}} = -\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^\top \mathbf{p}. \end{aligned} \tag{28}$$

We show that the Koopman eigenfunctions corresponding to the dynamical system (15) can be used to provide an integrable structure for the Hamiltonian system (28).

Proposition 2. *Following Assumption 3, let $\{\phi_{\lambda_k}(\mathbf{x}), \lambda_k\}$ for $k = 1, \ldots, n$ be the eigenfunctions eigenvalues pair of the Koopman generator corresponding to the system, $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$. Then, $\{\phi_{\lambda_k}(\mathbf{x}), \lambda_k\}$ and $\{H_0(\mathbf{x},\mathbf{p}), 0\}$ are the eigenfunctions eigenvalues pair of the Koopman generator associated with the Hamiltonian system (28).*

Proof: The action of the Koopman generator on $\psi(\mathbf{x},\mathbf{p})$ is given by

$$\mathcal{K}_{\mathcal{X}_{H_0}}\psi(\mathbf{x},\mathbf{p}) = \frac{\partial \psi}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) - \frac{\partial \psi}{\partial \mathbf{p}}\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^\top \mathbf{p}. \tag{29}$$

Since $\{\phi_{\lambda_k}, \lambda_k\}$ for $k = 1, \ldots, n$ form the eigenfunctions, eigenvalues pair of the Koopman generator corresponding to system (28) and $\phi_{\lambda_k}(\mathbf{x})$ are not function of $\mathbf{p}$, it follows that

$$\mathcal{K}_{\mathcal{X}_{H_0}}\phi_{\lambda_k}(\mathbf{x}) = \frac{\partial \phi_{\lambda_k}}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) = \lambda_k \phi_{\lambda_k}(\mathbf{x}).$$

Similarly, by taking $\psi(\mathbf{x},\mathbf{p}) = H_0(\mathbf{x},\mathbf{p})$ and using (29), we obtain

$$\begin{aligned}\mathcal{K}_{\mathcal{X}_{H_0}} H_0 &= \left(\frac{\partial H_0}{\partial \mathbf{x}}\right)\mathbf{f} - \left(\frac{\partial H_0}{\partial \mathbf{p}}\right)\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^\top \mathbf{p} \\ &= \mathbf{p}^\top \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)\mathbf{f} - \mathbf{f}^\top \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^\top \mathbf{p} = 0, \end{aligned} \tag{30}$$

i.e., eigenfunction with eigenvalue zero. □

We aim to show that the eigenfunctions, eigenvalues pair from Proposition 2 provide integrable structure to the nominal Hamiltonian H_0. Toward this goal, we want to determine the canonical change of coordinates for the unperturbed Hamiltonian system. This can be achieved using generating function, $W(\mathbf{x},t)$, that satisfies the following PDE [41], [42].

$$H_0\left(\mathbf{x}, \frac{\partial W(\mathbf{x},t)}{\partial \mathbf{x}}\right) + \frac{\partial W(\mathbf{x},t)}{\partial t} = 0. \tag{31}$$

Proposition 3. *The solution, $W(\mathbf{x},t)$, of the PDE (31) can be written as*

$$W(\mathbf{x},t) = \sum_{\mathbf{k}\in\mathbb{N}^n} \bar{w}_{\mathbf{k}} \prod_{i=1}^{N} \phi_{\lambda_i}^{k_i}(\mathbf{x}) e^{-k_i\lambda_i t}, \tag{32}$$

where $\bar{w}_{\mathbf{k}}$, for $\mathbf{k} = (k_1,\ldots,k_n)$ are constant coefficients and function of the initial state $W(\mathbf{x},0) =: W_0(\mathbf{x})$ at time $t = 0$ and $\{\phi_{\lambda_k}, \lambda_k\}$ are eigenfunction eigenvalue pair of the Koopman generator corresponding to the system $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$.

Proof: The initial state of the system (31) at $t = 0$ $W(\mathbf{x},0) =: W_0(\mathbf{x})$ admits the following Koopman decomposition (Definition 4)

$$W_0(\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{N}^n} \bar{w}_{\mathbf{k}} \prod_{i=1}^{N} \phi_{\lambda_i}^{k_i}(\mathbf{x}) \tag{33}$$

where $\mathbf{k} = (k_1,\ldots,k_n)$ and $\bar{w}_{\mathbf{k}}$ are the Koopman modes associated with eigenfunctions $\phi_{\lambda_1}^{k_1}(\mathbf{x})\ldots\phi_{\lambda_n}^{k_n}(\mathbf{x})$. Using the definition of nominal Hamiltonian, $H_0(\mathbf{x},\mathbf{p})$ from (27), the PDE (31) can be written as

$$\frac{\partial W}{\partial t} = -\left(\frac{\partial W}{\partial \mathbf{x}}\right)\mathbf{f}(\mathbf{x}). \tag{34}$$

Above is a Koopman PDE generated by vector field $\dot{\mathbf{x}} = -\mathbf{f}(\mathbf{x})$ [40, Chapter 7]. Hence the solution of the PDE can be written as

$$W(\mathbf{x},t) = W_0(\mathbf{s}_{-t}(\mathbf{x})), \tag{35}$$

where $\mathbf{s}_{-t}(\mathbf{x})$ is the solution of differential equation $\dot{\mathbf{x}} = -\mathbf{f}(\mathbf{x})$ (i.e., time reversed flow of vector field $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$). Above solution can also be written in terms of the Koopman operator as

$$W(\mathbf{x},t) = W_0(\mathbf{s}_{-t}(\mathbf{x})) = [\mathbb{U}_{-t}W_0](\mathbf{x}), \tag{36}$$

where $\mathbb{U}_{-t}$ is the Koopman operator associated with $\dot{\mathbf{x}} = -\mathbf{f}(\mathbf{x})$. Since $\{\phi_{\lambda_k}(\mathbf{x}), \lambda_k\}$ are the principal eigenfunctions, eigenvalues pair of the Koopman generator corresponding to system $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$, it follows that $\{\phi_{\lambda_k}, -\lambda_k\}$ are the principal eigenfunctions and eigenvalues pair of the Koopman generator corresponding to the system $\dot{\mathbf{x}} = -\mathbf{f}(\mathbf{x})$ as

$$\frac{\partial \phi_{\lambda_k}}{\partial \mathbf{x}}(-\mathbf{f}(\mathbf{x})) = -\lambda_k \phi_k(\mathbf{x}).$$

Since, $W_0(\mathbf{x})$ admits the decomposition (33), it follows that

$$W(\mathbf{x},t) = [\mathbb{U}_{-t}W_0](\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{N}^n} \bar{w}_{\mathbf{k}} \prod_{i=1}^{N} \phi_{\lambda_i}^{k_i}(\mathbf{x}) e^{-k_i\lambda_i t}. \tag{37}$$

□

Proposition 4. *Let $W(\mathbf{x},\mathbf{P},t)$ be the solution of the PDE (31), where the initial condition $W_0(\mathbf{x})$ is assumed to lie in the span of the principal eigenfunctions, i.e.,*

$$W_0(\mathbf{x}) = \sum_{j=1}^{n} P_j \phi_{\lambda_j}(\mathbf{x}), \tag{38}$$

for some constant P_j.[1] *Then*

$$p_j = \frac{\partial W(\mathbf{x},\mathbf{P},t)}{\partial x_j}, \quad X_j = \frac{\partial W(\mathbf{x},\mathbf{P},t)}{\partial P_j}, \quad j = 1,\ldots,n. \tag{39}$$

defines the canonical change of coordinates in which the nominal Hamiltonian dynamics (28) is completely integrable and hence of the form

$$\dot{X}_j = 0, \quad \dot{P}_j = 0, \quad j = 1,\ldots,n. \tag{40}$$

Proof: With $W_0(\mathbf{x})$ of the form (38), using the results of Proposition 3 it follows that

$$W(\mathbf{x},t) = \sum_{j=1}^{n} P_j \phi_{\lambda_j}(\mathbf{x}) e^{-\lambda_j t} =: W(\mathbf{x},P,t). \tag{41}$$

Define a canonical coordinates,

$$p_j = \frac{\partial W}{\partial x_j}, \quad X_j = \frac{\partial W}{\partial P_j}, \quad j = 1,\ldots,n. \tag{42}$$

Then we obtain

$$p_j(t) = \sum_{k=1}^{n} P_k \frac{\partial \phi_{\lambda_k}(\mathbf{x})}{\partial x_j} e^{-\lambda_k t}, \quad X_j(t) = \phi_{\lambda_j}(\mathbf{x}) e^{-\lambda_j t}.$$

Note that

$$\dot{X}_j = \frac{\partial \phi_{\lambda_j}}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) e^{-\lambda_j t} - \lambda_j e^{-\lambda_j t}\phi_{\lambda_j}(\mathbf{x}) = 0, \tag{43}$$

where we have use the fact that $\phi_{\lambda_j}(\mathbf{x})$ is the eigenfunction with eigenvalue λ_j i.e., $\frac{\partial \phi_{\lambda_j}}{\partial \mathbf{x}}\mathbf{f}(\mathbf{x}) = \lambda_j \phi_{\lambda_j}(\mathbf{x})$. Following (43) and using the fact that P_j are constant coefficient used in the expansion of W_0, we obtain the desired results. □

Remark 6. *Using the connection between the generating function, $W(\mathbf{x},\mathbf{P},t) = \mathbf{P}^\top e^{-\Lambda t}\Phi(\mathbf{x})$, and the Koopman eigenfunctions from Proposition 4, we arrive at the following canonical change of variables, $(\mathbf{X},\mathbf{P})$, written in compact notation as*

$$\mathbf{X} = e^{-\Lambda t}\Phi(\mathbf{x}), \quad \mathbf{p}(\mathbf{X},\mathbf{P},t) = \left(\frac{\partial \Phi}{\partial \mathbf{x}}\right)^\top e^{-\Lambda^\top t}\mathbf{P}, \tag{44}$$

[1] The above expansion of the initial state corresponds to the Koopman modes $\bar{w}_{0,\ldots,1_j,\ldots,0} = P_j$ with higher order modes being equal to zero.

where Λ is the block diagonal matrix in real Jordan canonical form consisting of eigenvalues of matrix $\mathbf{A}$ (Assumption 1) and $\Phi(\mathbf{x}) = (\phi_1(\mathbf{x}), \dots, \phi_n(\mathbf{x}))^\top$ is the vector of real eigenfunctions. Furthermore, we can write

$$\mathbf{x} = \Phi^{-1}(e^{\Lambda t}\mathbf{X}), \tag{45}$$

where, $\Phi^{-1}(\cdot)$ is the inverse of mapping Φ, which is known to exist as the principal eigenfunction forms a diffeomorphism in $\mathcal{P}_x$, mapping a nonlinear system to linear system (refer to discussion following Definition 5) and [19, Theorem 5.6, Proposition 5.8].

