Controllability of Scattering States of Quantum Mechanical Systems

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This paper provides a framework for the control of quantum mechanical systems with scattering states, i.e., systems with continuous spectra. We present the concept and prove a criterion of the approximate strong smooth controllability. Our results make non-trivial extensions from quantum systems with finite dimensional control Lie algebras to those with infinite dimensions. It also opens up many interesting problems for future studies.

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Recently, increasing research has been done on quantum mechanical systems with scattering states that possess practical applications [1, 2, 3, 4]. This has been a long-standing problem in the area of molecular control, where the attempts to breaking chemical bonds naturally evolve into various topics on discrete-continuum transitions of molecular states [2, 3, 5], i.e., photon-dissociation (from discrete to continuum), photon-association (from continuum to discrete) and laser catalysis (from continuum to continuum). Another prominent motivation is the continuous quantum computer [1, 2] that processes quantum information over continuous spectra. Serious theoretical studies have proved that they might be more sufficient in some tasks compared with their discrete counterparts.

These problems naturally fall under the system control theory [2, 3, 6, 10, 11, 12]. To the authors’ knowledge, most existing studies focus on finite dimensional bound-state quantum systems that have been strikingly successful in practice [3, 13, 14]. Very little has been done to scattering-state quantum control systems [7, 8, 15, 16] except some specialized discussions in the molecular control [5], where the calculation of controlled discrete-continuum transition probabilities are carried out along the lines of perturbation theory and adiabatic approximations under weak field assumptions.

Amongst various topics on quantum control, the controllability is of fundamental importance in understanding the physical mechanisms of quantum control [4, 8, 13, 12]. In this paper, we are investigating the controllability for a scattering-state quantum system that possesses an infinite dimensional control Lie algebra. As is well known in mathematics, the extension from finite dimensional Lie algebras to infinite dimensional Lie algebras is not trivial. Theoretically, the infinite dimensionality is the key to break through the HTC No-Go Theorem [1] so as to enable the ambitious control over a set of all scattering states. In these regards, our works make a quantum leap over the earlier result on finite dimensional systems, and that of [4, 8], which, although embraces the cases of both discrete [6] and continuous spectra [7], is still limited by the finite dimensionality of control Lie algebras.

Consider quantum control system in the form of the following Schrödinger equation:

\[
\frac{i\hbar}{\partial t} \psi(t) = \left[ H_0' + \sum_{j=1}^{m} u_j(t)H_j' \right] \psi(t), \quad \psi(0) = \psi_0. \tag{1}
\]

where the controls \( u_j(t) \) are real piecewise constant functions of time. The quantum state \( \psi(t) \) evolves in a separable Hilbert space \( \mathcal{H} \) that carries a unitary representation space of the symmetry algebra. The Hamiltonians \( H_0', H_1', \cdots, H_m' \) are Hermitian operators acting on \( \mathcal{H} \). For convenience, we rewrite (1) with skew-Hermitian operators \( H_i = H_i'/(i\hbar) \), i.e.,

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

In order to facilitate the analysis of system structures, we choose to embed the system in an algebraic framework based on an associated intrinsic symmetry algebra, say \( \mathcal{L} = \{L_1, \cdots, L_d\}_{\mathcal{L}A} \), of the quantum system under consideration. The subscript "LA" denotes the Lie algebra generated by the finite number of operators in the curly bracket. We assume that the Hamiltonians can be formally expressed as elements in the universal enveloping algebra \( E(\mathcal{L}) \) [17], i.e., in terms of polynomials of the generators of \( \mathcal{L} \). Obviously, the controllability Lie algebra \( \mathcal{A} = \{H_0, H_1, \cdots, H_m\}_{\mathcal{L}A} \) is a Lie subalgebra of \( E(\mathcal{L}) \).

