

Smooth controllability of infinite-dimensional quantum-mechanical systems

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Manipulation of infinite-dimensional quantum systems is important to controlling complex quantum dynamics with many practical physical and chemical backgrounds. In this paper, a general investigation is casted to the controllability problem of quantum systems evolving on infinite-dimensional manifolds. Recognizing that such problems are related with infinite-dimensional controllability algebras, we introduce an algebraic mathematical framework to describe quantum control systems possessing such controllability algebras. Then we present the concept of smooth controllability on infinite-dimensional manifolds, and draw the main result on approximate strong smooth controllability. This is a nontrivial extension of the existing controllability results based on the analysis over finite-dimensional vector spaces to analysis over infinite-dimensional manifolds. It also opens up many interesting problems for future studies.

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I. INTRODUCTION

The laboratory successes in coherent control of quantum dynamics in the late 1990s have dawned the dream of controlling quantum phenomena. Nowadays, advances in laser technologies and system control theory [1–4] have demonstrated the abilities of effectively manipulating microscopic systems both theoretically and experimentally. Owing to the unique quantum coherence, quantum control has manifested incredible novelties in contrast to the corresponding classical control schemes [5]. With new perspectives obtained from these achievements, more ambitious goals are being pursued to control complex quantum dynamics subject to issues such as large molecules [6], entanglements in quantum networks [7,8], and decoherence in open quantum systems [9,10]. Moreover, the developments of quantum measurements, which are in general weak and continuous in time, make it possible to implement feedback techniques to enhance the ability and robustness of control of nonunitary noisy evolutions of quantum states [8,11].

In this paper, we are concerned with quantum control of infinite-dimensional systems, especially those that contain continuous spectra, which are fundamental in many practical backgrounds. For example, as a long-standing problem in controlling ultrafast molecular dynamics, the attempts to break chemical bonds naturally fall under transitions of molecular states between discrete and continuous spectra [12–14]. More recently, motivation has been generated by the development of a continuous quantum computer [15,16] that processes quantum information encoded in continuous spectra. Serious theoretical studies have proved that they might be more sufficient in some tasks in comparison to their discrete counterparts.

A large class of infinite-dimensional quantum systems with discrete spectra can be well approximated to possess a finite number of levels under weak control field interactions that induce transitions between these levels. Mathematical treatments to such systems can then be largely simplified by linear approximations [17,18], perturbation theory or adiabatic approximations [14]. However, in intense-field circumstances numerous levels have to be taken into account because they become strongly coupled by multiphoton processes. For systems with continuous spectra, some of the above approximations will not be applicable even in weak-field cases due to the nonlocal nature of corresponding scattering states. To exert the use of physical resources in control, we need to put the study back into the infinite-dimensional prototype model of quantum-mechanical systems so that arbitrary spectral types can be universally handled. To the authors' knowledge, not much theoretical consideration has been received from this perspective. The first studies date back to the work of Huang, Tarn and Clark [1,19] in which analytic controllability is systematically studied based on group representation theory. Their work was later extended to time-dependent systems by Lan, Tarn, Chi, and Clark [20]. These results embrace both cases of discrete and continuous spectra [2,20], however, are still restricted to systems with finite-dimensional controllability algebras. Some other specific discussions can be found in Refs. [21–23].

In this paper, the study of infinite-dimensional quantum systems will be embedded in an algebraic framework that can deal with infinite-dimensional controllability Lie algebras. This framework also allows the use of strong fields and unbounded Hamiltonians to enforce control over the quantum states. On such a basis, we present new concepts of smooth controllability and extend the existing results to more general systems on infinite-dimensional manifolds. The organization of the paper is as follows. In Sec. II, we summarize the existing results and present the algebraic framework accompanied with preliminary examples. In Sec. III, we give the notions of smooth controllabilities based on the smooth

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domain. In Sec. IV, the main result is given and proved on approximate strong smooth controllability. In Sec. V, we discuss two typical examples. Finally, in Sec. VI, we draw conclusions and give our perspectives.

II. PROBLEM FORMULATION

Generally, quantum control systems can be written in the form of the following Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t} \psi(t) = (H'_0 + H'_I) \psi(t), \quad \psi(0) = \psi_0, \quad (1)$$

where the quantum state $\psi(t)$ evolves in a separable Hilbert space \mathcal{H} . The free (unperturbed or internal) Hamiltonian H'_0 of the quantum system is a Hermitian operator on \mathcal{H} . The H'_I refers to the interaction (control) Hamiltonian that is used to affect the quantum dynamics. In most situations, the interaction Hamiltonian can be decomposed into a sum $H'_I = \sum_{j=1}^m u_j(t) H'_j$, where the u_j 's are the controls that represent some classical fields interacting with the system through the Hamiltonians in the summation. To simplify the notations, we rewrite Eq. (1) with skew-Hermitian operators $H_i = (i\hbar)^{-1} H'_i$, which leads to the following quantum control system:

$$\frac{\partial}{\partial t} \psi(t) = \left[H_0 + \sum_{j=1}^m u_j(t) H_j \right] \psi(t), \quad \psi(0) = \psi_0. \quad (2)$$

Throughout this paper, we always assume that the controls are piecewise constant functions of time. A quantum state ψ' is said to be reachable from ψ if there exists a time instant T and some admissible (i.e., piecewise constant in this paper) controls over $[0, T]$ that steers the system from ψ to ψ' . Denote $\mathcal{R}(\psi)$ as the reachable set of all states that are reachable from ψ , and $\mathcal{R}_t(\psi)$ as the reachable set of all states that are reachable from ψ at a specified time $t > 0$.

The controllability issue concerns itself with the problem of whether or not the reachable set of the initial state can fill up a prescribed set of quantum states. In particular, let the manifold \mathbf{M} be the closure of the set of states [21]

$$\{e^{s_k H_{\alpha_k}} \cdots e^{s_1 H_{\alpha_1}} \psi_0; s_k \in \mathbb{R}; \alpha_k = 0, 1, \dots, m; k \in \mathbb{N}\}, \quad (3)$$

where $\psi_0 \in \mathcal{H}$ is the initial state, the reachable set of ψ_0 is obviously contained in \mathbf{M} because all possible control actions on the system are involved. In the rest parts of this paper, we will concentrate the studies on controllability properties on this manifold.

Controllability problem is of great interests mainly in two aspects. First, since the internal Hamiltonian H_0 may give rise to unwanted complex dynamics (e.g., chaos), the controllability characterizes the ability of the control system to fight against such complexities. Secondly, the yes or no answer of controllability provides important information in many practical problems, e.g., possibility of 100% ratio of preferred products in chemical reactions, or universality of quantum computation realized by some physical structures.

A. Existing results

Denote $\mathfrak{A} = \{H_0, H_1, \dots, H_m\}_{\text{LA}}$ the controllability algebra, where the subscript ‘‘LA’’ denotes the Lie algebra generated by operators in the curly bracket. For quantum control systems with a finite number of levels, the basic result is summarized as follows [24].

Theorem II.1. Suppose \mathcal{H} is a N -dimensional Hilbert space of quantum states and $S_{\mathcal{H}}$ is the unit sphere in \mathcal{H} . The system is controllable over $S_{\mathcal{H}}$, if the controllability algebra $\mathfrak{A} = \text{su}(N)$ or $\mathfrak{A} = \text{u}(N)$. For homogeneous quantum control systems, i.e., $H_0 = 0$, the condition is also a necessary condition.

Systems with an infinite number of levels are much more complicated because the Hamiltonians may bring severe domain constraints. Providing that some of them are unbounded operators [25], the system evolution will have to be restricted in a proper subset of quantum states in \mathcal{H} , on which the Hamiltonians are well defined, invariant, and the state evolution can be expressed globally in exponential form. For system with a finite-dimensional controllability Lie algebra $\mathfrak{A} = \{H_0, H_1, \dots, H_m\}_{\text{LA}}$, Huang, Tarn, and Clark [1] have suggested the analytic domain

$$\mathcal{D}_\omega = \left\{ \omega \in \mathcal{H}; \sum_{n=0}^{\infty} \sum_{1 \leq i_1, \dots, i_n \leq m} \frac{\|H_{i_1} \cdots H_{i_n} \omega\| s^n}{n!} < \infty \right\}$$

as a candidate. The existence of a dense analytic domain in \mathcal{H} (with respect to the Hilbert space topology) and corresponding group representation are guaranteed by the Nelson's theorem [26]). Based on the analytic domain, the notion of analytic controllability is as follows.