Using the notation in (44), the nominal Hamiltonian system in the transformed $(\mathbf{X}, \mathbf{P})$ coordinates can be written as

$$\dot{\mathbf{X}} = 0, \quad \dot{\mathbf{P}} = 0.$$

In [15] similar integrable structure was derived using integral of motions of Hamiltonian dynamical system. We next write the perturbed Hamiltonian $H_1(\mathbf{x}, \mathbf{p})$ in terms of the new canonical variables $(\mathbf{X}, \mathbf{P})$ as

$$H_1(\mathbf{x}, \mathbf{p}) = H_1(\mathbf{x}(\mathbf{X}, t), \mathbf{p}(\mathbf{X}, \mathbf{P}, t)) =: \bar{H}_1(\mathbf{X}, \mathbf{P}, t). \tag{46}$$

$$\bar{H}_1(\mathbf{X}, \mathbf{P}, t) = -\frac{1}{2}\mathbf{P}^\top e^{-\Lambda t}\left(\frac{\partial \Phi}{\partial \mathbf{x}}\right) R(\mathbf{x}) \left(\frac{\partial \Phi}{\partial \mathbf{x}}\right)^\top e^{-\Lambda^\top t}\mathbf{P} + q(\Phi^{-1}(e^{\Lambda t}\mathbf{X})). \tag{47}$$

The Hamiltonian system in the new coordinates $(\mathbf{X}, \mathbf{P})$ is given by

$$\dot{\mathbf{X}} = \frac{\partial \bar{H}_1}{\partial \mathbf{P}}, \quad \dot{\mathbf{P}} = -\frac{\partial \bar{H}_1}{\partial \mathbf{X}}. \tag{48}$$

The above discussion can be summarized in the form of the following theorem

Theorem 7. *Let $(\mathbf{X}(t), \mathbf{P}(t))$ be the solution of the Hamiltonian system (48), then the solution $(\mathbf{x}(t), \mathbf{p}(t))$ to the Hamiltonian system (9) is obtained from the canonical change of cooridnates (44)-(45).*

The proof relies on classical results from mechanics as the two Hamiltonian in $(\mathbf{x}, \mathbf{p})$ and $(\mathbf{X}, \mathbf{P})$ coordinates are related via generating function, $W(\mathbf{x}, \mathbf{P}, t)$ from Eq. (41). The above theorem proves that there are no approximations involved in arriving at the Hamiltonian system (48) from (9). However, the Hamiltonian system in $(\mathbf{X}, \mathbf{P})$ coordinates (48) is still nonlinear, and hence it is challenging to find the Lagrangian submanifold and, therefore, the HJ solution. We make the following approximations for the approximate computation of the Lagrangian submanifold and the HJ solution.

Approximation 1. *We simplify the Hamiltonian $\bar{H}_1(\mathbf{X}, \mathbf{P}, t)$ in (47) by making following approximation.*

$$\frac{\partial \Phi}{\partial \mathbf{x}}\mathbf{R}(\mathbf{x})\frac{\partial \Phi}{\partial \mathbf{x}}^\top \approx \mathbf{R}_1, \;\; \& \;\; q(\mathbf{x}) \approx \frac{1}{2}\Phi^\top \mathbf{Q}_1 \Phi, \tag{49}$$

where $\mathbf{R}_1$ and $\mathbf{Q}_1$ are some constant positive matrices. The approximation $\frac{\partial \Phi}{\partial \mathbf{x}}\mathbf{R}(\mathbf{x})\frac{\partial \Phi}{\partial \mathbf{x}}^\top \approx \mathbf{R}_1$ can be broken down as follows. First, the matrix $\mathbf{R}(\mathbf{x}) = \mathbf{g}(\mathbf{x})\mathbf{g}(\mathbf{x})^\top \approx \mathbf{R}_0$ is a constant matrix and will be true if the input matrix $\mathbf{g}(\mathbf{x}) = \mathbf{B}$ is constant, if not then $\mathbf{R}_0$ can be obtained as $\mathbf{R}_0 = \mathbf{g}(0)\mathbf{g}(0)^\top$. Second, the eigenfunction $\Phi(\mathbf{x})$ which admits a decomposition into linear and nonlinear parts, i.e., $\Phi(\mathbf{x}) = \mathbf{V}^\top\mathbf{x} + \mathbf{H}(\mathbf{x})$ (refer to Section III-C) is approximated as

$$\Phi(\mathbf{x}) \approx \mathbf{V}^\top \mathbf{x}.$$

Combining these, we can write

$$\begin{aligned}\frac{\partial \Phi}{\partial \mathbf{x}}\mathbf{R}(\mathbf{x})\frac{\partial \Phi}{\partial \mathbf{x}}^\top &= \left(\mathbf{V} + \frac{\partial \mathbf{H}}{\partial \mathbf{x}}\right)(\mathbf{R}_0 + \mathbf{R}(\mathbf{x}) - \mathbf{R}_0)\left(\mathbf{V} + \frac{\partial \mathbf{H}}{\partial \mathbf{x}}\right)^\top \\ &= \mathbf{V}\mathbf{R}_0\mathbf{V}^\top + O(|\mathbf{x}|^2) \approx \mathbf{V}\mathbf{R}_0\mathbf{V}^\top =: \mathbf{R}_1.\end{aligned} \tag{50}$$

The other approximation $q(\mathbf{x}) \approx \Phi^\top \mathbf{Q}_1 \Phi$ can be understood using Koopman mode decomposition (Definition 4). In particular, state cost can be projected along the eigenfunctions $\phi_i(\mathbf{x})\phi_j(\mathbf{x})$ for $i, j = 1, \dots, n$. In particular, for the case when the state cost is quadratic, i.e., $q(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top \mathbf{Q}_0 \mathbf{x}$, we have

$$\begin{aligned}\frac{1}{2}\Phi^\top \mathbf{Q}_1 \Phi &= \frac{1}{2}(\mathbf{V}^\top\mathbf{x} + \mathbf{H}(\mathbf{x}))^\top \mathbf{Q}_1 (\mathbf{V}^\top\mathbf{x} + \mathbf{H}(\mathbf{x})) \\ &= \frac{1}{2}\mathbf{x}^\top \mathbf{V}\mathbf{Q}_1\mathbf{V}^\top\mathbf{x} + O(|\mathbf{x}|^3) \approx \frac{1}{2}\mathbf{x}^\top \mathbf{Q}_0 \mathbf{x}\end{aligned} \tag{51}$$

and where $\mathbf{Q}_1$ is defined as $\mathbf{Q}_1 := \mathbf{V}^{-1}\mathbf{Q}_0(\mathbf{V}^\top)^{-1}$.

Using the above approximation, the Hamiltonian can be written as

$$\bar{H}_1(\mathbf{X}, \mathbf{P}, t) = -\frac{1}{2}\mathbf{P}^\top e^{-\Lambda t}\mathbf{R}_1 e^{-\Lambda^\top t}\mathbf{P} + \frac{1}{2}\mathbf{X}^\top e^{\Lambda^\top t}\mathbf{Q}_1 e^{\Lambda t}\mathbf{X}.$$

The nonlinear Hamiltonian system (48) get transformed to following linear Hamiltonian system.

$$\begin{pmatrix}\dot{\mathbf{X}} \\ \dot{\mathbf{P}}\end{pmatrix} = \begin{pmatrix}0 & -e^{-\Lambda t}\mathbf{R}_1 e^{-\Lambda^\top t} \\ -e^{\Lambda^\top t}\mathbf{Q}_1 e^{\Lambda t} & 0\end{pmatrix}\begin{pmatrix}\mathbf{X} \\ \mathbf{P}\end{pmatrix}. \tag{52}$$

The time-varying Hamiltonian system can be converted to time-invariant system by performing one more linear time-varying change of coordinates as

$$\bar{\mathbf{X}} = e^{\Lambda t}\mathbf{X}, \quad \bar{\mathbf{P}} = e^{-\Lambda^\top t}\mathbf{P}. \tag{53}$$

Writing (52) in $(\bar{\mathbf{X}}, \bar{\mathbf{P}})$ coordinates, we obtain

$$\begin{pmatrix}\dot{\bar{\mathbf{X}}} \\ \dot{\bar{\mathbf{P}}}\end{pmatrix} = \begin{pmatrix}\Lambda & -\mathbf{R}_1 \\ -\mathbf{Q}_1 & -\Lambda^\top\end{pmatrix}\begin{pmatrix}\bar{\mathbf{X}} \\ \bar{\mathbf{P}}\end{pmatrix} =: \mathcal{H}\begin{pmatrix}\bar{\mathbf{X}} \\ \bar{\mathbf{P}}\end{pmatrix}. \tag{54}$$

Since the system equations are linear, an analytical expression for the Lagrangian subspace and the HJ solution can be found. The problem of computing the Lagrangian subspace for the linear system can be reduced to the solution of the Riccatti equation. The results we present next are known in the literature in different forms. However, we offer these results in the spirit of the Koopman theory, which specializes in linear systems case. We assume that the Hamiltonian matrix $\mathcal{H}$ satisfies Assumption 2. The main result of this construction procedure is summarized in the following proposition.

Proposition 5. *For the linear Hamiltonian system (54) under Assumption 2 the Lagrangian subspace is given by*

$$\hat{\mathcal{L}}_l = \{(\bar{\mathbf{X}}, \bar{\mathbf{P}}) : \bar{\mathbf{P}} = \mathbf{L}\bar{\mathbf{X}},\ \ \mathbf{L} = -\mathbf{D}_2^{-1}\mathbf{D}_1\}, \tag{55}$$

where

$$\mathbf{D} = \begin{pmatrix} \mathbf{d}_1^\top \\ \vdots \\ \mathbf{d}_n^\top \end{pmatrix} = \begin{pmatrix} \mathbf{D}_1 & \mathbf{D}_2 \end{pmatrix} \in \mathbb{R}^{n\times 2n},\ \ \mathbf{D}_i \in \mathbb{R}^{n\times n},\ i = 1, 2. \tag{56}$$

and $\mathbf{d}_j^\top$ for $j = 1, \ldots, n$ are the left eigenvectors associated with eigenvalues with positive real part of the Hamiltonian matrix $\mathcal{H}$.

