

Controllability of quantum mechanical systems: from conical eigenvalue intersections to Lie bracket conditions

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Abstract— We study the controllability of a closed control-affine quantum system driven by two or more external fields. We provide a sufficient condition for controllability in terms of existence of conical intersections between eigenvalues of the Hamiltonian in dependence of the controls seen as parameters. The spectral condition appears naturally in the adiabatic control framework and yields approximate controllability in the infinite-dimensional case. In the finite-dimensional case it implies that the system is Lie-bracket generating when lifted to the group of unitary transformations, and in particular that it is exactly controllable. Hence, Lie algebraic conditions are deduced from purely spectral properties.

I. INTRODUCTION

In this paper we consider a closed quantum system of the form

$$\begin{aligned} i\dot{\psi}(t) &= H(u(t))\psi(t) \\ &= (H_0 + \sum_{j=1}^m u_j(t)H_j)\psi(t), \end{aligned} \quad (1)$$

where $\psi(\cdot)$ describes the state of the system evolving in the unit sphere \mathcal{S} of a finite- or infinite-dimensional complex Hilbert space \mathcal{H} . The control $u(\cdot) = (u_1(\cdot), \dots, u_m(\cdot))$ takes values in a subset U of \mathbb{R}^m and represents external fields. The Hamiltonian $H(u)$ is a self-adjoint operator on \mathcal{H} for every $u \in U$.

System (1) is exactly (respectively, approximately) controllable if every point of \mathcal{S} can be steered to (respectively, steered arbitrarily close to)

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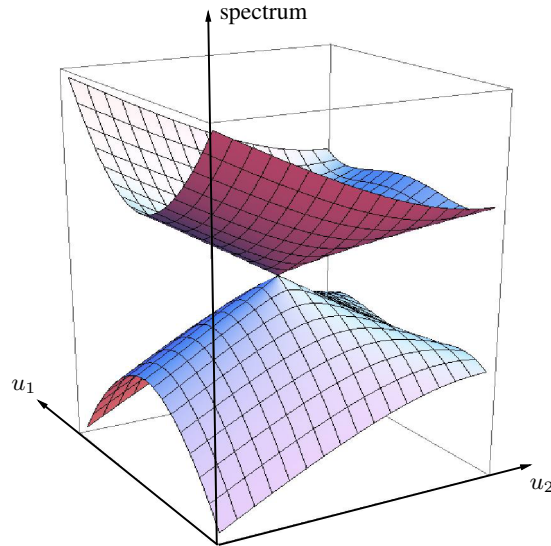


Fig. 1. A conical intersection when $m = 2$: the surfaces represent two eigenvalues of $H(u_1, u_2)$ as functions of u_1 and u_2 .

any other point of \mathcal{S} , by an admissible trajectory of (1).

In [2], in the case $m = 2$, it is shown how to exploit the existence of *conical intersections* (see Figure 1 and Definition 1) between every pair of subsequent eigenvalues to induce an approximate population transfer from any eigenstate to any other eigenstate or any nontrivial superposition of eigenstates (without controlling the relative phases). This kind of partial controllability is named *spread controllability* in [2].

In this paper we study the whole controllability implications of the conditions ensuring spread controllability, namely the existence of conical intersections between every pair of subsequent eigenvalues. A relevant advantage of these conditions is that

they consist in qualitative structural properties of the spectrum of $H(u)$ as a function of $u \in U$. This might be useful when the explicit expression of the Hamiltonian is not known, but one has information about its spectrum (as it happens in many experimental situations).

In the following we say that *the spectrum of $H(\cdot)$ is conically connected* if all eigenvalue intersections are conical, each pair of subsequent eigenvalues is connected by a conical intersections such that all other eigenvalues are simple (see Figure 2). A notable property of conical connectedness is that it is a structurally stable property for $m = 2$ (when restricted to real Hamiltonians) and for $m = 3$. This structural stability dates back to the 1920s ([1], [6]) and is discussed in more details in Section II-A (see Remark 2).