Definition II.1 (Analytic Controllability). Quantum-mechanical control system (2) is said to be analytically controllable on \mathbf{M} if the reachable set $\mathcal{R}(\psi) = \mathbf{M} \cap \mathcal{D}_\omega$ for all $\psi \in \mathbf{M} \cap \mathcal{D}_\omega$. If the reachable set $\mathcal{R}_t(\psi)$ equals to $\mathbf{M} \cap \mathcal{D}_\omega$ for all $\psi \in \mathbf{M} \cap \mathcal{D}_\omega$ at any time $t > 0$, the system is said to be strongly analytically controllable.

Huang, Tarn, and Clark (HTC) presented a criterion of strong analytic controllability [1].

Theorem II.2. Suppose the controllability algebra \mathfrak{A} is finite dimensional and the analytic domain exists. Let the Lie algebra $\mathfrak{B} = \{H_1, \dots, H_r\}_{\text{LA}}$ and $\mathfrak{C} = \{\text{ad}_{H_0}^k \mathfrak{B}; k = 0, 1, \dots\}_{\text{LA}}$, where $\text{ad}_{H_0}^0 \mathfrak{B} = \mathfrak{B}$ and $\text{ad}_{H_0}^{k+1} \mathfrak{B} = [H_0, \text{ad}_{H_0}^k \mathfrak{B}]$. The system (2) is strongly analytically controllable if the following conditions are satisfied. (1) $[\mathfrak{B}, \mathfrak{C}] \subseteq \mathfrak{B}$ and (2) for any $\phi \in \mathbf{M} \cap \mathcal{D}_\omega$, $\dim \mathfrak{C}(\phi) = \dim \mathbf{M}$.

Interested readers are further referred to Ref. [20] for extended results on time-dependent quantum control systems. A common restriction of these results is that at most a finite-dimensional manifold \mathbf{M} in finite- or infinite-dimensional Hilbert spaces can be taken into consideration, because the corresponding controllability Lie algebra \mathfrak{A} is finite dimensional. This limitation is manifested more clearly in the following HTC no-go theorem [1]:

Theorem II.3. The system (2) is not strongly analytically controllable on $S_{\mathcal{H}}$, if the controllability Lie algebra \mathfrak{A} is finite dimensional.

The negative assertion of no-go theorem implies strongly the necessity to explore quantum systems with infinite-dimensional controllability algebras in order to drive systems over infinite-dimensional manifolds. This is the primary motivation of the study in this paper.

B. Algebraic model and preliminary examples

Quantum Hamiltonians in traditional models are usually expressed as combinations of kinetic and potential energies according to the Hamiltonian formulation of mechanics. Specialized scalar or vector potentials are applied to affect the quantum dynamics. For example, the dipole interaction of an electrical field with atoms or molecules are widely used for quantum control [3]. Such expressions are physically explicit, however, not convenient for calculation in structural analysis of quantum control systems with complicated Hamiltonians. In this regard, we adopt an algebraic framework that has been systematically applied to study atomic structure and molecular spectroscopy [27,28]. The method is rooted on an intrinsic symmetry Lie algebra that describes the quantum system under consideration, whose quantum observables are functions of the generators of the symmetry algebra. Each of these physical observables can serve as a control Hamiltonian interacting with external fields by some realizable physical means, although, not necessarily under present laboratory conditions. Rather broad classes of symmetries can be unified in this framework, such as geometrical, dynamical, or even *a priori* prescribed symmetries [25], hence the formulation benefits in gaining deeper insights into the physical mechanism of quantum control.

In this paper, we are concerned with quantum control systems associated with finite-dimensional symmetry algebras, say $\mathcal{L}=\{L_1, \dots, L_d\}_{\text{LA}}$. Assume that the system Hamiltonians H_0, H_1, \dots, H_m can be expressed as skew-symmetric polynomials of the generators of \mathcal{L} , i.e., elements in the so-called universal enveloping algebra $E(\mathcal{L})$ (roughly speaking, the minimal associative algebra of polynomial operators in terms of the generators in \mathcal{L} that contains \mathcal{L} , see Refs. [25,29] for a rigorous definition). Apparently, $E(\mathcal{L})$ is also an infinite-dimensional Lie algebra equipped with the standard definition of Lie bracket $[X, Y]=XY-YX$, where $X, Y \in E(\mathcal{L})$. Apparently, the controllability algebra $\mathfrak{A}=\{H_0, H_1, \dots, H_m\}_{\text{LA}}$ is a Lie subalgebra of $E(\mathcal{L})$.

From the well-known Poincaré-Birkhoff-Witt theorem ([29], p.138), all the ordered polynomials

$$\{L_1^{\alpha_1} \cdots L_d^{\alpha_d}; \alpha_1 \cdots \alpha_d \in \mathbb{N}\}$$

consist of a basis of $E(\mathcal{L})$. Denote $E^{(n)}(\mathcal{L})$ the subspace of elements in $E(\mathcal{L})$ whose orders are no greater than n , we obtain a graded algebra structure

$$E^{(1)}(\mathcal{L}) \subset E^{(2)}(\mathcal{L}) \subset \cdots \subset E^{(n)}(\mathcal{L}) \subset \cdots$$

that decomposes the infinite-dimensional vector space $E(\mathcal{L})$ into finite-dimensional subspaces. In this structure, the computation with differential operators can be replaced by algebraic operations that are easier to carry out on the graded finite-dimensional subspaces. This facilitates the noncommu-

tative analysis [30] over an infinite-dimensional algebra.

To understand the concepts of symmetry algebra, infinite-dimensional controllability Lie algebra, and infinite-dimensional manifold, we present several illustrative examples of quantum systems with Pöschl-Teller potentials. As one of the known solvable potentials in the literature [2,27,28], Pöschl-Teller potential has been widely used to describe stretching or bending vibrations states in molecules. In the following, various algebraic models of Pöschl-Teller potentials will be presented via separation of variables under special coordinate systems.

Example 1. The first approach applies the so-called potential algebra $\text{su}(1,1)=\{L'_x, L'_y, L'_z\}_{\text{LA}}$ as the symmetry algebra, where L'_z is a compact operator and L'_x, L'_y are noncompact operators. Their commutation relations read

$$[L'_x, L'_y] = iL'_z, [L'_y, L'_z] = -iL'_x, [L'_z, L'_x] = -iL'_y.$$

The $\text{su}(1,1)$ can be realized in Cartesian coordinates

$$L'_x = -i \left(y \frac{\partial}{\partial z} + z \frac{\partial}{\partial y} \right),$$

$$L'_y = -i \left(x \frac{\partial}{\partial z} + z \frac{\partial}{\partial x} \right),$$

$$L'_z = -i \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right),$$

where L'_x and L'_y are the pseudoangular momentum operators along x and y axes, and L'_z is the angular momentum operator along the z axis. We change them to the hyperbolic coordinates

$$x = \cosh \rho \cos \phi, y = \cosh \rho \sin \phi, z = \sinh \rho,$$

with a succeeding similarity transformation $U = \cosh^{1/2} \rho$ on the wave function. Then, we simultaneously diagonalize the Casimir operator $C = L'^2_x + L'^2_y - L'^2_z$ and L'_z with simultaneous eigenvectors $\{|j, m\rangle = u^m_j(\rho) e^{im\phi}\}$:

$$C|j, m\rangle = j(j+1)|j, m\rangle, \quad L'_z|j, m\rangle = m|j, m\rangle,$$

where the j and m take values in the unitary representations of $\text{su}(1,1)$:

$$D^+_j: j = \frac{1}{2}, 1, \frac{3}{2}, \dots; \quad m = j, j+1, \dots;$$

$$D^-_j: j = \frac{1}{2}, 1, \frac{3}{2}, \dots; \quad m = -j, -j-1, \dots;$$

$$C^0_j: j > 0; \quad m = 0, \pm 1, \dots;$$

$$C^{1/2}_j: j > \frac{1}{4}; \quad m = \pm \frac{1}{2}, \pm \frac{3}{2}, \dots.$$