The algebraic modelling method covers a wide class of quantum control systems such as harmonic oscillator [6] and hydrogen atom [8]. A paradigm closely related to this paper is the continuous quantum computer modelled as [11]:

\[
\frac{i\hbar}{\partial t} \psi(x,t) = \left[ \left( p^2 + x^2 \right) + u_1 p + u_2 x + u_3 (x^2 + p^2) + u_4 (xp + px) + u_5 (x^2 + p^2)^2 \right] \psi(t), \tag{3}
\]

where \( p = -i\hbar \partial_x \), \( [x, p] = i\hbar \). Here the Heisenberg algebra \( h(1) = \{x, p, i\}_{\mathcal{L}A} \) plays the role of the symmetry algebra of the system. The Hamiltonians for quantum computation are derived from quantization of classical variables of a harmonic oscillator into the universal enveloping algebra \( E(h(1)) \) [18, 19]. Comparing this system with the example of harmonic oscillator in [6]:

\[
\frac{i\hbar}{\partial t} \psi(x,t) = \left[ \left( p^2 + x^2 \right) + u_1 p + u_2 x \right], \tag{4}
\]
one can observe the distinction between these two systems: the controllability algebra of (3) is infinite dimensional, while that of (4) is finite dimensional. As indicated in [1], the infinite dimensionality is necessary for universality of quantum computation using this model.

The symmetry algebras of scattering-state quantum mechanical systems are necessarily noncompact. From the theory of unitary representation, \( \mathcal{H} \) has to be an infinite dimensional Hilbert space in which the quantum state prevails [17, 20]. Also due to the noncompactness, the unboundedness of Hamiltonians brings severe domain constraints [17]. Thus one has to specify a dense subset of \( \mathcal{H} \) on which the Hamiltonians are well-defined, invariant and the state-evolution can be expressed globally in exponential form. For systems with finite dimensional control Lie algebras , Huang, Tarn and Clark [6] suggested the analytic domain (the existence is ensured by Nelson’s theorem [21]):

\[
\mathcal{D}_0 = \left\{ \omega \in \mathcal{H} : \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{1 \leq n_1, \cdots, n_d \leq d} \| H_{n_1} \cdots H_{n_d} \omega \| s^n < \infty \right\}
\]

as a candidate, on which they present the notion of analytic controllability. The state-evolution of these systems are therefore restricted on a locally finite dimensional manifold with finite directions to move towards.

However, there does not exist, in general, a dense analytic domain for \( \mathcal{A} \) as an infinite dimensional Lie subalgebra of \( \mathcal{E}(\mathcal{L}) \). Nevertheless, as implied in [22], the existence of analytic domain is not necessary for the exponential formula. A natural choice is to enlarge the analytic domain to the collection of differentiable vectors of the associated symmetry algebra \( \mathcal{L} \):

\[
\mathcal{D}_0 = \{ \phi \in \mathcal{H} : \| L_1^{s_1} \cdots L_n^{s_n} \phi \| < \infty; s_i = 0, 1, 2, \cdots \}. \]

Given an insight into the space structure, \( \mathcal{D}_0 \) forms a complete Frechet space endowed with a locally convex topology that makes the Hamiltonians continuous [22, 23]. With this topology, the control algebra \( \mathcal{A} \) can be exponentiated to form a Frechet (or ILH-) Lie transformation group \( \mathcal{G} \) [22, 24] acting on \( \mathcal{D}_0 \). Parallel with the analytic domain, we call \( \mathcal{D}_0 \) the smooth domain. For instance, the smooth domain for (3) is the Schwartz domain

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

**Remark 1** The smooth domain provides a natural characterization of scattering states. Denote the dual space of \( \mathcal{D}_0 \) by \( \mathcal{D}_0^* \); we obtain a triad of linear spaces, i.e., the rigged Hilbert space [23]:

\[
\mathcal{D}_0 \subset \mathcal{H} \subset \mathcal{D}_0^*,
\]

with \( \mathcal{D}_0 \) dense in \( \mathcal{H} \) and \( \mathcal{H} \) dense in \( \mathcal{D}_0^* \). While \( \mathcal{D}_0 \) contains all experimentally preparable states for (3), the scattering states can be specified as vectors in \( \mathcal{D}_0^* \) which have run out of the Hilbert space \( \mathcal{H} \). Since \( \mathcal{D}_0 \) is dense in \( \mathcal{D}_0^* \), the system can approach arbitrarily close to any scattering state if all states in the smooth domain is reachable. From this viewpoint, we can make sense of the dynamical control over nonphysical scattering states.