Refer to the Appendix for the proof. We next show that the matrix $\mathbf{L}$ from Proposition 5 satisfies the Riccatti equation.

Proposition 6. *The matrix $\mathbf{L}$ from Proposition 5 satisfies the Riccatti equation*

$$\Lambda^\top \mathbf{L} + \mathbf{L}\Lambda - \mathbf{L}\mathbf{R}_1\mathbf{L} + \mathbf{Q}_1 = 0, \tag{57}$$

and the spectrum of the closed loop linear system $\Lambda - \hat{\mathbf{R}}\mathbf{L}$ is in the left half plane.

Refer to Appendix for the proof. The Lagrangian submanifold can now be computed as follows. From (55), we have

$$\bar{\mathbf{P}} = \mathbf{L}\bar{\mathbf{X}} \implies \text{from Eq.(53)} \implies e^{-\Lambda^\top t}\mathbf{P} = \mathbf{L}e^{\Lambda t}\mathbf{X}.$$

Pre-multiplying the above by $\frac{\partial \Phi}{\partial \mathbf{x}}$ and using (44), we obtain

$$\mathbf{p} = \left(\frac{\partial \Phi}{\partial \mathbf{x}}\right) e^{-\Lambda^\top t}\mathbf{P} = \left(\frac{\partial \Phi}{\partial \mathbf{x}}\right)\mathbf{L}e^{\Lambda t}\mathbf{X} = \left(\frac{\partial \Phi}{\partial \mathbf{x}}\right)\mathbf{L}\Phi(\mathbf{x}).$$

We thus obtain the following expression for the approximate Lagrangian submanifold

$$\hat{\mathcal{L}} = \left\{(\mathbf{x}, \mathbf{p}) : \mathbf{p} = \left(\frac{\partial \Phi}{\partial \mathbf{x}}\right)^\top \mathbf{L}\Phi(\mathbf{x})\right\}. \tag{58}$$

We know that the Lagrangian submanifold is obtained as a gradient of a scalar value function i.e., $\mathbf{p} = \frac{\partial V}{\partial \mathbf{x}}$. Hence from (58), we obtain

$$V(\mathbf{x}) = \frac{1}{2}\Phi(\mathbf{x})^\top \mathbf{L}\Phi(\mathbf{x}). \tag{59}$$

as the approximate HJ solution. This suggests that the approximated optimal cost is quadratic in Koopman eigenfunction coordinates where following the results of Proposition 6, the matrix $\mathbf{L}$ is obtained as a solution of the Riccatti equation.

Remark 8. *We observe from (58) that the Riccatti solution from the linearized HJ equation is obtained as a particular case of the Lagrangian submanifold construction proposed in procedure one. In particular, the special case will correspond to the eigenfunctions $\Phi(\mathbf{x})$ being approximated as a linear function of $\mathbf{x}$, i.e., $\Phi(\mathbf{x}) = \mathbf{V}^\top\mathbf{x}$ with $\mathbf{V}^\top\mathbf{A} = \Lambda\mathbf{V}^\top$. In this case, we have*

$$V(\mathbf{x}) = \frac{1}{2}\Phi^\top(\mathbf{x})\mathbf{L}\Phi(\mathbf{x}) = \frac{1}{2}\mathbf{x}^\top\mathbf{V}\mathbf{L}\mathbf{V}^\top\mathbf{x} = \frac{1}{2}\mathbf{x}^\top\mathbf{P}_r\mathbf{x}.$$

Since we know that the matrix $\mathbf{L}$ satisfies the Riccatti equation (57) it then follows that the matrix $\mathbf{P}_r$ satisfies following Riccatti equation

$$\mathbf{A}^\top\mathbf{P}_r + \mathbf{P}_r\mathbf{A} - \mathbf{P}_r\mathbf{R}_0\mathbf{P}_r + \mathbf{Q}_0 = 0,$$

where $\mathbf{A} = (\mathbf{V}^{-1})^\top\Lambda\mathbf{V}^\top$ and $\mathbf{Q}_0, \mathbf{R}_0$ are as given in (50)-(51). This proves that the Riccatti solution is embedded in the proposed approximation of the HJ solution obtained using procedure one.

Summary: The approximation of the Lagrangian submanifold and the HJ solution using procedure one are given by Eqs. (58) and (59) respectively, where $\Phi(\mathbf{x})$ are the principal Koopman eigenfunction of the uncontrolled system $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ and the $\mathbf{L}$ is obtained as the solution of Riccatti equation (57).

B. Koopman Eigenfunctions of Hamiltonian System : Procedure Two

While the procedure one makes use of eigenfunctions of the uncontrolled system, $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$, the procedure two relies on the eigenfunctions of the Hamiltonian system for the approximation of the Lagrangian submanifold and the HJ solution. The Hamiltonian system is repeated here for convenience.

$$\begin{aligned} \dot{\mathbf{x}} &= \mathbf{f}(\mathbf{x}) - \mathbf{R}(\mathbf{x})\mathbf{p} \\ \dot{\mathbf{p}} &= -\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)^\top \mathbf{p} + \frac{1}{2}\left(\frac{\partial \mathbf{p}^\top\mathbf{R}(\mathbf{x})\mathbf{p}}{\partial \mathbf{x}}\right)^\top - \frac{\partial q}{\partial \mathbf{x}}^\top. \end{aligned} \tag{60}$$

The linearization of the nonlinear Hamiltonian system at the origin is given by following the Hamiltonian matrix

$$\mathcal{H}_1 = \begin{pmatrix} \mathbf{A} & -\mathbf{R}_2 \\ -\mathbf{Q}_2 & -\mathbf{A}^\top \end{pmatrix}, \tag{61}$$

where $\mathbf{A} = \frac{\partial \mathbf{f}}{\partial \mathbf{x}}(0), \mathbf{R}_2 = \mathbf{R}(0)$, and $\mathbf{Q}_2 = \frac{\partial^2 q}{\partial \mathbf{x}^2}(0)$. Following Assumption 1, we know that the equilibrium point is hyperbolic, with eigenvalues forming a mirror image along the imaginary axis. Furthermore, similar to procedure one, we assume the Hamiltonian matrix $\mathcal{H}_1$ satisfies Assumption 2.

The Hamiltonian dynamical system is a $2n$-dimensional system; hence, it has $2n$ principal eigenfunctions. However, we are only interested in computing n out of the $2n$ eigenfunctions. Which of the n eigenfunctions to compute will depend on the HJ equation under consideration. For example, in the optimal control problem, the Lagrangian submanifold is the subset of the stable manifold [1, Proposition 11.2.2] as the optimal control is stabilizing. Hence, for the optimal control problem, we would compute the eigenfunctions corresponding to the eigenvalues with positive real part, as the joint zero-level curves of the unstable eigenfunctions constitute the stable manifold (Corollary 1). Let $\Phi_u(\mathbf{z}) : T^\star\mathcal{M} \to \mathbb{R}^n$ with $\mathbf{z} \in \mathcal{P}_z$ be the eigenfunctions corresponding to the eigenvalues with positive real part. The stable manifold is then given by

$$\mathcal{M}_s = \{\mathbf{z} \in \mathcal{P}_z : \Phi_u(\mathbf{z}) = 0\}. \tag{62}$$

The Lagrangian submanifold is obtained from the stable manifold as a graph of the gradient of the scalar function

$V(\mathbf{x})$, i.e.,

$$\mathcal{L} = \left\{ \mathbf{z} \in \mathcal{M}_s : \left(\mathbf{x}, \mathbf{p} = \frac{\partial V}{\partial \mathbf{x}}^\top \right) \right\}. \tag{63}$$

The scalar valued function, $V(\mathbf{x})$, will be the solution of the HJ equation.

Remark 9. *Our ultimate objective is to approximate the Lagrangian submanifold, $\mathcal{L}$, in Eq. (63) and the HJ solution, V, but not the eigenfunctions, Φ_u, of the Hamiltonian system per se. The eigenfunctions of the Hamiltonian system are used as an intermediate step towards approximation of the HJ solution. With this ultimate goal in mind, we observe that the Lagrangian submanifold is a subset of stable invariant manifold characterized by a set of all $(\mathbf{x}, \mathbf{p})$ such that $\mathbf{p} - \frac{\partial V}{\partial \mathbf{x}}^\top = 0$, i.e., linear function of $\mathbf{p}$. This linear parameterization of the Lagrangian submanifold in variable $\mathbf{p}$ is crucial in selecting basis functions for approximating the Koopman eigenfunctions. In particular, we choose the basis functions to be linear in the variable $\mathbf{p}$ for the approximation of the Koopman eigenfunctions.*

Our main contribution towards approximating the Koopman eigenfunction is presented in Section III-C. In this section, we will assume that the principal eigenfunctions are approximated and demonstrate their application for the computation of the Lagrangian submanifold and the HJ solution. Towards this goal, we first write the Hamiltonian system (60) in the compact form and split it into linear and nonlinear parts as

$$\dot{\mathbf{z}} = \mathbf{F}(\mathbf{z}) = \mathcal{H}_1 \mathbf{z} + \mathbf{F}_n(\mathbf{z}), \tag{64}$$

where, $\mathbf{z} = (\mathbf{x}^\top, \mathbf{p}^\top)^\top$, $\mathcal{H}_1$ is given in (61) and $\mathbf{F}_n(\mathbf{z}) = \mathbf{F}(\mathbf{z}) - \mathcal{H}_1 \mathbf{z}$. We now introduce a few notations to facilitate the following discussion. Let $\mathbf{W}^\top$ consists of the left eigenvectors of the Hamiltonian matrix $\mathcal{H}_1$ (Eq. (61)) i.e., $\mathbf{W}^\top \mathcal{H}_1 = \Lambda_{\mathbf{F}} \mathbf{W}^\top$ with $\Lambda_{\mathbf{F}}$ corresponds to the matrix of eigenvalues of $\mathcal{H}_1$ in real Jordan canonical form. The matrix $\mathbf{W}^\top \in \mathbb{R}^{2n \times 2n}$ admits following decomposition

$$\mathbf{W}^\top = \begin{pmatrix} \mathbf{W}_u^\top \\ \mathbf{W}_s^\top \end{pmatrix} \in \mathbb{R}^{2n \times 2n}, \tag{65}$$

where $\mathbf{W}_u^\top \in \mathbb{R}^{n \times 2n}, \mathbf{W}_s^\top \in \mathbb{R}^{n \times 2n}$ corresponds to unstable and stable linear subspace respectively. Following the decomposition of the Hamiltonian system into linear and nonlinear parts, the principal eigenfunction can also be decomposed into linear and nonlinear parts as follows.