Finally, we arrive at the time-independent Schrödinger equation subject to Pöschl-Teller potentials

$$\left(-\frac{d^2}{d\rho^2} - \frac{m^2 - \frac{1}{4}}{\cosh^2 \rho} \right) u^m_j(\rho) = \left(j + \frac{1}{2} \right)^2 u^m_j(\rho).$$

The free Hamiltonian reads $H_0 = a(C+1/4)$, $a > 0$ is some constant. It possesses discrete (corresponding to D^+_j and D^-_j

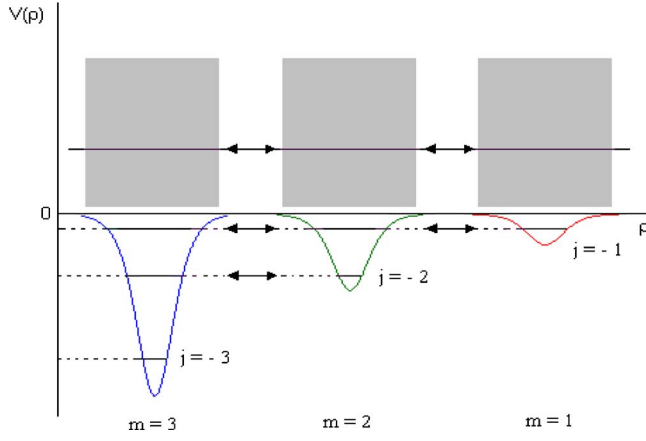


FIG. 1. (Color online) State transitions in example 1 with Pöschl-Teller potentials.

representations) or continuous (corresponding to C_j^0 and $C_j^{1/2}$ representations) spectra. The potential strength $m^2 - 1/4$ is labeled by the eigenvalues of L'_z . Choosing control Hamiltonians from the universal enveloping algebra of the potential algebra, we can realize the quantum control over this system, for instance, by the other two operators in the potential algebra [2]:

$$i\hbar \frac{\partial}{\partial t} \psi(t) = \left[\left(C + \frac{1}{4} \right) + u_1 L'_x + u_2 L'_y \right] \psi(t). \quad (4)$$

Because both the control Hamiltonians commute with the free Hamiltonian, they are not able to move the energy level labelled by the eigenvalue $(j+1/2)^2$ of H_0 . However, as shown in Fig. 1 [27], they can alter the potential strength because the corresponding operator L'_z does not commute with the control Hamiltonians. Hence these quantum controls weaken or strengthen potentials while conserving the system energy. It is not difficult to verify that the controllability Lie algebra $\mathfrak{A} = \{C + \frac{1}{4}, L'_x, L'_y, L'_z\}_{\text{LA}}$ is a four-dimensional Lie subalgebra of $E(\text{su}(1, 1))$. From the HTC theorem, this system is strongly analytically controllable.

Example 2. The second approach describes the scattering states in Pöschl-Teller potentials. The corresponding symmetry algebra is called scattering algebra $\text{su}(1, 1) = \{L'_x, L'_y, L'_z\}_{\text{LA}}$ with operators L'_y compact and L'_x, L'_z noncompact. The commutation relations read

$$[L'_x, L'_y] = -iL'_z, \quad [L'_y, L'_z] = -iL'_x, \quad [L'_z, L'_x] = iL'_y.$$

Here the $\text{su}(1, 1)$ algebra takes a different realization

$$L'_x = -i \left(y \frac{\partial}{\partial z} + z \frac{\partial}{\partial y} \right),$$

$$L'_y = -i \left(x \frac{\partial}{\partial z} - z \frac{\partial}{\partial x} \right),$$

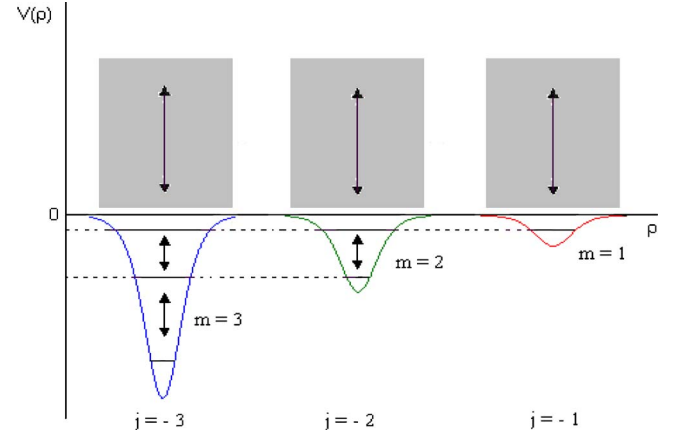


FIG. 2. (Color online) State transitions in examples 2 and 3 under Pöschl-Teller potentials.

$$L'_z = -i \left(x \frac{\partial}{\partial y} + y \frac{\partial}{\partial x} \right),$$

where L'_x and L'_z are the pseudoangular momentum operators along x and z axes, and L'_y is the angular momentum operator along y axis. Followed by hyperbolic coordinate transformation

$$x = \cos \varrho \cosh \phi, \quad y = \cos \varrho \sinh \phi, \quad z = \sin \varrho$$

and a succeeding similarity transformation $\rho = \tanh^{-1} \cos \varrho$ on the wave function, the simultaneous diagonalization of the operators $C = L'^2_x - L'^2_y + L'^2_z$ and L'_z with simultaneous eigenvectors $\{|j, m\rangle = u^m_j(\rho) e^{im\phi}\}$:

$$C|j, m\rangle = j(j+1)|j, m\rangle, \quad j = 0, \frac{1}{2}, 1, \frac{3}{2}, 2, \dots,$$

$$L'_z|j, m\rangle = m|j, m\rangle, \quad m \in \mathbb{R},$$

gives the time-independent Schrödinger equation subject to Pöschl-Teller potential

$$\left(-\frac{d^2}{d\rho^2} - \frac{j(j+1)}{\cosh^2 \rho} \right) u^m_j(\rho) = m^2 u^m_j(\rho).$$

The free Hamiltonian reads $H_0 = aL'^2_z$, where $a > 0$ is a constant. The system possesses a positive continuous spectrum $\{E = am^2, m \in \mathbb{R}\}$ because L'_z is noncompact. The potential strength $j(j+1)$ is related to the Casimir operator C . Consider quantum control system using two operators in the scattering algebra [2]:

$$i\hbar \frac{\partial}{\partial t} \psi(t) = [aL'^2_z + u_1 L'_x + u_2 L'_y] \psi(t), \quad (5)$$

the potential strength is a conservative quantity because the corresponding Casimir operator commutes with all system Hamiltonians. As shown in the upper part of Fig. 2 [27], the controls affect only the change of energies in continuous spectra. The controllability algebra $\mathfrak{A} = \{aL'^2_z, L'_x, L'_y\}_{\text{LA}}$ is an infinite-dimensional Lie algebra and contains arbitrarily high-order elements in $E(\text{su}(1, 1))$. Therefore, the former results cannot be used here.