The main results of the paper about the relations between conically connected spectra and controllability are the following:

- if \mathcal{H} is finite-dimensional and the spectrum of $H(\cdot)$ is conically connected then $\text{Lie}\{H(u) \mid u \in U\}$ is equal to $\mathfrak{u}(n)$ if the trace of $H(u)$ is nonzero for some $u \in U$ or $\mathfrak{su}(n)$ otherwise. In particular (1) is exactly controllable and the same is true for its lift in $U(n)$ or $SU(n)$;
- if \mathcal{H} is infinite-dimensional and the spectrum of $H(\cdot)$ is conically connected then (1) is approximately controllable.

II. CONICAL INTERSECTIONS AND EXACT CONTROLLABILITY IN FINITE DIMENSION

A. Basic definitions and facts

A general controlled closed quantum system evolving in a finite-dimensional Hilbert space can be written as

$$i\dot{\psi}(t) = H(u(t))\psi(t), \quad (2)$$

where $\psi : [0, T] \rightarrow S^{2n-1} \subset \mathbb{C}^n$ denotes the state of the system and $H(u)$ is a Hermitian matrix smoothly depending on $u \in U \subset \mathbb{R}^m$. From now on let us take $n \geq 2$, otherwise the controllability problem is trivial.

Naturally associated with (2) is its lift on the unitary group $U(n)$,

$$i\dot{g}(t) = H(u(t))g(t), \quad (3)$$

which is right-invariant and permits to write the solution $\psi(\cdot)$ of (2) starting from ψ_0 as $\psi(t) = g(t)\psi_0$ where $g(\cdot)$ is the solution of (3) starting from the identity.

It is well known that (3) is controllable in $U(n)$ if and only if the Lie algebra generated by $\{iH(u) \mid u \in U\}$ is equal to $\mathfrak{u}(n)$. If the trace of each matrix $H(u)$, $u \in U$, is zero, then (3) is well posed in $SU(n)$ and its exact controllability in $SU(n)$ is equivalent to the condition $\text{Lie}\{iH(u) \mid u \in U\} = \mathfrak{su}(n)$.

In order to deduce the controllability properties of (2) from those of (3) one has to turn towards the classification of transitive actions of subgroups of $U(n)$ onto $S^{2n-1} \subset \mathbb{C}^n$. As a consequence, system (2) is exactly controllable if and only if

$$\text{Lie}\{iH(u) \mid u \in U\} \supseteq \begin{cases} \mathfrak{su}(n) & \text{if } n \text{ is odd,} \\ \text{an algebra conjugate to} \\ \mathfrak{sp}(n/2) & \text{if } n \text{ is even.} \end{cases} \quad (4)$$

(See [4].)

Of special interests for this paper are closed control-affine quantum system driven by m external fields, satisfying the following assumption:

- (A)** Let $m \geq 2$ and U be an open and connected subset of \mathbb{R}^m . We assume that $H(\cdot)$ is control-affine, i.e., it has the form

$$H(u) = H_0 + u_1H_1 + \dots + u_mH_m.$$

In the following, under assumption **(A)**, we focus on the controllability of the system

$$i\dot{\psi}(t) = (H_0 + u_1(t)H_1 + \dots + u_m(t)H_m)\psi(t), \\ \psi(t) \in S^{2n-1}, \quad (5)$$

and its lift

$$i\dot{g}(t) = (H_0 + u_1(t)H_1 + \dots + u_m(t)H_m)g(t), \\ g(t) \in U(n). \quad (6)$$

A crucial hypothesis that we shall use to prove exact controllability of (6) (and hence, in particular, of (5)) is the existence of conical intersections (in the space of controls) between consecutive energy levels, and the fact that these conical intersections occur at distinct points in the space of controls. More precisely:

Definition 1: Let **(A)** be satisfied. Let $\Sigma(u) = \{\lambda_1(u), \dots, \lambda_n(u)\}$ be the spectrum of $H(u)$,

where the eigenvalues $\lambda_1(u) \leq \dots \leq \lambda_n(u)$ are counted according to their multiplicities. We say that $\bar{u} \in U$ is a *conical intersection* between the eigenvalues λ_j and λ_{j+1} if $\lambda_j(\bar{u}) = \lambda_{j+1}(\bar{u})$ has multiplicity two and there exists a constant $c > 0$ such that for any unit vector $v \in \mathbb{R}^m$ and $t > 0$ small enough we have

$$\lambda_{j+1}(\bar{u} + tv) - \lambda_j(\bar{u} + tv) > ct. \quad (7)$$

See Figure 1 for the picture of a conical intersection.

Remark 2: Conical intersections are not pathological phenomena. On the contrary, they happen to be generic for $m = 3$ or for $m = 2$, when restricted to real Hamiltonians, in the following sense.

Let us first consider the case $m = 2$. Let $\text{sym}(n)$ be the set of all $n \times n$ symmetric real matrices. Then, generically with respect to the pair (H_1, H_2) in $\text{sym}(n) \times \text{sym}(n)$ (i.e., for all (H_1, H_2) in an open and dense subset of $\text{sym}(n) \times \text{sym}(n)$), for each $u = (u_1, u_2) \in \mathbb{R}^2$ and $\lambda \in \mathbb{R}$ such that λ is a multiple eigenvalue of $H_0 + u_1H_1 + u_2H_2$, the eigenvalue intersection u is conical. Moreover, each conical intersection u is structurally stable, in the sense that small perturbations of H_0, H_1 and H_2 give rise, in a neighborhood of u , to conical intersections for the perturbed H . See Section III for a version of this result in infinite dimension and [2] for more details.

In the case $m = 3$, let $\text{Herm}(n)$ be the space of $n \times n$ Hermitian matrices. Then, generically with respect to the triple (H_1, H_2, H_3) in $\text{Herm}(n)^3$, for each $u = (u_1, u_2, u_3) \in \mathbb{R}^3$ and $\lambda \in \mathbb{R}$ such that λ is a multiple eigenvalue of $H_0 + u_1H_1 + u_2H_2 + u_3H_3$, the eigenvalue intersection u is conical. Structural stability also holds, in the same sense as above. See [3] for more details and a discussion on the infinite-dimensional counterpart of these properties.

The following definition identifies the Hamiltonians for which we can guarantee exact controllability from qualitative properties of their spectra. Roughly speaking we require all their eigenvalues to be connected by conical intersections and the conical intersections to occur at different points in the space of controls.

Definition 3: Let **(A)** be satisfied. We say that the spectrum $\Sigma(\cdot)$ of $H(\cdot)$ is *conically connected* if all

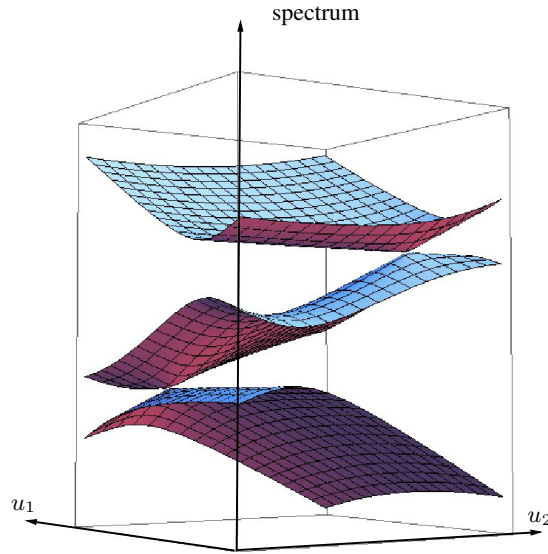


Fig. 2. A conically connected spectrum in the case $m = 2$.

eigenvalue intersections are conical and for every $j = 1, \dots, n - 1$, there exists a conical intersection $\bar{u}_j \in U$ between the eigenvalues λ_j, λ_{j+1} , with $\lambda_l(\bar{u}_j)$ simple if $l \neq j, j + 1$.