The smooth domain and the exponentiated Frechet Lie group have already laid a technical basis in system analysis of the controllability properties. Let \( \mathcal{M} \) be the closure of the set

\[
\{ \exp(s_1 H_{\alpha_1}) \cdots \exp(s_k H_{\alpha_k}) \psi_0 | s_i \in \mathbb{R}, \alpha_k = 0, 1, \cdots, m, k \in \mathbb{N} \}
\]

for the initial state \( \psi_0 \in \mathcal{D}_0 \). Note \( \mathcal{M} \) is allowed to be an infinite dimensional sub-manifold of \( S_\mathcal{H} \), the unit sphere in \( \mathcal{H} \). Apparently, \( \mathcal{M} \) is the maximal set of possibly reachable states from \( \psi_0 \). Here we give the definition of controllability to be studied in this paper:

**Definition 1 (Smooth Controllability)** Denote \( \mathcal{R}(\psi) \) as the reachable set of the initial quantum state \( \psi_0 \in \mathcal{M} \cap \mathcal{D}_0 \) by all quantum states that can be driven from \( \psi_0 \) under properly adjusted controls. Quantum mechanical control system (2) is said to be approximately smoothly controllable if \( \mathcal{R}(\psi) = \mathcal{M} \cap \mathcal{D}_0 \) (the closure is with respect to the locally convex topology of \( \mathcal{D}_0 \)). Moreover, the system is said to be approximately strongly smoothly controllable if the closure of reachable set \( \mathcal{R}(\psi) \) at any time \( t > 0 \) equals to \( \mathcal{M} \cap \mathcal{D}_0 \).

**Remark 2** The prevailing definition of quantum controllability implicitly assigns the manifold \( \mathcal{M} \) to \( S_\mathcal{H} \), the unit sphere in \( \mathcal{H} \). This definition can be taken as a special case of that given here. It is another interesting and important problem to investigate when the reachable set of a controllable system covers \( S_\mathcal{H} \).

Now we are standing at the same starting point as in previous studies, where the existing results [4] can be naturally extended to quantum mechanical systems with infinite dimensional control algebras. Note that only finite control parameters are available to affect the state-evolution, repeated switching operations can generate only finite directions within any finite time interval. Therefore, at most approximate controllability can be achieved over an infinite dimensional manifold \( \mathcal{M} \) under piecewise constant controls. Nevertheless, from a practical point of view, approximate controllability is already enough for most situations. The following is our main result:

**Theorem 1** Let the Lie algebra \( \mathcal{B} = \{ H_1, \cdots, H_m \} \) and \( \mathcal{C} = \{ ad_{H_0}^j H_i, j = 0, 1, \cdots, i = 1, \cdots, m \} \), where \( ad_{H_0}^j H_i = H_i, ad_{H_0}^j H_i = [H_0, ad_{H_0}^{j-1} H_i] \). The system (2) is approximately strongly smoothly controllable if the following conditions are satisfied:

1. \([\mathcal{B}, \mathcal{C}] \subseteq \mathcal{B} \);
2. For any \( \phi \in \mathcal{M} \cap \mathcal{D}_0 \), \( \mathcal{C}(\phi) = \mathcal{A}(\phi) \) and they are infinite dimensional.
proof} Due to the space limitation, we present a condensed proof in this paper. Recall that the primary obstacle for controllability analysis is the presence of free evolution which can not be artificially adjusted. From a system theoretical point of view, the basic idea is to find out enough "adjustable" flows generated by interactions between the system Hamiltonians, so that the free evolution governed by $H_0$ can be cancelled and recreated. This in turn leads to the approximate strong smooth controllability prevailing over $\mathbf{M} \cap \mathcal{D}_\infty$.