Example 3. The third example describes bound states in

Pöschl-Teller potentials with a compact dynamical Lie algebra $\text{su}(2)=\{L'_x, L'_y, L'_z\}_{\text{LA}}$. In a similar way, we first realize this algebra in Cartesian coordinate system

$$L'_x = -i \left(y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right),$$

$$L'_y = -i \left(x \frac{\partial}{\partial z} - z \frac{\partial}{\partial x} \right),$$

$$L'_z = -i \left(x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right),$$

where L'_j is the angular momentum operator along the j axis, $j=x, y, z$. Changing them into spherical coordinates

$$x = \cos \varrho \cos \phi, \quad y = \cos \varrho \sin \phi, \quad z = \sin \varrho$$

followed by a similarity transformation $\rho = \cos^{-1} \text{sech } \varrho$ on the wave function, and the simultaneous diagonalization of the operators $C = L'^2_x + L'^2_y + L'^2_z$ and L'_z with simultaneous eigenvectors $\{|j, m\rangle = u_j^m(\rho) e^{im\phi}\}$

$$C|j, m\rangle = j(j+1)|j, m\rangle, \quad j = \frac{1}{2}, 1, \frac{3}{2}, 2, \dots,$$

$$L'_z|j, m\rangle = m|j, m\rangle, \quad m = -j, \dots, j,$$

we can get the time-independent Schrödinger equation subject to Pöschl-Teller potentials

$$\left(-\frac{d^2}{d\rho^2} - \frac{j(j+1)}{\cosh^2 \rho} \right) u_j^m(\rho) = -m^2 u_j^m(\rho).$$

The free Hamiltonian reads $H_0 = -aL'^2_z$, where $a > 0$ is a constant. The potential strength is labeled by the eigenvalues of the Casimir operator, while the quantum number m labels the $(2j+1)$ bound states in the j th potential. Consider the following control system [31]:

$$i\hbar \frac{\partial}{\partial t} \psi(t) = [aL'^2_z + u_1 L'_x + u_2 L'_y] \psi(t), \quad (6)$$

with control Hamiltonians selected from the $\text{su}(2)$ algebra. As shown in the lower part of Fig 2, the control Hamiltonians serve to shift discrete energy levels in Pöschl-Teller potentials. They cannot affect the potential strength, nor can they drive the system out of discrete spectra to the continuum. More interestingly, this example shows that controllability algebra can still be infinite dimensional even if the symmetry algebra is compact.

The above three examples reveal rich symmetry properties in the same Pöschl-Teller potentials by which system can be represented by simple algebraic variables. The concepts of infinite-dimensional Lie algebra and infinite-dimensional manifold should not be confused with the infinite-dimensional systems (distributed-parameter systems [32]) widely used in the literature. All the three examples are infinite dimensional systems since they are described by partial differential equations and their solutions are functions. However, in the first example, the controllability algebra is finite dimensional and the corresponding manifold is a finite-

dimensional submanifold of infinite-dimensional manifolds. This is different from the finite-dimensional manifolds contained in a finite-dimensional vector space, since the generators of the algebras consists of unbounded operators and the solution of the Schrödinger equations are functions rather than vectors in finite-dimensional vector spaces.

III. SMOOTH CONTROLLABILITY

No doubt that the domain problem is also nontrivial for systems with infinite-dimensional controllability Lie algebras. Normally, it is not difficult to find an analytic domain for the symmetry algebra \mathcal{L} , however, this domain is not invariant under the actions of high-order operators in its universal enveloping algebra $E(\mathcal{L})$. In fact, it has been demonstrated that analytic domain is nonexistent for most infinite dimensional Lie algebras [33]. Therefore, one needs to seek another proper domain for the universal enveloping algebra.

What we are going to choose is the larger set of differentiable vectors of \mathcal{L} :

$$\mathcal{D}_\infty = \{ \phi \in \mathcal{H} : \|L_1^{s_1} \cdots L_d^{s_d} \phi\| < \infty; \forall s_i = 0, 1, 2, \dots \}, \quad (7)$$

which is well defined and invariant for all operators in $E(\mathcal{L})$, hence can be taken as a candidate. Parallel with the analytic domain, we call \mathcal{D}_∞ the smooth domain. Topologically, the smooth domain occupies a special inverse limit Hilbert (ILH) vector space structure that is inherited from, but completely different with, the Hilbert space structure of \mathcal{H} (see Appendix A). This ILH structure also makes it possible to generate an infinite-dimensional ILH transformation group on \mathcal{H} from the universal enveloping algebra $E(\mathcal{L})$ [34], which establishes a solid mathematical basis for the following discussions on infinite-dimensional quantum control systems.

Moreover, the smooth domain has crucial physical meanings on describing scattering states, which can be intuitively depicted as limits of bound states whose wave packets spread widely in the configuration space. By definition, \mathcal{D}_∞ represents the set of bound states on which all the system observables (elements in the universal enveloping algebra) and their commutations act legally, hence is comprised of all experimentally preparable states produced by the quantum control system (2). Denote the dual space of \mathcal{D}_∞ by \mathcal{D}_∞^* , i.e., the space of continuous antilinear functionals on \mathcal{D}_∞ . The scattering states can be represented as ideal vectors in the larger set \mathcal{D}_∞^* that do not have finite norm in \mathcal{H} [35,36]. Mathematically, the triad of linear spaces

$$\mathcal{D}_\infty \subset \mathcal{H} \subset \mathcal{D}_\infty^*$$

forms a so-called rigged Hilbert space [35,36] with \mathcal{D}_∞ dense in \mathcal{H} and \mathcal{H} dense in \mathcal{D}_∞^* (with respect to the weak topology of \mathcal{D}_∞^*). So \mathcal{D}_∞ is also dense in \mathcal{D}_∞^* . This shows that scattering states can be identified as the ideal limits of some sequences of bound states in \mathcal{D}_∞ (note that the limit is called “ideal” because it is outside the Hilbert space and is not converged to with respect to the usual Hilbert space topology).

Consider the manifold \mathbf{M} defined by Eq. (3), which, corresponding to infinite-dimensional controllability algebras, is

in general infinite dimensional. Parallel with the analytic controllability, we present rigorous controllability concepts of quantum control systems over this manifold.

Definition III.1 (smooth controllability). Quantum-mechanical control system (2) is said to be smoothly controllable if the reachable set $\mathcal{R}(\psi) = \mathbf{M} \cap \mathcal{D}_\infty$ for all $\psi \in \mathbf{M} \cap \mathcal{D}_\infty$.

Definition III.2 (strong smooth controllability). The system is said to be strongly smoothly controllable if the reachable set $\mathcal{R}_t(\psi) = \mathbf{M} \cap \mathcal{D}_\infty$ for all $\psi \in \mathbf{M} \cap \mathcal{D}_\infty$ at any time $t > 0$.

In the context of this paper, where only piecewise constant controls are considered, the system can never be completely smoothly controllable on an infinite-dimensional manifold \mathbf{M} unless an infinite number of switches are applied [1]. Hence we have to turn to the following weakened definition.

Definition III.3 (approximate smooth controllability). Quantum-mechanical control system (2) is said to be approximately smoothly controllable on \mathbf{M} if the reachable set $\mathcal{R}(\psi)$ is dense (with respect to the ILH topology) in $\mathbf{M} \cap \mathcal{D}_\infty$ for all $\psi \in \mathbf{M} \cap \mathcal{D}_\infty$.

Definition III.4 (approximate strong smooth controllability). The system is said to be approximately strongly smoothly controllable if the reachable set $\mathcal{R}_t(\psi)$ is dense in $\mathbf{M} \cap \mathcal{D}_\infty$ (with respect to the ILH topology) for all $\psi \in \mathbf{M} \cap \mathcal{D}_\infty$ at any time $t > 0$.

The consideration of differential vectors has been suggested by Huang, Tarn, and Clark in Ref. [1] as a possible extension of the analytic controllability. In this paper, we put it into a rigorous setting. The smooth domain not only enlarges the system domain, but also gives a nice topology by which one can carry out strict controllability analysis. More important a by-product is that the smooth domain provides an explicit picture of the control of scattering-state quantum systems, which are non physical in a strict sense. Nevertheless, taking scattering states as ideal limits of bound states in the smooth domain, we can directly translate the knowledge of controllability properties on the smooth domain \mathcal{D}_∞ to scattering states in the dual space \mathcal{D}_∞^* in the sense of an ideal limit.

IV. MAIN RESULTS

The foregoing mathematical preliminaries provide a technical basis for us to explore quantum systems with infinite-dimensional controllability algebras. In this section, we will study the approximate strong smooth controllability of quantum control systems over the manifold \mathbf{M} defined by Eq. (3). The main difficulty will be that only a finite number of controls are available to guide the quantum states all over the infinite-dimensional manifold \mathbf{M} , while fighting against the possibly complex free evolution.