$$\mathbb{R}^n \ni \Phi_u(\mathbf{z}) = \mathbf{W}_u^\top \begin{pmatrix} \mathbf{x}^\top & \mathbf{p}^\top \end{pmatrix}^\top + \mathbf{U} \Gamma_M(\mathbf{z}), \tag{66}$$

where, $\mathbf{W}_u^\top \mathbf{z}$ is the linear part and $\mathbf{U}\Gamma_M(\mathbf{z})$ is the nonlinear part. Similar decomposition also applies to eigenfunctions corresponding to eigenvalue with negative real parts. The nonlinear part of the eigenfunction is approximated by the term $\mathbf{U}\Gamma_M(\mathbf{z})$, where $\mathbf{U} \in \mathbb{R}^{n \times M}$ and $\Gamma_M(\mathbf{z}) : T^\star \mathcal{M} \to \mathbb{R}^M$ are the finite basis functions used in the approximation. Our proposed computational framework for approximating the nonlinear part of the eigenfunctions is presented in Section III-C. The main contribution and conclusion of Section III-C is that the matrix $\mathbf{U}$ can be obtained as a solution to the least square problem using data. Following Remark 9, the basis functions are assumed to be of the form

$$\Gamma_M(\mathbf{z}) = \begin{pmatrix} \Xi_1^\top(\mathbf{x}) & (\Xi_2(\mathbf{x})\mathbf{p})^\top \end{pmatrix}^\top \in \mathbb{R}^M. \tag{67}$$

where $\Xi_1(\mathbf{x}) \in \mathbb{R}^N$ and $\Xi_2(\mathbf{x}) \in \mathbb{R}^{(M-N) \times n}$. Since $\mathbf{U}\Gamma_M(\mathbf{z})$ captures the pure nonlinear part of the eigenfunctions, we chose basis function $\Gamma_M(\mathbf{z})$ such that $\frac{\partial \Gamma_M}{\partial \mathbf{z}}(0) = 0$. Given the form of $\mathbf{W}_u$ and $\Gamma_M(\mathbf{z})$, we can decompose (66) to determine the stable manifold as the joint zero-level set of unstable eigenfunctions

$$0 = \Phi_u(\mathbf{x}, \mathbf{p}) := \mathbf{W}_u^\top \begin{pmatrix} \mathbf{x} \\ \mathbf{p} \end{pmatrix} + \begin{pmatrix} \mathbf{U}_{11} & \mathbf{U}_{12} \end{pmatrix} \begin{pmatrix} \Xi_1(\mathbf{x}) \\ \Xi_2(\mathbf{x})\mathbf{p} \end{pmatrix}, \tag{68}$$

where we split the matrix $\mathbf{U}$ with $\mathbf{U}_{11} \in \mathbb{R}^{n \times N}, \mathbf{U}_{12} \in \mathbb{R}^{n \times (M-N)}$. Following (62) and (63), the objective is to find Lagrangian submanifold of the form $\mathbf{p} = \frac{\partial V}{\partial \mathbf{x}}^\top$ for some unknown function V such that $\Phi_u(\mathbf{x}, \mathbf{p} = \frac{\partial V}{\partial \mathbf{x}}^\top) = 0$. We seek the following form of the Lagrangian submanifold consisting of linear and nonlinear terms

$$\mathbf{p} = \frac{\partial V}{\partial \mathbf{x}}^\top =: \mathbf{p}_l + \mathbf{p}_n. \tag{69}$$

Substituting the assumed form of the Lagrangian submanifold from (69) in (68), we obtain

$$\begin{aligned} &\mathbf{W}_{u1}^\top \mathbf{x} + \mathbf{W}_{u2}^\top (\mathbf{p}_l + \mathbf{p}_n) + \mathbf{U}_{11} \Xi_1(\mathbf{x}) \\ &+ \mathbf{U}_{12} \Xi_2(\mathbf{x})(\mathbf{p}_l + \mathbf{p}_n) = 0. \end{aligned} \tag{70}$$

Equating the linear and nonlinear terms, we obtain

$$\mathbf{W}_{u1}^\top \mathbf{x} + \mathbf{W}_{u2}^\top \mathbf{p}_l = 0 \implies \mathbf{p}_l := \mathbf{J}_l \mathbf{x} = -(\mathbf{W}_{u2}^\top)^{-1} \mathbf{W}_{u1} \mathbf{x}$$

where, the invertibility of matrix $\mathbf{W}_{u2}$ follows from the fact the Hamiltonian matrix $\mathcal{H}_1$ satisfies Assumption 2 (refer to the proof of Proposition 5 in the Appendix). The optimal $\mathbf{J}_l^\star$ and hence $\mathbf{p}_l^\star$ is given by

$$\mathbf{p}_l^\star = \mathbf{J}_l^\star \mathbf{x} = -(\mathbf{W}_{u2}^\top)^{-1} \mathbf{W}_{u1}^\top \mathbf{x}. \tag{71}$$

We notice, following results of Propositions 5 and 6, that $\mathbf{J}_l^\star$ matches with the solution of Riccatti equation. In particular $\mathbf{P} := \mathbf{V}\mathbf{J}_l^\star \mathbf{V}^\top$, where $\mathbf{V}^\top \mathbf{A} = \Lambda \mathbf{V}$ satisfies the following Riccatti equation

$$\mathbf{A}^\top \mathbf{P} + \mathbf{P}\mathbf{A} - \mathbf{P}\mathbf{R}_2\mathbf{P} + \mathbf{Q}_2 = 0, \tag{72}$$

Substituting the $\mathbf{p}_l^\star$ in Eq. (70) we obtain following equation for the nonlinear part

$$\mathbf{W}_{u_2}^\top \mathbf{p}_n + \mathbf{U}_{11} \Xi_1(\mathbf{x}) + \mathbf{U}_{12} \Xi_2(\mathbf{x}) \mathbf{p}_l^\star + \mathbf{U}_{12} \Xi_2(\mathbf{x}) \mathbf{p}_n = 0. \tag{73}$$

As $\mathbf{p}_l^\star = \mathbf{J}_l^\star \mathbf{x}$ is a known linear function of $\mathbf{x}$ from Eq. (71), we define $\mathbf{G}_1(\mathbf{x}) := \mathbf{U}_{11} \Xi_1(\mathbf{x}) + \mathbf{U}_{12} \Xi_2(\mathbf{x}) \mathbf{J}_l^\star \mathbf{x} \in \mathbb{R}^n$ and $\mathbf{G}_2(\mathbf{x}) := \mathbf{W}_{u_2}^\top + \mathbf{U}_{12} \Xi_2(\mathbf{x}) \in \mathbb{R}^{n \times n}$. With this definition, we can write (73) as

$$\mathbf{G}_1(\mathbf{x}) + \mathbf{G}_2(\mathbf{x}) \mathbf{p}_n = 0. \tag{74}$$

Under the assumption that $\mathbf{G}_2(\mathbf{x})$ is invertible, we can obtain $\mathbf{p}_n$ as

$$\mathbf{p}_n^\star = -\mathbf{G}_2(\mathbf{x})^{-1} \mathbf{G}_1(\mathbf{x}). \tag{75}$$

The invertibility assumption on $\mathbf{G}_2(\mathbf{x})$ can be viewed as the nonlinear generalization of invertibility of matrix $\mathbf{W}_{u2}$. The invertibility of $\mathbf{W}_{u_2}$ follows from Assumption 2 (refer to the proof of Propostion 5 in Appendix). Combining (71) and (75), the approximation of the Lagrangian submanifold is given by

$$\mathbf{p}^\star = -(\mathbf{W}_{u2}^\top)^{-1}\mathbf{W}_{u1}^\top \mathbf{x} - \mathbf{G}_2(\mathbf{x})^{-1}\mathbf{G}_1(\mathbf{x}). \tag{76}$$

There is a similarity between the formula for linear $\mathbf{p}_l$ in Eq. (71) and nonlinear, $\mathbf{p}_n$ in Eq. (75). Both these formula has same functional form where $\mathbf{G}_2(\mathbf{x})$ and $\mathbf{G}_1(\mathbf{x})$ can be viewed as nonlinear generalization of $\mathbf{W}_{u_2}$ and $\mathbf{W}_{u_1}$ respectively. It suffices to use (76) if we are only interested in computing the optimal control. Alternatively, if we are interested in computing the optimal cost, we proceed as follows. Let $\Xi_3(\mathbf{x}) \in \mathbb{R}^{M_1}$ be the basis function satisfying $\frac{\partial \Xi_3(0)}{\partial \mathbf{x}} = 0$ and $V_n(\mathbf{x}) = \frac{1}{2}\Xi_3^\top(\mathbf{x})\mathbf{J}_n\Xi_3(\mathbf{x})$, for some positive $\mathbf{J}_n \in \mathbb{R}^{M_1 \times M_1}$, be the parametrization of the optimal cost function corresponding to terms containing higher than quadratic nonlinearity. Then substituting for $\mathbf{p}_n = \frac{\partial V}{\partial \mathbf{x}}^\top = \frac{\partial \Xi_3}{\partial \mathbf{x}}^\top \mathbf{J}_n \Xi_3(\mathbf{x}) = \bar{\Xi}_3 \mathrm{vec}(\mathbf{J}_n)$ in Eq. (74). The $\mathrm{vec}(\mathbf{J}_n) \in \mathbb{R}^{\frac{M_1(M_1+1)}{2}}$ is the vector form of the matrix $\mathbf{J}_n$ and $\bar{\Xi}_3(\mathbf{x}) \in \mathbb{R}^{n \times M_1}$ is obtained from $\frac{\partial \Xi_3}{\partial \mathbf{x}}$ and $\Xi_3(\mathbf{x})$. Using (74), we can write the following optimization problem to solve for $\mathbf{J}_n$.