We need to implement this idea in a strict way. A Hamiltonian $X$ is said to be strongly attainable if its integral curve passing any $\psi_0 \in \mathbf{M} \cap \mathcal{D}_\infty$ is contained in the closure of the infinitesimal-time reachable set $\mathcal{R}_0(\psi_0) = \bigcap_{t > 0} \mathcal{R}_{<t}(\psi_0)$, where $\mathcal{R}_{<t}(\psi_0)$ denotes the reachable set within $t$ units of time. The collection of strongly attainable Hamiltonians form a Lie algebra, i.e. they are closed under linear combination and commutation operations. This novel property is obvious from the well-known Trotter’s formula \cite{25}:

\[
\begin{align*}
\exp s(X + Y)\phi &= \lim_{n \to \infty}[\exp(sX/n)\exp(sY/n)^n]\phi, \\
\exp s[X,Y]\phi &= \lim_{n \to \infty}[\exp(\sqrt{s/n}X)\exp(\sqrt{s/n}Y) - \exp(-\sqrt{s/n}Y)\exp(-\sqrt{s/n}X)]^n\phi.
\end{align*}
\]

Now we seek strongly attainable Hamiltonians. Apparently, the control Hamiltonians $H_1, \ldots, H_m$ are strongly attainable, because they dominate the system evolution if we tune the controls sufficiently large (see detailed proof in \cite{26}). Thus the spanned Lie algebra $\mathcal{B}$ is strongly attainable.

Subsequently, we investigate the interaction of a strongly attainable Hamiltonian $H \in \mathcal{B}$ with the free Hamiltonian $H_0$. From the Campbell-Baker-Hausdorff formula \cite{24},

\[
\exp(tH)\exp sH_0 \exp(-tH)\phi = \exp \left\{ s(H_0 + t[H,H_0]) + \frac{t^2}{2}[H,[H,sH_0]] + \cdots \right\} \phi,
\]

where $\phi \in \mathbf{M} \cap \mathcal{D}_\infty$ we observe that the higher order terms on the right hand side are all strongly attainable Hamiltonians in $\mathcal{B}$ under the condition $[H_0,\mathcal{B}] \subseteq \mathcal{B}$. So we have

\[
\exp s(H_0 + t[H,H_0])\psi_0 \subseteq \mathcal{R}_s(\psi_0), \quad s > 0,
\]

by which we derive that

\[
\exp(\pm s[H,H_0])\psi_0 = \lim_{n \to \pm \infty} \exp \left( \frac{1}{n} [H_0 + t[H,H_0]] \right) \psi_0 \subseteq \lim_{n \to \pm \infty} \mathcal{R}_n(\psi_0) = \mathcal{R}_0(\psi_0).
\]

Thus we proved that the first-order term $[H,H_0]$ is strongly attainable. Inductively by repeated commutation operations, the system evolution can be guided along any flows generated by Hamiltonians in $ad_{H_0}^{\pm} \mathcal{B}$ for every integer $k$ with arbitrary precision. Therefore, the Lie algebra $\mathcal{C}$ is strongly attainable. This is to say, the integral manifold $(exp \mathcal{C})\psi_0$ of $\mathcal{C}$, which coincides with $\mathbf{M}$ under the condition $\mathcal{C}(\phi) = \mathcal{A}(\phi)$ for any $\phi \in \mathbf{M} \cap \mathcal{D}_\infty$, is contained in $\mathcal{R}_0(\psi_0)$.

Therefore, the system can be steered arbitrary closely to any state in $\mathbf{M} \cap \mathcal{D}_\infty$ at any time $t > 0$, because

\[
\mathbf{M} \cap \mathcal{D}_\infty \subseteq \exp(tH_0)(\exp \mathcal{A})\psi_0 = \exp(tH_0)(\exp \mathcal{C})\psi_0 \subseteq \mathcal{R}_0(\psi_0) \subseteq \mathbf{M} \cap \mathcal{D}_\infty.
\]

Thus $\mathcal{R}_0(\psi_0) = \mathbf{M} \cap \mathcal{D}_\infty$, i.e., the system is approximately strongly smoothly controllable over $\mathbf{M}$.