In the following, the discussion will be focused on the quantum control system of the unitary propagators:

$$\frac{d}{dt}U(t) = \left[H_0 + \sum_{j=1}^m u_j(t)H_j \right] U(t), \quad U(0) = I, \quad (8)$$

where the system propagator satisfies $\psi(t) = U(t)\psi_0$ and belongs to the infinite-dimensional Lie group \mathcal{G} generated by

the controllability algebra \mathfrak{A} . Controllability properties of system (2) can be derived from this system, because the manifold \mathbf{M} can be equivalently expressed as the orbit, $\mathbf{M} = \{U\psi_0, U \in \mathcal{G}\}$, of \mathcal{G} passing the initial state ψ_0 . Providing that a dense subset of propagators in \mathcal{G} can be generated from Eq. (8), the system will be consequently smoothly controllable on \mathbf{M} . Our basic idea is to construct unitary transformations in \mathcal{G} by repeatedly switching control interactions so that the free evolution can be cancelled and recreated, hence forms a dense subset of \mathcal{G} as the number of switches increase. Concretely, we are looking for a class of strongly “adjustable” flows (i.e., one-dimensional subgroups in \mathcal{G}) generated by the so-called strongly attainable Hamiltonians.

Definition IV.1. Denote the infinitesimal-time reachable set $\mathcal{R}_0(\psi) = \bigcap_{t>0} \mathcal{R}_{\leq t}(\psi)$, where $\mathcal{R}_{\leq t}(\psi)$ denotes the reachable set within t units of time. A time-independent Hamiltonian X is said to be strongly attainable if its integral curve $\{\exp(Xt)\psi, t \in \mathbb{R}\}$ passing any $\psi \in \mathbf{M} \cap \mathcal{D}_\infty$ is contained in the closure of $\mathcal{R}_0(\psi)$. A set of Hamiltonians is said to be strongly attainable if each element in this set is strongly attainable.

The strongly attainable Hamiltonians represent Hamiltonians of which the generated unitary propagators can be achieved in an arbitrary small time interval. We are going to seek plenty of strongly attainable Hamiltonians for the system (8) so that flows passing ψ_0 can be generated to steer the system with full freedom in a dense subset of the infinite-dimensional manifold \mathbf{M} , which leads to the approximate strong smooth controllability of Eq. (2). Before presenting the main result, we will prove several preliminary lemmas and theorems. Readers interested in the main result may proceed directly to theorem IV.3 and examples in Sec. V.

To apply these ideas, we will repeatedly use the Campbell-Baker-Hausdorff formula that is already well established on infinite-dimensional Lie groups [29,37]:

$$X_s Y_t = \exp \left(sX + tY + \frac{st}{2}[X, Y] + \frac{s^2 t}{12}[X, [X, Y]] + \frac{st^2}{12}[Y, [Y, X]] + \dots \right)$$

and the Trotter’s formula [38,39]

$$(X + Y)_s \phi = \lim_{n \rightarrow \infty} (X_{s/n} Y_{s/n})^n \phi, \quad (9)$$

$$[X, Y]_s \phi = \lim_{n \rightarrow \infty} (X_{\sqrt{s/n}} Y_{\sqrt{s/n}}^{-1} X_{\sqrt{s/n}}^{-1} Y_{\sqrt{s/n}})^n \phi, \quad (10)$$

where X_s and Y_t are the flows generated by X and Y , respectively. First, one can identify the following properties of strongly attainable Hamiltonians.

Lemma IV.1. Let X and X_1, \dots, X_α be strongly attainable Hamiltonians, then (1) $(X_{i_n})_{s_n} \cdots (X_{i_1})_{s_1} \psi \in \mathcal{R}_0(\psi)$, for all $n \in \mathbb{N}$, $i_1, \dots, i_n \in \{1, \dots, \alpha\}$, $s_1, \dots, s_n \in \mathbb{R}$ and $\psi \in \mathcal{D}_\infty$ and (2) $(H_0)_t X_s \psi \in \mathcal{R}_t(\phi)$, $X_s (H_0)_t \psi \in \mathcal{R}_t(\phi)$, for all $\psi \in \mathcal{R}_t(\phi)$, $t > 0$, and $s \in \mathbb{R}$.

Proof. Let $U(t, \mathbf{u}(\cdot))$ be the system propagator under control $\mathbf{u}(\cdot) = (u_1(\cdot), \dots, u_m(\cdot))$. According to the definition of strongly attainable Hamiltonians, for arbitrary positive number ϵ and arbitrary positive time t , there exist a sequence of

unitary propagators $U_{1,t/n}, \dots, U_{n,t/n}$ such that $U(t/n, \mathbf{u}^k(\cdot)) = U_{k,t/n}$ for some $\mathbf{u}^k(\cdot)$, and satisfies

$$\|[(X_{i_k})_{s_k} - U_{k,t/n}](X_{i_{k-1}})_{s_{k-1}} \cdots (X_{i_1})_{s_1} \psi\| < \frac{\epsilon}{n}.$$

Because $U_{k,t/n}$'s are unitary operators,

$$\begin{aligned} & \| (X_{i_n})_{s_n} (X_{i_{n-1}})_{s_{n-1}} \cdots (X_{i_1})_{s_1} \psi - U_{n,t/n} U_{n-1,t/n} \cdots U_{1,t/n} \psi \| \\ & < \| [(X_{i_n})_{s_n} - U_{n,t/n}](X_{i_{n-1}})_{s_{n-1}} \cdots (X_{i_1})_{s_1} \psi \| + \cdots \\ & + \| U_{n,t/n} U_{n-1,t/n} \cdots [(X_{i_1})_{s_1} - U_{1,t/n}] \psi \| \\ & = \| [(X_{i_n})_{s_n} - U_{n,t/n}](X_{i_{n-1}})_{s_{n-1}} \cdots (X_{i_1})_{s_1} \psi \| \\ & + \cdots + \| (X_{i_1})_{s_1} \psi - U_{1,t/n} \psi \| < \epsilon. \end{aligned}$$

From the choices of $U_{1,t/n}, \dots, U_{n,t/n}$, it is obvious that $U_{n,t/n} U_{n-1,t/n} \cdots U_{1,t/n} \psi \in \overline{\mathcal{R}_t(\psi)}$ for any $t > 0$. So $(X_{i_k})_{s_k} (X_{i_{k-1}})_{s_{k-1}} \cdots (X_{i_1})_{s_1} \psi \in \overline{\mathcal{R}_t(\psi)}$. As to the second assertion, we similarly choose U_τ such that $\| (H_0)_t X_s \psi - (H_0)_t U_\tau \psi \| < \epsilon$. Then

$$\begin{aligned} & \| (H_0)_t X_s \psi - (H_0)_{t-\tau} U_\tau \psi \| < \| (H_0)_t X_s \psi - (H_0)_t U_\tau \psi \| \\ & + \| (H_0)_t U_\tau \psi - (H_0)_{t-\tau} U_\tau \psi \|. \end{aligned}$$

Because of the continuity of the one-parameter group $\{(H_0)_t\}_{t \in \mathbb{R}}$, the second term goes to zero as $\tau \rightarrow 0$. Therefore $(H_0)_t X_s \psi \in \overline{\mathcal{R}_t(\psi)}$. Similar is the proof for $X_s (H_0)_t \psi \in \overline{\mathcal{R}_t(\psi)}$.

Lemma IV.2. X is strongly attainable if and only if $(H_0 + cX)_t \psi \in \overline{\mathcal{R}_t(\psi)}$ for all $c \in \mathbb{R}$.