$$\min_{\mathbf{J}_n \geq 0} \|\mathcal{B}\mathrm{vec}(\mathbf{J}_n) - \mathcal{A}\|, \tag{77}$$

where

$$\mathcal{B} = \left(\bar{\mathbf{G}}_2(\mathbf{x}_1)^\top, \ldots, \bar{\mathbf{G}}_2(\mathbf{x}_L)^\top\right)^\top,\ \mathcal{A} = \left(\mathbf{G}_1(\mathbf{x}_1)^\top, \ldots, \mathbf{G}_1(\mathbf{x}_L)^\top\right)^\top$$

with $\bar{G}_2(\mathbf{x}) := \mathbf{G}_2(\mathbf{x})\bar{\Xi}_3(\mathbf{x})$ and $\{\mathbf{x}_k\}_{k=1}^L$ are the sampled data points. The solution of the above optimization problem, $\mathbf{J}_n^\star$, will be used to write the optimal cost function as

$$V(\mathbf{x}) = \frac{1}{2}(\mathbf{x}^\top \mathbf{J}_l^\star \mathbf{x} + \Xi_3(\mathbf{x})^\top \mathbf{J}_n^\star \Xi_3(\mathbf{x})). \tag{78}$$

So procedure two, leads to two formulas for optimal control. Based on (76), we obtain following expression for the optimal control

$$\mathbf{u}^\star = -\mathbf{D}^{-1}\mathbf{g}^\top \left((\mathbf{W}_{u2}^\top)^{-1}\mathbf{W}_{u1}^\top \mathbf{x} + \mathbf{G}_2(\mathbf{x})^{-1}\mathbf{G}_1(\mathbf{x})\right), \tag{79}$$

and using (78), we obtain

$$\mathbf{u}^\star = -\mathbf{D}^{-1}\mathbf{g}^\top \left(\mathbf{J}_l^\star \mathbf{x} + \frac{\partial \Xi_3}{\partial \mathbf{x}}^\top \mathbf{J}_n^\star \Xi_3\right). \tag{80}$$

Furthermore, the HJ solution (78) can be used to construct the Lagrangian submanifold as

$$\mathbf{p} = \mathbf{J}_l^\star \mathbf{x} + \frac{\partial \Xi_3}{\partial \mathbf{x}}^\top \mathbf{J}_n^\star \Xi_3(\mathbf{x}). \tag{81}$$

We comment on the approximation of the Lagrangian submanifold in Eq. (76) at the end of subsection III-C.

Summary: Using procedure two, we obtain two different formulas for the Lagrangian submanifold given by (76) and (81). The solution of HJ equation and optimal cost function is given by (78).

C. Computation of Principal Eigenfunctions: Convergence Analysis

There are several approaches available for the computation of the Koopman operator, including results that provide sample complexity-based error bounds in the computation [20]–[23]. This section presents results for directly approximating the principal Koopman spectrum. We do not approximate the Koopman operator itself. Following Remark 3, the results are presented for the dynamical system in the form (15). Using Assumption 1 and Remark 4 , we can decompose the system (15) into linear and nonlinear parts as

$$\dot{\mathbf{z}} = \mathbf{F}(\mathbf{z}) = \mathbf{E}\mathbf{z} + (\mathbf{F}(\mathbf{z}) - \mathbf{E}\mathbf{z}) =: \mathbf{E}\mathbf{z} + \mathbf{F}_n(\mathbf{z}). \tag{82}$$

For the simplicity of presentation and continuity of notations, we present approximation results for eigenfunctions with real eigenvalues; the extension to the complex case is straightforward. Let λ be the Koopman generator's eigenvalues and also of $\mathbf{E}$. The eigenfunction corresponding to eigenvalue λ admits the decomposition into linear and nonlinear parts.

$$\phi_\lambda(\mathbf{z}) = \mathbf{w}^\top \mathbf{z} + h(\mathbf{z}), \tag{83}$$

where $\mathbf{w}^\top \mathbf{z}$ and $h(\mathbf{z})$ are the eigenfunction's linear and purely nonlinear parts, respectively. Substituting (83) in (19) and using (82), we obtain following equations to be satisfied by $\mathbf{w}$ and $h(\mathbf{z})$

$$\mathbf{w}^\top \mathbf{E} = \lambda \mathbf{w}^\top,\ \ \frac{\partial h}{\partial \mathbf{z}}\mathbf{F}(\mathbf{z}) - \lambda h(\mathbf{z}) + \mathbf{w}^\top \mathbf{F}_n(\mathbf{z}) = 0. \tag{84}$$

So, the linear part of the eigenfunction can be found as the left eigenvector with eigenvalue λ of matrix $\mathbf{E}$, and the nonlinear term satisfies the linear partial differential equation. We have the following proposition for the finite-dimensional approximation of $h(\mathbf{z})$ using finite basis functions. We make the following assumption on the basis functions.

Assumption 4. *We assume that the basis function $\Gamma_M = \{\gamma_j\}_{j=1}^M$ with $\gamma_j : \mathcal{Z} \to \mathbb{R}$ are μ linearly independent i.e.,*

$$\mu\{\mathbf{z} \in \mathcal{Z} : \mathbf{c}^\top \Gamma(\mathbf{z}) = 0\} = 0. \tag{85}$$

Also with no loss of generality we assume that $\{\frac{\partial \gamma_j}{\partial \mathbf{x}}\mathbf{F} - \lambda\gamma_j\}_{j=1}^M$ for any given eigenvalue λ of $\mathbf{E}$ are also μ linearly independent. Because if not then there exists a vector $\mathbf{c}$ such that $\frac{\partial \mathbf{c}^\top \Gamma_M}{\partial \mathbf{z}}\mathbf{F} = \lambda \mathbf{c}^\top \Gamma_M$. Hence, $\mathbf{c}^\top \Gamma_M$ is precisely the nonlinear part of the eigenfunction corresponding to eigenvalue λ and can be taken out of consideration to approximate.

Typically, the measure μ can be taken to be equivalent to Lebesgue. Let $\mathcal{F}_M = \mathrm{span}\{\gamma_1, \ldots, \gamma_M\}$ and $\mathcal{F} = \mathcal{L}_2(\mu)$ for some positive measure μ on $\mathcal{Z}$ with inner product $\langle f, g\rangle_{\mathcal{L}_2(\mu)} = \int_{\mathcal{Z}} f(\mathbf{z})g(\mathbf{z})d\mu(\mathbf{z})$.

Definition 6. *Given a countable set of functions $\Gamma = \{\gamma_j\}_1^\infty$, with $\gamma_j : \mathcal{Z} \to \mathbb{R}$, define $\mathcal{G}(\Gamma, \mathcal{Z})$ to be set of all linear combinations of elements in Γ that converge pointwise at each $\mathbf{z} \in \mathcal{Z}$ w.r.t measure μ.*

The main results of this section relies on the following Lemma and the proof follows along the lines of proof of [5, Lemma 14] on the Galerkin approximation.

Lemma 1. *If the set $\{\gamma_j\}_1^\infty$ is linearly independent and $\frac{\partial\gamma_j}{\partial\mathbf{z}}\mathbf{F}-\lambda\gamma_j \in \mathcal{G}(\Gamma,\mathcal{Z})$, then for all M,*

$$\operatorname{rank}(\mathbf{J}_\mu) = M, \tag{86}$$

where $\mathbf{J}_\mu := \left\langle (\frac{\partial\Gamma_M}{\partial\mathbf{z}}\mathbf{F}-\lambda\Gamma_M), \Gamma_M\right\rangle_m$ [2]

Proof: Since, $\{\gamma_j\}_1^\infty$ is linearly independent and $\frac{\partial\gamma_j}{\partial\mathbf{z}}\mathbf{F}-\lambda\gamma_j \in \mathcal{G}(\Gamma,\mathcal{Z})$, we have

$$\frac{\partial\gamma_j}{\partial\mathbf{z}}\mathbf{F}-\lambda\gamma_j = \sum_{k=1}^{\infty} c_{kj}\gamma_j(\mathbf{z}) = \mathbf{c}_j^\top\Gamma(\mathbf{z}).$$

We can write

$$\mathbf{J}_\mu = \begin{pmatrix} \left\langle \mathbf{c}_1^\top\Gamma, \gamma_1\right\rangle & \dots & \left\langle \mathbf{c}_M^\top\Gamma, \gamma_1\right\rangle \\ \vdots & \dots & \vdots \\ \left\langle \mathbf{c}_1^\top\Gamma, \gamma_M\right\rangle & \dots & \left\langle \mathbf{c}_M^\top\Gamma, \gamma_M\right\rangle \end{pmatrix}$$
$$= \begin{pmatrix} \langle\Gamma,\Gamma_M\rangle_m \mathbf{c}_1 & \dots & \langle\Gamma,\Gamma_M\rangle_m \mathbf{c}_M \end{pmatrix} = \langle\Gamma,\Gamma_M\rangle_m \mathcal{D}, \tag{87}$$

where $\mathcal{D} := [\mathbf{c}_1,\dots,\mathbf{c}_M]$, and hence $\operatorname{rank}(\mathbf{J}_\mu) = \operatorname{rank}(\langle\Gamma,\Gamma_M\rangle\mathcal{D})$. Now rank of $\langle\Gamma,\Gamma_M\rangle$ is M as $\{\gamma_j\}$ are linearly independent. Hence the proof will follow if we can show that rank of $\mathcal{D}$ is M. Following Assumption 4, we know that the set $\{\frac{\partial\gamma_j}{\partial\mathbf{z}}\mathbf{F}-\lambda\gamma_j\}_1^\infty = \{\mathbf{c}_j^\top\Gamma\}_1^\infty$ is linearly independent and hence the Gram matrix for M of these vectors

$$\begin{pmatrix} \left\langle \mathbf{c}_1^\top\Gamma, \mathbf{c}_1^\top\Gamma\right\rangle & \dots & \left\langle \mathbf{c}_1^\top\Gamma, \mathbf{c}_M^\top\Gamma\right\rangle \\ \vdots & & \vdots \\ \left\langle \mathbf{c}_M^\top\Gamma, \mathbf{c}_1^\top\Gamma\right\rangle & \dots & \left\langle \mathbf{c}_M^\top\Gamma, \mathbf{c}_M^\top\Gamma\right\rangle \end{pmatrix} = \mathcal{D}^\top\langle\Gamma,\Gamma\rangle_m\mathcal{D}$$

has rank equal to M. Now since Γ is linearly independent, $\operatorname{rank}(\langle\Gamma,\Gamma\rangle_m) = M$ and hence rank of $\mathcal{D}$ is equal to M. □

Theorem 10. *Under Assumption 4, the optimal Galerkin projection for the nonlinear term of the eigenfunction, i.e., $h(\mathbf{z})$ corresponding to eigenvalue λ is given by $\Gamma_M^\top(\mathbf{z})\mathbf{u}^\star$, where $\mathbf{u}^\star$ is obtained as the unique solution of following linear equations.*

$$\mathbf{J}_\mu\mathbf{u} = -\mathbf{b}_\mu, \tag{88}$$

where, $\mathbf{b}_\mu := \left\langle \mathbf{w}^\top\mathbf{F}_n, \Gamma_M\right\rangle_v$ and $\mathbf{J}_\mu$ is as defined in (86).