Physically, our result enables one to use finite controls to modulate the superposition of innumerable scattering states so as to resist the irreversible dispersion of wavepacket of scattering-state quantum systems. The fact is somewhat amazing and has been earlier questioned by Zhao and Rice \cite{4} for the presence of chaos. Actually, as they also recognized later, the essence of controllability is not altered because controllability problems always concern themselves with evolution on finite time internals, although the presence of chaos do make the control much more complicated.

To illuminate the ideas presented in this paper, we will discuss an example described in \cite{17}. The example is typically associated with an integral dimensional control algebra. The algebraic model characterizes the scattering states of particles subject to Pöschl-Teller potentials based on a scattering algebra $so(2,1) = \{ L_x, L_y, L_z \}_{LA}$ with $L_x$ compact and $L_y, L_z$ noncompact (see \cite{3} for detail), which commutation relations read:

\[
[L_x, L_y] = -iL_z, \quad [L_y, L_z] = -iL_x, \quad [L_z, L_x] = iL_y.
\]

We consider a control system as follows:

\[
i\hbar \frac{\partial}{\partial t} \psi(t) = [aL_y^2 + u_1 L_x + u_2 L_y + u_3 L_z^2] \psi(t).
\]

The noncompact free Hamiltonian $aL_y^2$ generates a continuous spectrum. Let $|j,m\rangle$ be the simultaneous eigenvectors of the compact generator $L_x$ and the Casimir operator $C = L_y^2 - L_x^2 - L_z^2$, the smooth domain of $\psi(t)$ is

\[
\mathcal{D}_\infty = \{ x = \sum_{m=-\infty}^{\infty} x_m | j,m \rangle \mid \lim_{|m| \to \infty} m^n x_m = 0, \forall n \in \mathbb{N} \}
\]

as described in \cite{27}.

It is not difficult to verify inductively that any element in $E(so(2,1))$, including the free Hamiltonian, may be generated by repeated commutations and linear combinations of the control Hamiltonians. Hence the Lie algebras $\mathcal{A}, \mathcal{B}, \mathcal{C}$ coincide with $E(so(2,1))$. Let $\mathbf{M}$ be the integral manifold of $\mathcal{A}$ through $\psi_0$. According to Theorem \textbf{1}, strong approximate smooth controllability follows on $\mathbf{M}$. We conjecture that $\mathbf{M}$ is dense in the unit sphere $S_M$, but the rigorous proof has not been found.

From the above derivation, the first-order control Hamiltonians manifest fundamental significance for shaping the quantum wavepacket by modulating the interaction of control
Hamiltonians. At the first glance, the operators $K_{\pm} = L_x \pm i L_y$ resemble the ladder operators of harmonic oscillators which is well-known for "raising" and "lowering" of energy levels. But intuitively, the "ladder" operators are not allowed to generate well-known for "raising" and "lowering" of energy levels. But

find by simple calculations that arises from the fact that $K_{\pm}$ can only operate on the superposition of scattering states, but illegally upon the scattering states that are outside the Hilbert space \[28\]. Interested readers are referred to \[28\] for more details.

The use of high-order operators in the universal enveloping algebra enables one to expand an infinite dimensional algebra by finite control Hamiltonians, so that the quantum state can be driven to an infinite dimensional manifold. Thus the high-order terms are important to enhance the control of quantum systems. As shown in the optical scheme for continuous quantum computation \[1\], the key operation is chosen as the nonlinear Kerr process \[4\] in equation (3) as a higher order terms. This high order term plays an essential role in achieving universality of quantum computation over continuous variables.

In conclusion, this paper provides a clearer understanding of quantum control over infinite dimensional manifolds of scattering states. Our result advances the existing results to a broader landscape. Back to the cases of finite dimensional control algebras, the extension of analytic controllability to the larger smooth domain, which has been conjectured in \[3\], can be taken as a trivial corollary of Theorem 1. The extension to infinite dimensional manifolds makes it possible to explore full control over the whole set of scattering states. It opens up many interesting problems for study, e.g. the control between discrete and continuous spectra and the control of resonances.

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