Proof. To prove the sufficiency, we estimate the deviation between the system evolution with that in absence of H_0 by integrating the differential equation

$$\frac{d}{ds} (\epsilon H_0 + X)_{t-s} X_s \psi = -(\epsilon H_0 + X)_{t-s} (\epsilon H_0) X_s \psi$$

over the time interval $[0, t]$:

$$\begin{aligned} & \| (\epsilon H_0 + X)_t \psi - X_t \psi \| \leq \int_0^t \| (\epsilon H_0 + X)_{t-s} \| \| (\epsilon H_0) X_s \psi \| ds \\ & \leq \epsilon M t, \end{aligned} \quad (11)$$

where $\| (\epsilon H_0 + X)_{t-s} \| = 1$ by unitarity, $0 < M = \sup_{[0,t]} \| H_0 X_s \psi \| < \infty$. Hence for fixed t and ψ , $\lim_{\epsilon \rightarrow 0} \| (\epsilon H_0 + X)_t \psi - X_t \psi \| = 0$. This is to say, the integral curve $X_t \psi$ can be arbitrarily close to $(\epsilon H_0 + X)_t \psi = (H_0 + \epsilon^{-1} X)_{et} \psi \in \overline{\mathcal{R}_{et}(\psi)}$ for ϵ small enough. Therefore $X_t \psi \in \overline{\mathcal{R}_0(\psi)}$, i.e., X is strongly attainable.

Conversely, if X is strongly attainable, the necessity can be shown from the Trotter's formula

$$(H_0 + cX)_s \psi = \lim_{n \rightarrow \infty} [(H_0)_{s/n} (cX)_{s/n}]^n \psi,$$

in which the term at the right hand side belongs to the closure of $\mathcal{R}_t(\psi)$ by repeatedly using lemma IV.1 (2). The end of proof.

Lemma IV.3. Denote \mathfrak{A}_S the collection of strongly attainable Hamiltonians. \mathfrak{A}_S is a Lie algebra containing $\mathfrak{B} = \{H_1, \dots, H_r\}_{\text{LA}}$.

Proof. Suppose $X, Y \in \mathfrak{A}_S$ is strongly attainable. The

strong attainability of cX for arbitrary nonzero $c \in \mathbb{R}$ is obvious. Using Trotter's formula and applying lemma IV.1 (1), we observe that the right-hand sides of Eqs. (9) and (10) belongs to the closure of the infinitesimal-time reachable set, so both $X+Y$ and $[X, Y]$ are strongly attainable. This proves the Lie algebra property of \mathfrak{A}_S . On the other hand, the control Hamiltonians H_1, \dots, H_m are strongly attainable according to lemma IV.2. Therefore the Lie algebra \mathfrak{B} that is generated by H_1, \dots, H_m is a strongly attainable Lie subalgebra of \mathfrak{A}_S .

Theorem IV.1. The Lie algebra \mathfrak{C} is strongly attainable if the algebraic condition $[\mathfrak{B}, \mathfrak{C}] \subseteq \mathfrak{B}$ is satisfied.

Proof. It is sufficient to prove that $\text{ad}_{H_0}^k H \in \mathfrak{A}_S$ for arbitrary integer k and strongly attainable Hamiltonian $H \in \mathfrak{B}$. We invoke the Campbell-Baker-Hausdorff formula [29]

$$\begin{aligned} H_{-t}(H_0)_s H_t \psi = & \left(H_0 + t \text{ad}_{H_0} H \right. \\ & \left. + \frac{t^2}{2} \int_0^1 (\theta - 1)^2 H_{-\theta t} \text{ad}_{H_0}^2 H_0 H_{\theta t} d\theta \right)_s \psi, \end{aligned}$$

where $t \in \mathbb{R}$. The last term

$$R_1 = \frac{t^2}{2} \int_0^1 (\theta - 1)^2 H_{-\theta t} \text{ad}_{H_0}^2 H_0 H_{\theta t} d\theta$$

is the Lagrange remainder. Under the condition $[\mathfrak{B}, \mathfrak{C}] \subseteq \mathfrak{B}$, the term $\text{ad}_{H_0}^2 H_0$ is strongly attainable, hence its translation $H_{-\theta t} \text{ad}_{H_0}^2 H_0 H_{\theta t}$ by a strongly attainable Hamiltonian H is also strongly attainable (by lemma IV.1). Taking the integral as a limit of summations, we can see that the Lagrange remainder is also strongly attainable. Applying Trotter's formula, we have

$$(H_0 + t \text{ad}_{H_0} H)_s \psi = \lim_{n \rightarrow \infty} [H_{-t/n} (H_0)_{s/n} H_{t/n} (-R_1)_{s/n}]^n \psi,$$

of which the right-hand side is contained in the closure of reachable set $\overline{\mathcal{R}_s(\psi)}$ by lemma IV.1. Hence $(H_0 + t \text{ad}_{H_0} H)_s \psi \in \overline{\mathcal{R}_s(\psi)}$, which implies that $\text{ad}_{H_0} H$ is strongly attainable from lemma IV.2. Thus we proved the strong attainability of $\text{ad}_{H_0} \mathfrak{B}$.

Inductively, assume the subspace of Hamiltonians $\mathfrak{C}_k = \{\text{ad}_{H_0}^j \mathfrak{B}, j=0, \dots, k\} \subset \mathfrak{C}$ is strongly attainable for some positive integer k . Employ again the Campbell-Baker-Hausdorff formula

$$\begin{aligned} & (\text{ad}_{H_0}^k H)_{-t} (H_0)_s (\text{ad}_{H_0}^k H)_t \psi \\ & = \left(H_0 - t \text{ad}_{\text{ad}_{H_0}^k H} H_0 + \frac{t^2}{2} \int_0^1 (\theta - 1)^2 (\text{ad}_{H_0}^k H)_{-\theta t} \right. \\ & \quad \left. \times \text{ad}_{\text{ad}_{H_0}^k H}^2 H_0 (\text{ad}_{H_0}^k H)_{\theta t} d\theta \right)_s \psi \\ & = \left(H_0 + t \text{ad}_{H_0}^{k+1} H + \frac{t^2}{2} \int_0^1 (\theta - 1)^2 (\text{ad}_{H_0}^k H)_{-\theta t} \right. \end{aligned}$$

$$\times [\text{ad}_{H_0}^{k+1} H, \text{ad}_{H_0}^k H] (\text{ad}_{H_0}^k H)_{\theta} d\theta \Big|_s \psi. \quad (12)$$

Making use of the formula [40]

$$[\text{ad}_{H_0}^{k+1} H, \text{ad}_{H_0}^k H] = \sum_{j=0}^k (-1)^j \binom{k}{j} \text{ad}_{H_0}^{k-j} [\text{ad}_{H_0}^{k+j+1} H, H] \subseteq \mathfrak{C}_k$$

together with the condition $[\mathfrak{B}, \mathfrak{C}] \subseteq \mathfrak{B}$, we can see the strong attainability of the Lagrange remainder R_k in Eq. (12) from the assumption that \mathfrak{C}_k is strongly attainable. Using Trotter's formula, we have

$$(H_0 + t \text{ad}_{H_0}^{k+1} H)_s \psi = \lim_{n \rightarrow \infty} [(\text{ad}_{H_0}^k H)_{-t} (H_0)_{s/n} (\text{ad}_{H_0}^k H)_t \times (-R_k)_{s/n}]^n \psi,$$

where the right-hand side is contained in the closure of reachable set $\mathcal{R}_s(\psi)$ by lemma IV.1. Similarly, we can prove in the same line as carried above that each element in the subspace $\text{ad}_{H_0}^{k+1} \mathfrak{B}$ is strongly attainable. Therefore, we inductively prove the strong attainability of \mathfrak{C}_{k+1} . In conclusion, \mathfrak{C} is strongly attainable.

Next, we cite a useful theorem to connect the strongly attainable Hamiltonians with the reachable sets $\mathcal{R}_t(\psi)$.

Theorem IV.2 [40–42]. Let $I(\psi, \mathfrak{C}) = (\exp \mathfrak{C})\psi$ be the maximal connected integral manifold of \mathfrak{C} containing the point ψ . Then $\mathcal{R}_t(\psi) \subseteq I(\psi, \mathfrak{C})$, where $I(\psi, \mathfrak{C}) = (H_0)_t I(\psi, \mathfrak{C}) = I((H_0)_t \psi, \mathfrak{C})$.