Proof: We seek to find a finite-dimensional approximation of $h(\mathbf{z})$ using the finite basis function $\Gamma_M(\mathbf{z})$ as

$$h(\mathbf{z}) \approx \sum_k^M u_k\bar{\gamma}_k(\mathbf{z}) = \Gamma_M(\mathbf{z})^\top\mathbf{u}.$$

Substituting the above expression in (84), we can write the approximation error as

$$\text{error} = (\frac{\partial\Gamma_M}{\partial\mathbf{z}}\mathbf{F}-\lambda\Gamma_M(\mathbf{z}))^\top\mathbf{u} + \mathbf{w}^\top\mathbf{F}_n(\mathbf{z}). \tag{89}$$

The objective is to determine the vector $\mathbf{u}$ such that the projection of the error on the finite basis $\{\gamma_k\}_{k=1}^M$ is equal to zero for all $\mathbf{z}$. Hence, we obtain

$$\left\langle \left(\frac{\partial\Gamma_M}{\partial\mathbf{z}}\mathbf{F}-\lambda\Gamma_M(\mathbf{z})\right), \Gamma_M\right\rangle_m \mathbf{u} = -\left\langle \mathbf{w}^\top\mathbf{F}_n(\mathbf{z}), \Gamma_M\right\rangle_v.$$

[2] subscripts $m(v)$ are used to signify that matrix (vector) respectively.

where the inner product is in $\mathcal{L}_2(\mu)$. The uniqueness of solution follows from Lemma 1, where the matrix $\mathbf{J}_\mu = \left\langle (\frac{\partial\Gamma_M}{\partial\mathbf{z}}\mathbf{F}-\lambda\Gamma_M(\mathbf{z})), \Gamma_M\right\rangle_m$ is proved to have rank M and hence invertible. The optimal solution $\mathbf{u}^\star$ is given by

$$\mathbf{u}^\star = -{\mathbf{J}_\mu}^{-1}\mathbf{b}_\mu \quad \square \tag{90}$$

In general, computing the integral and inner product in $\mathcal{L}_2(\mu)$ would be computationally expensive. Instead, the inner product can be replaced by a dot product using empirical measure. Let $\{\mathbf{z}_1,\dots,\mathbf{z}_L\}$ be the finite data points drawn independent identically distributed (i.i.d) random w.r.t. μ from $\mathcal{Z}$. Let $\hat{\mu}_L$ be the associated empirical measure i.e., $\hat{\mu}_L = \frac{1}{L}\sum_k^L \delta_{\mathbf{z}_k}$, with $\delta_{\mathbf{z}_k}$ the Dirac-delta measure. We then have $\int_{\mathcal{Z}} f(\mathbf{z})d\hat{\mu}_L = \frac{1}{L}\sum_k^L f(\mathbf{z}_k)$. With the use of this empirical measure, we can write the Eq. (88) to determine the approximate coefficient vector $\mathbf{u}_L$ as the solution of finite linear equations.

$$\underbrace{\frac{1}{L}\sum_{k=1}^{L}\Gamma_M(\mathbf{z}_k)\left(\frac{\partial\Gamma_M}{\partial\mathbf{z}}(\mathbf{z}_k)\mathbf{F}(\mathbf{z}_k)-\lambda\Gamma_M(\mathbf{z}_k)\right)^\top}_{\mathbf{J}_{\hat{\mu}_L}}\mathbf{u}_L$$
$$= -\underbrace{\frac{1}{L}\sum_{k=1}^{L}\mathbf{w}^\top\mathbf{F}_n(\mathbf{z}_k)\Gamma_M(\mathbf{z}_k)}_{\mathbf{b}_{\hat{\mu}_L}}. \tag{91}$$

Following Assumption 4, the matrix $\mathbf{J}_{\hat{\mu}_L}$ will be invertible with probability one for $L \geq M$ as the samples $\{\mathbf{z}_k\}_1^L$ are drawn i.i.d. The solution for $\mathbf{u}_L$ is given by

$$\mathbf{u}_L^\star = -\left(\mathbf{J}_{\hat{\mu}_L}\right)^{-1}\mathbf{b}_{\hat{\mu}_L}. \tag{92}$$

We have following results.

Lemma 2. *Let Assumption 4 hold true and $\phi_\lambda^{ML}(\mathbf{z}) = \mathbf{w}^\top\mathbf{z} + \Gamma_M^\top(\mathbf{z})\mathbf{u}_L^\star$ and $\phi_\lambda^M(\mathbf{z}) = \mathbf{w}^\top\mathbf{z} + \Gamma_M^\top(\mathbf{z})\mathbf{u}^\star$, where $\mathbf{u}^\star$ and $\mathbf{u}_L^\star$ are the solutions of (90) and (92) respectively. Then,*

$$\lim_{L\to\infty}\|\phi_\lambda^{ML} - \phi_\lambda^M\| = 0, \tag{93}$$

where $\|\cdot\|$ is any norm on $\mathcal{F}_M$.

Proof: Since the linear part, $\mathbf{w}^\top\mathbf{z}$ of the eigenfunction is common in both ϕ_λ^M and ϕ_λ^{ML}, we only need to show (93) for the nonlinear terms. We have by strong law of large number

$$\lim_{L\to\infty}\Gamma_M^\top(\mathbf{z})\mathbf{J}_{\hat{\mu}_L}^{-1}\mathbf{b}_{\hat{\mu}_L} = \Gamma_M^\top(\mathbf{z})\mathbf{J}_\mu^{-1}\mathbf{b}_\mu. \tag{94}$$

with probability one since the matrix inverse operation is continuous and the samples are drawn i.i.d. □

Remark 11. *Since the samples, $\{\mathbf{z}_k\}$, are drawn i.i.d. random in the approximation of ϕ_λ^M, the law of large number can be applied to study the convergence rate of $\phi_\lambda^{ML} \to \phi_\lambda^M$ as a function of data size L. Using the central limit theorem, this rate of convergence will be proportion to $\frac{1}{\sqrt{L}}$ [46]. Using the results of this section, we can claim that the expression for the Lagrangian submanifold (76) is the optimal Galerkin projection of the Lagrangian submanifold on the basis function spanned by $\Gamma_M(\mathbf{z})$ as defined in (67).*

IV. Simulation Results

This section presents numerical examples based on procedures one and two for approximating the Lagrangian submanifolds. All the simulation codes are developed in MATLAB and run on a computer with 16 GB of RAM and a 3.8 GHz Intel Core i7 processor. The total simulation time for each example was less than a minute.

A. Example 1

For our first example, procedures one and two can be carried out analytically as the eigenfunctions of the uncontrolled system, and the Hamiltonian system can be computed analytically. The control dynamics of the two-dimensional example are given as follows.

$$\begin{pmatrix}\dot{x}_1\\ \dot{x}_2\end{pmatrix} = \alpha\begin{pmatrix}-\cos x_2(x_1-2x_2)+4(x_1+\sin x_2)\\ x_1-2x_2+2(x_1+\sin x_2)\end{pmatrix}+\begin{pmatrix}1\\0\end{pmatrix}u, \tag{95}$$

where $\alpha = \frac{1}{\cos x_2+2}$. We consider the quadratic state cost $q(\mathbf{x}) = \frac{1}{2}((x_1-2x_2)^2+(x_1+\sin x_2)^2)$, and the control cost to be $\frac{1}{2}u^2$. For procedure one, we work with the eigenfunctions of the uncontrolled system which along with the eigenvalues are given by

$$\Phi(\mathbf{x}) = \begin{bmatrix}\phi_1\\ \phi_2\end{bmatrix} = \begin{bmatrix}x_1-2x_2\\ x_1+\sin x_2\end{bmatrix}, \quad \Lambda = \begin{bmatrix}-1 & 0\\ 0 & 2\end{bmatrix}. \tag{96}$$

In Fig. 1, we show the plots of the eigenfunctions of the uncontrolled system. Approximation 1 made in procedure one for this example is not an approximation as

$$\mathbf{R}(\mathbf{x}) = \mathbf{B}\mathbf{B}^\top = \begin{pmatrix}1 & 0\\ 0 & 0\end{pmatrix}, \frac{\partial\Phi}{\partial\mathbf{x}} = \begin{pmatrix}1 & -2\\ 1 & \cos x_2\end{pmatrix}, q(\mathbf{x}) = \frac{1}{2}\Phi^\top\Phi,$$

and hence

$$\frac{\partial\Phi}{\partial\mathbf{x}}\mathbf{B}\mathbf{B}^\top\frac{\partial\Phi}{\partial\mathbf{x}}^\top = \begin{pmatrix}1 & 1\\ 1 & 1\end{pmatrix} = \mathbf{R}_1, \quad \mathbf{Q}_1 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}$$

are indeed constant matrices. Based on the steps outlined for procedure one, the Lagrangian submanifold and the optimal cost function are given by

$$\mathbf{p}^\star = \frac{\partial V}{\partial\mathbf{x}}, \quad V(\mathbf{x}) = \frac{1}{2}\Phi^\top\mathbf{L}\Phi. \tag{97}$$

where, $\mathbf{L}$ is obtained as the solution of Riccatti equation (57) and the optimal control input equal to

$$\mathbf{L} = \begin{pmatrix}0.49 & -0.62\\ -0.62 & 5.35\end{pmatrix}, \mathbf{u}^\star = -4.61x_1 - 0.263x_2 - 4.74\sin x_2. \tag{98}$$