Proof. Because the admissible control are piecewise constant, we can always decompose the system flow into pulses driven by constant controls. Consider the single pulse, we have by Trotter's formula and Campbell-Baker-Hausdorff formula

$$(H_0 + H)_t \psi = \lim_{n \rightarrow \infty} [(H_0)_{t/n} H_{t/n}]^n \psi \\ = \lim_{n \rightarrow \infty} (H_0)_t \{ (H_0)_{-[(n-1)t/n]} H_{t/n} (H_0)_{-[(n-1)t/n]} \} \\ \times \cdots \{ (H_0)_{-t/n} H_{t/n} (H_0)_{t/n} \} (H_0)_{-t/n} \psi, \quad (13)$$

where $H = \sum_{i=1}^m u_i H_i$ are the control Hamiltonian. Because

$$(H_0)_{-s} H_i (H_0)_s \psi = \exp \left\{ tH - st[H_0, H] + \frac{s^2 t}{2} [H_0, [H_0, H]] - \cdots \right\} \psi \in \exp \mathfrak{C} \psi,$$

so each part in the curly brackets in Eq. (14) generates a unitary propagator in $\exp \mathfrak{C}$. Hence $\mathcal{R}_t(\psi) \subseteq I(\psi, \mathfrak{C})$. Inductively, suppose the conclusion establishes for k pulses, then for $(k+1)$ pulses with $t_1 + \cdots + t_{k+1} = t$, let $t' = t_1 + \cdots + t_k$,

$$(H_0 + H^{(k+1)})_{t_{k+1}} (H_0 + H^{(k)})_{t_k} \cdots (H_0 + H^{(1)})_{t_1} \psi \\ \in [\exp \mathfrak{C} (H_0)_{t_{k+1}}] (H_0)_{t'} I(\psi, \mathfrak{C}) \\ \in \exp \mathfrak{C} (H_0)_t I(\psi, \mathfrak{C})$$

$$= (H_0)_t [(H_0)_{-t'} \exp \mathfrak{C} (H_0)_{t'}] I(\psi, \mathfrak{C}) \\ = (H_0)_t I(\psi, \mathfrak{C}).$$

Thus the conclusion establishes for $(k+1)$ pulses. The end of proof.

Having the above properties of the strongly attainable Hamiltonians and reachable sets in hand, now we can draw the main result of the approximate strong smooth controllability.

Theorem IV.3. The system (2) is approximately strongly smoothly controllable if the following conditions are satisfied: (1) $[\mathfrak{B}, \mathfrak{C}] \subseteq \mathfrak{B}$ and (2) For any $\phi \in \mathbf{M} \cap \mathcal{D}_\infty$, $\mathfrak{C}(\phi) = \mathfrak{A}(\phi)$ and they are infinite dimensional.

Proof. From theorem IV.2, \mathfrak{C} is strongly attainable under the first condition. According to lemma IV.1, we have $I(\psi, \mathfrak{C}) = (H_0)_t \exp \mathfrak{C} \psi \subseteq \mathcal{R}_t(\psi)$ for some initial state $\psi \in \mathbf{M} \cap \mathcal{D}_\infty$. On the other hand, from theorem IV.2, $\mathcal{R}_t(\psi) \subseteq I(\psi, \mathfrak{C})$. Hence $\mathcal{R}_t(\psi) = I(\psi, \mathfrak{C})$.

By Frobenius theorem ([34], p. 215), the condition $\mathfrak{C}(\phi) = \mathfrak{A}(\phi)$ for any $\phi \in \mathbf{M} \cap \mathcal{D}_\infty$ guarantees that \mathfrak{A} and \mathfrak{C} have identical maximal integral manifold passing ψ , i.e., $\exp \mathfrak{A} \psi = \exp \mathfrak{C} \psi = \mathbf{M} \cap \mathcal{D}_\infty$. Since $H_0 \in \mathfrak{A}$, the unitary transformation $(H_0)_t$ leaves \mathbf{M} invariant. Thus we arrive at the final conclusion:

$$\overline{\mathcal{R}_t(\psi)} = (H_0)_t (\exp \mathfrak{C}) \psi = (H_0)_t (\mathbf{M} \cap \mathcal{D}_\infty) = \mathbf{M} \cap \mathcal{D}_\infty.$$

V. EXAMPLES

To illuminate the ideas presented in this paper, we proceed to discuss several examples in this section.

Example 1. The first paradigm comes from the model of continuous quantum computation over continuous variables proposed by Lloyd and Braunstein [15]. The scheme encodes quantum information in the continuous spectrum of the position operator of a harmonic oscillator. The control task then becomes the manipulation of superpositions of eigenstates of the position operator by the following control systems:

$$i \frac{\partial}{\partial t} \psi(x, t) = [p^2 + x^2 + u_1(xp + px) + u_2 p + u_3 x + u_4(x^2 + p^2)^2] \psi(x, t), \quad (15)$$

where the commutation of the position operator x and the momentum operator $p = -i\hbar \partial_x$ reads $[x, p] = i\hbar$. Here the Heisenberg algebra $\mathfrak{h}(1) = \{x, p, i\}_{LA}$ plays the role of the symmetry algebra of the system. The smooth domain for the Heisenberg algebra $\mathfrak{h}(1) = \{x, p, i\}$ is the Schwartz space

$$\left\{ v(x) \in L^2(\mathbb{R}) : \sup_{\alpha, \beta \geq 0} \left| x^\alpha \left(\frac{d}{dx} \right)^\beta v(x) \right| < \infty \right\}.$$

As argued in Ref. [15], arbitrary functions of variable x and p can be approximated by repeatedly switching operations of the control Hamiltonians, i.e. all the polynomials of x and p in $E(\mathfrak{h}(1))$ can be generated by commutations and linear combinations of the control operators

$$H_1 = xp + px, \quad H_2 = p, \quad H_3 = x, \quad H_4 = (x^2 + p^2)^2.$$

This is actually equivalent to say that all these polynomial Hamiltonians are strongly attainable according to the terminology used in this paper. According to theorem IV.3, the system (15) is approximately strongly smoothly controllable. In quantum computation field, this amounts to the universality of continuous quantum computation using model (15).

Physically, the linear optical interactions are used to shift phase by x and translate the coordinate by p ; the second-order operator $px+xp$ provides a squeezer operation. The nonlinear Kerr Hamiltonian $(x^2+p^2)^2$, which plays essential roles in producing many interesting physical phenomena such as entangled photons, is applied here to explode up an infinite-dimensional controllability algebra that is necessary for controllability over the whole continuous spectrum. It is also easy to verify that many other higher-order operators in $E(h(1))$ can replace the Kerr Hamiltonian for the same goal of controllability [15].

Example 2. The physical model of the second example has been described in Sec. II. The scattering states in Pöschl-Teller potentials are characterized using a noncompact symmetry algebra $\mathfrak{su}(1, 1)$. Let $|j, k\rangle$, $k=j, j+1, \dots$, be simultaneous eigenvectors of the compact generator L'_y and the Casimir operator C for some fixed integer $j > 0$. These vectors expand a Hilbert space \mathcal{H}_j . The smooth domain contained in \mathcal{H}_j consists of the “fast decreasing sequences”

$$\mathcal{D}_\infty = \left\{ x = \sum_{k=j}^{\infty} x_k |j, k\rangle \mid \lim_{|k| \rightarrow \infty} k^n x_k = 0, \forall n \in \mathbb{N} \right\} \quad (16)$$

as described in Ref. [43]. The scattering states are contained in the set of “slow increasing sequences”

$$\mathcal{D}_\infty^* = \left\{ x = \sum_{k=j}^{\infty} x_k |j, k\rangle \mid \lim_{|k| \rightarrow \infty} k^{-n} x_k = 0, \forall n \in \mathbb{N} \right\} \quad (17)$$

For the quantum control system (5), one can verify inductively that the controllability algebra $\mathfrak{A} = E(\mathfrak{su}(1, 1))$ (see proof in Appendix B), which generates a unitary representation of the volume-preserving diffeomorphism group $\text{diff}S^{1,1}$ over a hyperboloid surface $S^{1,1} = \text{SU}(1, 1)/\text{SO}(1, 1)$ [44]. Denote \mathbf{M} the orbit of $\text{diff}S^{1,1}$ passing the initial state $\psi \in \mathcal{D}_\infty \cap \mathcal{H}_j$.