For procedure two, the eigenvalues of the Hamiltonian are given by $(2.14, 1.19, -2.14, -1.19)$, and the eigenfunctions corresponding to the unstable eigenvalues are given by

$$\begin{pmatrix}-0.20\phi_1(\mathbf{x}) - 0.67\phi_2(\mathbf{x}) + 0.67P_1 + 0.20P_2\\ -0.39\phi_1(\mathbf{x}) - 0.11\phi_2(\mathbf{x}) + 0.90P_1 + 0.08P_2\end{pmatrix},$$

where $(P_1, P_2)^\top = \mathbf{P} = (\frac{\partial\Phi}{\partial\mathbf{x}}^\top)^{-1}\mathbf{p}$. We notice that the eigenfunctions of the Hamiltonian system are obtained as linear combinations of the eigenfunctions of the uncontrolled system. This will always be the case when the Approximation 1 is no longer an approximation but is exact, as is the case with this example. The optimal cost and control for procedures 1 and 2 are the same for this example and are given in Eqs. (97) and (98) respectively. In Fig. 2, we show the plot for the optimal cost and control input obtained using procedures 1, 2, and LQR control. The optimal cost and control input using LQR control is given by

$$u_{lqr} = -5.06x_1 - 5.74x_2, \; V_{lqr} = \frac{1}{2}\mathbf{x}^\top\begin{pmatrix}2.53 & 2.87\\ 2.87 & 7.59\end{pmatrix}\mathbf{x}. \tag{99}$$

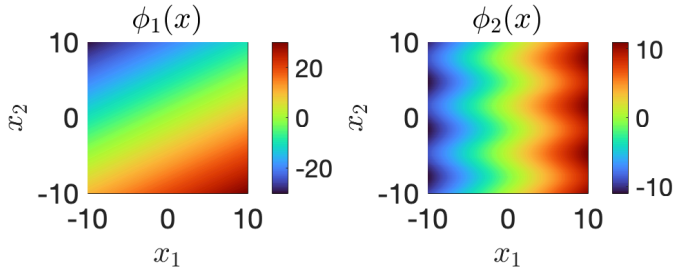

Fig. 1: Eigenfunctions $\phi_1(\mathbf{x}), \phi_2(\mathbf{x})$ of the uncontrolled system

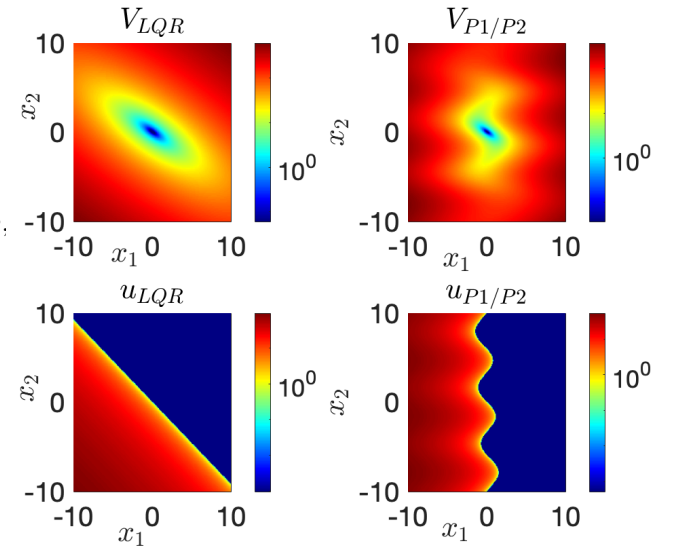

Fig. 2: Value function of LQR control and Proc. 1 and Proc.2 (top). Feedback contorol law for LQR, Proc. 1, and Proc.2 (bottom).

We compare the analytical results presented above with those obtained using our proposed framework. In particular, we use the approach outlined in Section III-C to approximate the Koopman eigenfunctions and the HJ solution. We also compare the results obtained using our proposed framework with one obtained using the Taylor series approximation [13], [14]. We use the polynomial basis function to approximate the Koopman eigenfunctions for a fair comparison with the Taylor series-based solution. For the Taylor series approximation of the HJ solution, we Taylor expand the vector field (95) around the origin as

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \mathbf{B}u = \mathbf{A}\mathbf{x} + \mathbf{F}_2(\mathbf{x}) + \mathbf{F}_3(\mathbf{x}) + \cdots + \mathbf{B}u.$$

where $\mathbf{F}_j(\mathbf{x})$ is the part of the vector field containing nonlinear terms of order j. Similarly, the value function, $V(\mathbf{x})$, the control input, $k(\mathbf{x})$, and the cost function, $q(\mathbf{x})$, are expanded in Taylor series as follows:

$$V(\mathbf{x}) = \sum_{j=2}^{\infty} V_j(\mathbf{x}),\ u = \mathbf{K}\mathbf{x} + \sum_{j=2}^{\infty} k_j(\mathbf{x}),\ q(\mathbf{x}) = \sum_{j=2}^{\infty} q_j(\mathbf{x})$$

where $V_2(\mathbf{x}) = \mathbf{x}^\top \mathbf{P}\mathbf{x}$ and $\mathbf{K} = -\mathbf{B}^\top \mathbf{P}$ with $\mathbf{P}$ being the solution of Riccatti equation. $V_j(\mathbf{x})$ and $k_j(\mathbf{x})$ are the cost function and control input containing nonlinear terms of order j. In [13, Eq. 2.21] [14, Eq. 2.9], it has been shown that the $V_{j>2}(\mathbf{x})$ satisfy a recursive equation, where V_j is function of $V_k(\mathbf{x})$ with $k < j$, $\mathbf{F}_\ell(\mathbf{x})$ for $\ell \leq j$ and $q_j(\mathbf{x})$. For more details on this derivation, refer to [13], [14]. In Fig. 3, we show the normalized error plot between the analytical Koopman eigenfunction, $\phi_2(\mathbf{x})$, of the uncontrolled system and the one, approximated from data with finite basis, $\phi_2^{ML}(\mathbf{x})$, i.e., $\frac{\|\phi_2^{ML} - \phi_2\|}{\|\phi_2\|}$ as the function of data length, L. The results are presented using the boxplots where the red line denotes the mean and the 75^{th} and 25^{th} quartiles are represented by the upper and lower edges of the blue box, and the red stars represent the outliers.

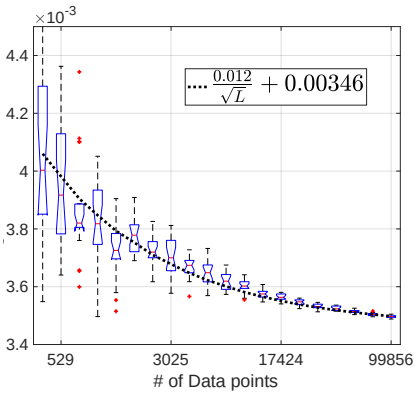

Fig. 3: Eigenfunction error vs data length

We choose the polynomial basis function of degree five and hence $M = 18$. The plot shows the error decays at the rate of $\frac{1}{\sqrt{L}}$ (Remark 11) and validates the results of Lemma 2. Now, let $V^\star(\mathbf{x})$, $V_T(\mathbf{x})$, and V_K be the analytical, Taylor series-based, and Koopman spectrum-based approximated HJ solutions, respectively. In Fig. 4 we show the plot for the point-wise error between $|V^\star(\mathbf{x}) - V_T(\mathbf{x})|$ and $|V^\star(\mathbf{x}) - V_K(\mathbf{x})|$. The error with the Taylor series-based approximated solution is an order of magnitude higher than the proposed Koopman spectrum-based HJ solution. This demonstrates the effectiveness of the developed framework over the solution obtained using the Taylor series.

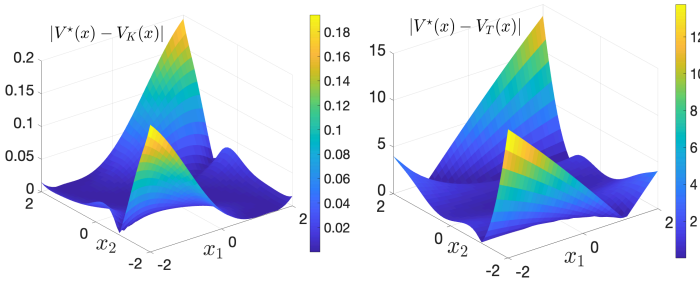

Fig. 4: Comparison of optimal cost function error: $|V^\star(\mathbf{x}) - V_K(\mathbf{x})|$ (left) and $|V^\star(\mathbf{x}) - V_T(\mathbf{x})|$ (right).

B. Example 2

Our second example is controlled 2-D nonlinear oscillator.

$$\begin{aligned} \dot{x}_1 &= x_2 \\ \dot{x}_2 &= -x_1 - x_2(1 - (1 + 2\sin x_1)^2) + (1 + 2\sin x_1)u. \end{aligned} \tag{100}$$

For this example, the optimal control can be determined analytically when $q(\mathbf{x}) = x_2^2$ and the control cost is u^2. The optimal control input is given by $u^\star = -(1 + 2\sin x_1)x_2$ and optimal cost is $V(\mathbf{x}) = \mathbf{x}^\top \mathbf{x}$. We used the methodology developed in Section III-C to approximate the eigenfunctions. We used $1e^4$ initial condition uniformly distributed over the domain $[-3, 3] \times [-3, 3]$ to approximate eigenfunctions. The polynomial basis function of maximum degree three is used to approximate the Koopman eigenfunctions of the uncontrolled system. For procedure two, the eigenfunctions of the Hamiltonian system are approximated using basis functions $\Xi_1(\mathbf{x})$ (with reference to Eq. 67) as polynomial basis with maximum degree 3 excluding linear terms, and $\Xi_2(\mathbf{x}) = (\text{diag}(x_1), \text{diag}(x_2), \ldots, \text{diag}(x_1^i x_2^j), \ldots, \text{diag}(x_2^3))^\top$, where $\text{diag}(x_1^i x_2^j) \in \mathbb{R}^{2\times 2}$ with $i + j \leq 3$. The domain for the eigenfunction computation is $[-3, 3]^4$ with $1e^5$ points used in the approximation of eigenfunction. For this example, the optimal control is approximated using (80) and the optimal cost using (78) with $\Xi_3(\mathbf{x})$ again chosen to be the polynomial basis of maximum degree three. In Fig 6, we show the plots comparing different control inputs, the true optimal, procedure one and two, and LQR. We notice that the optimal control input obtained using procedures 1 and 2 closely matches true optimal control; in contrast, the LQR optimal control is different than the true optimal. In Fig. 7, we compare the closed-loop trajectories with the initial condition at $(-1.8, 1.8)$. We notice that the controller obtained using the LQR control fails to stabilize the system. In Fig. 5, we compare the control input and cumulative cost obtained using procedures one and two and true optimal control. We notice that procedure two performs slightly better than procedure one, matching the control input and cumulative cost of the true optimal control. In procedure two, we directly work with the eigenfunctions of the Hamiltonian system. Using procedure one, we have made the Approximation 1, which is the source of error compared to procedure two and explains the better performance of procedure two. On the other hand, in procedure one, we have to compute the eigenfunctions of a lower, n-dimensional uncontrolled system instead of $2n$-dimensional Hamiltonian system in procedure two. While procedure two performs better than procedure one for this example, the choice between the two will depend on multiple factors such as the validity of Approximation 1 and computational efforts required for the eigenfunction computation.

V. Conclusions

This paper combines tools from linear Koopman operator theory and differential geometry to provide a novel approach for the approximate computation of the HJ solution. We present two different procedures based on the spectrum of the Koopman operator for the computation of the Lagrangian submanifold, which are instrumental in solving the HJ equation. Furthermore, given the significance of the HJ equation in

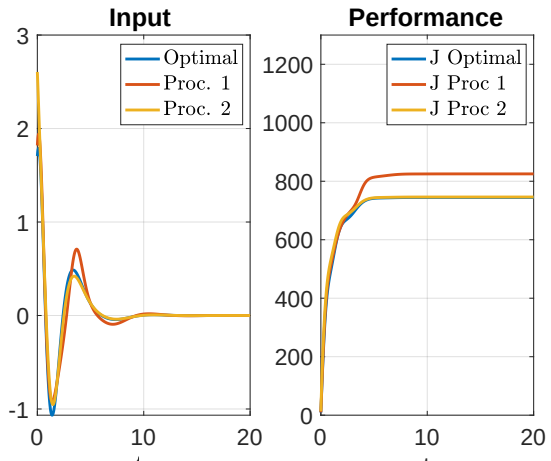

Fig. 5: Comparison of control input and cumulative cost using Proc.1, Proc.2, and true optimal control. Proc. 2 cumulative cost is right on top of true cumulative cost.

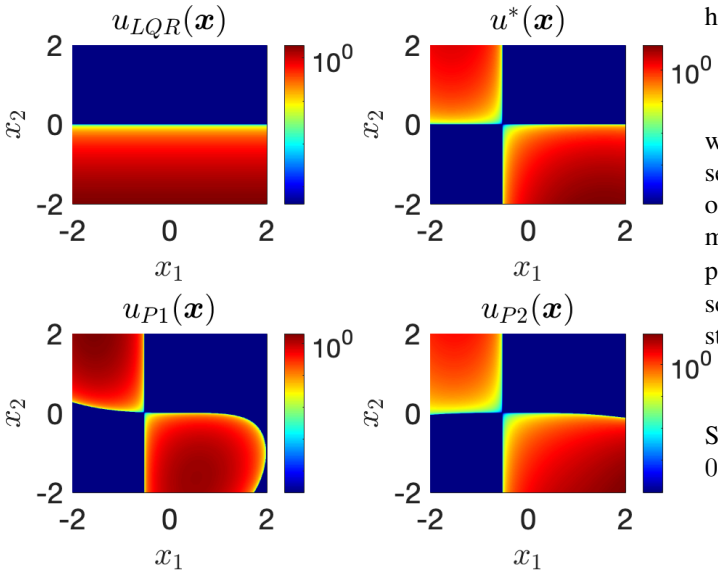

Fig. 6: Comparison of optimal feedback controllers.

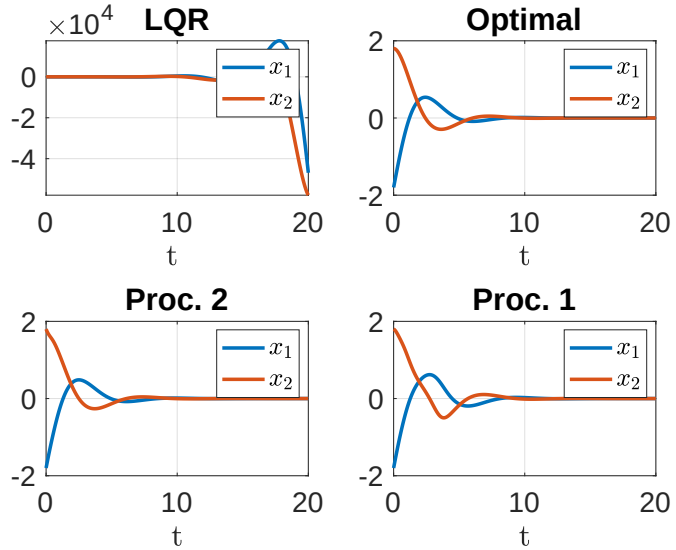

Fig. 7: Comparison of state trajectories with LQR control input, Proc. 1 and Proc. 2.

various problems in system theory, the proposed methodology involving the Koopman operator can be extended in several different directions, including analysis and synthesis of a control system and robust control. The proposed approach is also the most promising direction for extending existing results in linear control theory to the nonlinear control system by exploiting the spectral properties of the Koopman operator. Future research efforts will focus on implementing the two procedures in the data-driven setting.

APPENDIX

Proof: (*Proof of Proposition 5*). Following Assumption 2, we know that the Hamiltonian matrix, $\mathcal{H}$, has no eigenvalues on the $j\omega$ axis. Let $\mathbf{d}_1^\top, \ldots, \mathbf{d}_n^\top$ be the left eigenvectors associated with eigenvalues with positive real part. Following Corollary 1, the stable subspace of the linear system is characterized by the joint zero-level sets of Koopman eigenfunctions corresponding to eigenvalues with a positive real part, and hence the stable subspace is characterized as

$$\mathbb{E}_s = \{(\bar{\mathbf{X}}, \bar{\mathbf{P}}) : \mathbf{D}\begin{pmatrix}\bar{\mathbf{X}}\\ \bar{\mathbf{P}}\end{pmatrix} = \mathbf{D}_1\bar{\mathbf{X}} + \mathbf{D}_2\bar{\mathbf{P}} = 0\},$$

where the matrix $\mathbf{D}, \mathbf{D}_1, \mathbf{D}_2$ are as defined in (56). We seek the parameterization of the stable subspace in terms of $\bar{\mathbf{X}}$, and hence we write $\bar{\mathbf{P}} = \mathbf{L}\bar{\mathbf{X}}$ for some symmetric matrix $\mathbf{L}$. Symmetric $\mathbf{L}$ follows from the fact that we seek parameterization of the form $\bar{\mathbf{P}} = \frac{\partial V(\bar{\mathbf{X}})}{\partial \bar{\mathbf{X}}}$, i.e., a gradient of a scalar value function $V = \frac{1}{2}\bar{\mathbf{X}}^\top\mathbf{L}\bar{\mathbf{X}}$. Substituting for $\bar{\mathbf{P}}$ in the stable subspace equation, we obtain

$$\mathbf{D}_1\bar{\mathbf{X}} + \mathbf{D}_2\mathbf{L}\bar{\mathbf{X}} = (\mathbf{D}_1 + \mathbf{D}_2\mathbf{L})\bar{\mathbf{X}} = 0. \tag{101}$$

Since the above has to be true for all $\bar{\mathbf{X}}$, we need $\mathbf{D}_1 + \mathbf{D}_2\mathbf{L} = 0$. Following Assumption 2, (14) is equivalent to

$$\mathbb{E}_s^\perp \oplus \begin{pmatrix}I\\ 0\end{pmatrix} = \mathbb{R}^{2n}. \tag{102}$$

Now since matrix $\mathbf{D}$ span the space orthogonal to $\mathbb{E}_s$ i.e., $\mathbb{E}_s^\perp$, (102) is equivalent to the invertability of $\mathbf{D}_2$ matrix Hence, we obtain $\mathbf{L} = \mathbf{D}_2^{-1}\mathbf{D}_1$. This gives us the required expression for the Lagrangian subspace in $\bar{\mathbf{X}}, \bar{\mathbf{P}}$ coordinates. □

Proof: (*Proof of Proposition 6*) Since, the matrix $\mathbf{D}$ from Proposition 5 consists of left eigenvectors with eigenvalues with positive real part, say $\bar{\Lambda}$, of the Hamiltonian $\mathcal{H}$, it forms an invariant subspace and satisfies

$$\begin{pmatrix}\mathbf{D}_1 & \mathbf{D}_2\end{pmatrix}\begin{pmatrix}\Lambda & -\hat{\mathbf{R}}\\ -\hat{\mathbf{Q}} & -\Lambda^\top\end{pmatrix} = \bar{\Lambda}\begin{pmatrix}\mathbf{D}_1 & \mathbf{D}_2\end{pmatrix}. \tag{103}$$

Premultiplying by $\mathbf{D}_2$ inverse, we obtain

$$\begin{pmatrix}-\mathbf{L} & I\end{pmatrix}\begin{pmatrix}\Lambda & -\hat{\mathbf{R}}\\ -\hat{\mathbf{Q}} & -\Lambda^\top\end{pmatrix} = \mathbf{D}_2{-}1\bar{\Lambda}\mathbf{D}_2\begin{pmatrix}-\mathbf{L} & I\end{pmatrix}. \tag{104}$$

Postmultiply by $\begin{pmatrix}I\\ \mathbf{L}\end{pmatrix}$, we obtain

$$\mathbf{L}\Lambda + \Lambda^\top\mathbf{L} - \mathbf{L}\hat{\mathbf{R}}\mathbf{L} + \hat{\mathbf{Q}} = 0. \tag{105}$$

and

$$\Lambda - \hat{\mathbf{R}}\mathbf{L} = -\mathbf{D}_2^\top\bar{\Lambda}^\top\mathbf{D}_2^{-1\top} \implies \sigma(\Lambda - \hat{\mathbf{R}}\mathbf{L}) = \sigma(-\bar{\Lambda}). \quad \square$$

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