However, although we have an infinite dimensional controllability algebra \mathfrak{A} , the algebra $\mathfrak{B} = \{L'_x, L'_y\}_{\text{LA}} = \mathfrak{su}(1, 1)$ is too small to fulfil the condition in theorem IV.3. Hence nothing can be told according to the results obtained in this paper. Nevertheless, if one can apply an extra second-order control Hamiltonian L'^2_x , which leads to the following control system:

$$i\hbar \frac{\partial}{\partial t} \psi(t) = [aL'^2_z + u_1 L'_x + u_2 L'_y + u_3 L'^2_x] \psi(t), \quad (18)$$

the second-order control Hamiltonian helps to explode up an infinite-dimensional Lie algebra \mathfrak{B} that coincides with $\mathfrak{A} = E(\mathfrak{su}(1, 1))$. According to theorem IV.3, strong approximate smooth controllability follows on \mathbf{M} .

Let us give some physical insights. At the first glance, the operators $K'_\pm = L'_x \pm L'_y$ resemble the ladder operators in harmonics oscillators. But intuitively, the “ladder” operators are not allowed to generate discrete shift of levels on a continuous spectrum. In fact, K'_\pm shift eigenvalues of L'_z by $\pm i$ units [45], which is of course absurd because the Hermitian L'_z has a real continuous spectrum. As interpreted in Refs. [45,46], the contradiction originates from the fact that K'_\pm act illegally upon the scattering states that are outside the Hilbert space. Their operations are only well defined on the wave packets of superposition of scattering states. Interested readers may refer to Refs. [45,46] for more details.

The second-order Hamiltonian $L'^2_x = (K'_+ + K'_-)^2/4$ is also essential in expanding an infinite-dimensional controllability algebra as well as the Kerr Hamiltonian in the first example. Any other second-order operator that does not commute with H_0 functions equivalently in controllability. As analogs of the Kerr nonlinear process, these operators generate higher-order harmonics on $\text{SU}(1, 1)$. On the other hand, whatever higher-order operators in $E(\mathfrak{su}(1, 1))$ are applied, they can never move the system state out of the continuous spectrum due to the symmetry predetermined by the scattering algebra.

VI. CONCLUSION

This paper provides a clearer understanding of system control of infinite-dimensional quantum-mechanical systems. The presented framework may be applied to quantum control systems with finite or infinite dimensions, and with bound states or scattering states. Back to the cases of finite dimensional controllability algebras, the extension of analytic controllability to the larger smooth domain, which has been conjectured in Ref. [1], can be taken as a corollary of theorem IV.3. Most important is that the results open up much broader applications to infinite-dimensional manifolds.

As has been earlier discussed by Zhao and Rice [13], control of scattering-state system can be significantly influenced by the presence of chaos. Since the strong controllability property is not altered because the evolution always concerns itself on finite time intervals, our results affirm that quantum scattering-state control system can be “strong” enough to overcome the chaos. However, controllability not in the strong sense is indeed more complicated because chaotic dynamics manifests itself on long time intervals.

In the examples in Sec. V, the manifold \mathbf{M} is not characterized in detail. We conjecture that they are at least dense in the unit sphere, which is most interesting to researchers on controllability studies, but rigorous proofs have not been found. Generally, it is a further task to investigate whether the system is controllable on some prescribed manifolds. Providing that the condition in theorem IV.3 is satisfied, this problem can be reduced to the transitivity of the strong ILH-Lie group \mathcal{G} over $S_{\mathcal{H}}$ (*N.B.* a group is said to be transitive if any two points on the manifold can be connected by some transformation in \mathcal{G} [29]). While a complete list for finite-dimensional systems has given in Refs. [47,48], it is worth exploring the problem of classifying all possible controllability algebras that act transitively over the hypersphere. This remains to be studied in the future.

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APPENDIX A

In the viewpoint of functional analysis, the smooth domain can be related to the inverse limit Hilbert (ILH) chains [34] defined as follows.

Definition A.1 (ILH space). Let $N(d)$ be the set of integers k such that $k \geq d$, where d is an integer. A family of complete locally convex topological vector (CLCTV) spaces $\{E, E^k; k \in N(d)\}$ is called an ILH chain if the following conditions are satisfied.

(1) Each E^k , $k \in N(d)$ is a Hilbert space, E^{k+1} is embedded continuously in E^k , and the image is dense in E^k .

(2) $E = \bigcap_{k \in N(d)} E^k$, and the topology of E is given by the inverse limit of $\{E^k; k \in N(d)\}$, where the inverse limit topology is the weakest topology such that the natural embedding $E \rightarrow E^k$ is continuous for every $k \in N(d)$.

For the universal enveloping algebra $E(\mathcal{L})$ considered in this paper, the smooth domain (7) can be equivalently expressed as an ILH space $\mathcal{D}_\infty = \bigcap_{k \in \mathbb{N}} \mathcal{H}_k$ by a series of Hilbert spaces $\mathcal{H} = \mathcal{H}_0 \supset \mathcal{H}_1 \supset \dots$ completed by the class of scalar products [30]

$$(\phi, \psi)_k = \langle \phi, \Delta^{k/2} \psi \rangle, \quad k = 0, 1, 2, \dots,$$

where the Nelson operator $\Delta = I + L_1^2 + \dots + L_d^2$ and $\langle \cdot, \cdot \rangle$ is the inner product of \mathcal{H} . To properly define the series of Hilbert spaces, the Nelson operator is required to be essential self-adjoint. With respect to this ILH-topology, the elements in the universal enveloping algebra are continuous and the uni-

versal enveloping algebra itself can be exponentiated to form an infinite-dimensional Frechet (or ILH) Lie transformation group [29,34] acting on \mathcal{D}_∞ . This group is no longer a Hilbert Lie group that covers most finite dimensional Lie groups. Geometrically, the tangent space of the group manifold at each group element is an ILH space instead of a Hilbert space. Interested readers may consult [29,34] for more details.

APPENDIX B

Let $L_\alpha = -iL'_\alpha$, $\alpha = x, y, z$. To prove this fact, it is enough to show that every ordered $L_x^p L_y^q L_z^r$ can be generated from the Poincaré-Birkhoff-Witt theorem [29]. Let $l = p + q + r$. The case for $l=1$ is obvious. Assume the case for $l=n-1$ is correct, we prove the validity for $l=n$. First, if one of $L_x^p L_y^q L_z^r$ for which $p+q+r=n$ can be generated, any other of such operators can be generated, because we have

$$\begin{aligned} [L_x^p L_y^q L_z^r, L_x] &= L_x^p [L_y^q, L_x] L_z^r + L_x^p L_y^q [L_z^r, L_x] \\ &= -q L_x^p L_y^{q-1} L_z^{r+1} - r L_x^p L_y^{q+1} L_z^{r-1} + Q_{n-1}, \end{aligned}$$

where Q_{n-1} denotes the terms of order less than n . Continuing calculating the commutations $\text{ad}_x^k(L_x^p L_y^q L_z^r)$, we can obtain $q+r+1$ operators in which the orders of L_y and L_z range from $(q+r, 0)$ to $(0, q+r)$. Since the operators with different (q, r) indices are linearly independent, we can obtain any $L_x^p L_y^q L_z^r$ after proper linear combination of these commutations and operators with order less than n . Similarly, we can obtain any $L_x^p L_y^q L_z^r$ and $L_x^p L_y^q L_z^r$ from $L_x^p L_y^q L_z^r$. Therefore any $L_x^p L_y^q L_z^r$ can be generated from $L_x^p L_y^q L_z^r$.

So the case of $l=n$ is valid if at least one $L_x^p L_y^q L_z^r$ of order n can be generated by lower order terms. This can be easily verified since $[L_x^2, L_x^{n-2} L_y] = 2L_x^{n-1} L_y + Q_{n-1}$. Hence all the Lie algebras \mathfrak{A} , \mathfrak{B} , \mathfrak{C} coincide with $E(\text{su}(1, 1))$.

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