See Figure 2 for a conically connected spectrum.

B. Conical connectedness implies exact controllability

The main result of Section II is the following theorem.

Theorem 4: Let **(A)** be satisfied and assume that the spectrum $\Sigma(\cdot)$ of $H(\cdot)$ is conically connected. Then the Lie algebra generated by $\{iH(u) \mid u \in U\}$ is either $\mathfrak{u}(n)$ or $\mathfrak{su}(n)$ (in the case $H_0, \dots, H_m \in \mathfrak{su}(n)$). Hence, system (6) is either exactly controllable in $U(n)$ or well-posed and exactly controllable in $SU(n)$.

III. CONICAL INTERSECTIONS AND APPROXIMATE CONTROLLABILITY IN INFINITE DIMENSION

In this section we extend the controllability analysis of the previous section to systems of the form (5) evolving in infinite-dimensional spaces.

Consider a separable infinite-dimensional complex Hilbert space \mathcal{H} . In this section we make the following assumption:

(A[∞]) Let $m \geq 2$ and U be an open and connected subset of \mathbb{R}^m . Assume that the Hamiltonian $H(\cdot)$ has the form

$$H(u) = H_0 + u_1 H_1 + \cdots + u_m H_m, \\ u = (u_1, \dots, u_m) \in U,$$

where H_0, \dots, H_m are self-adjoint operators on \mathcal{H} , with H_0 bounded from below and H_1, \dots, H_m bounded.

With a Hamiltonian $H(\cdot)$ as in assumption (A[∞]) we can associate the control system

$$i\dot{\psi}(t) = (H_0 + u_1(t)H_1 + \cdots + u_m(t)H_m)\psi(t), \\ \psi(t) \in \mathcal{S}, \quad (8)$$

where \mathcal{S} is the unit sphere of \mathcal{H} .

Existence of solutions of (8) for u of class L^∞ and H_1, \dots, H_m bounded is classical (see [5]).

A typical case for which (A[∞]) is satisfied is when $H_0 = -\Delta + V$, where Δ is the Laplacian on a domain $\Omega \subset \mathbb{R}^d$ (with suitable boundary conditions if $\Omega \neq \mathbb{R}^d$), V is a regular enough real-valued potential bounded from below, $\mathcal{H} = L^2(\Omega, \mathbb{C})$, and H_1, \dots, H_m are multiplication operators by L^∞ real-valued functions.

The main technical assumption of this section is the following.

(B) The spectrum of H_0 is discrete without accumulation points and each eigenvalue has finite multiplicity.

Under assumptions (A[∞]) and (B) the spectrum of $H(u)$, $u \in U$, with eigenvalues repeated according to their multiplicities, can be described by $\Sigma^\infty(u) = \{\lambda_j(u)\}_{j \in \mathbb{N}}$ with $\lambda_j(u) \leq \lambda_{j+1}(u)$ for every $j \in \mathbb{N}$ and each $\lambda_j(\cdot)$ continuous on U . In analogy with Definition 3, we say that $\Sigma(\cdot)$ is *conically connected* if all eigenvalue intersections $\lambda_j = \lambda_{j+1}$, $j \in \mathbb{N}$, are conical (the definition of conical intersection extends trivially to this case) and for every $j \in \mathbb{N}$ there exists a conical intersection $\bar{u}_j \in U$ between the eigenvalues λ_j, λ_{j+1} , with $\lambda_l(\bar{u}_j)$ simple if $l \neq j, j+1$.

Remark 5: Recall from [2] that conical intersections are generic in the case $m = 2$ in the reference case where $\mathcal{H} = L^2(\Omega, \mathbb{C})$, $H_0 = -\Delta + V_0 : D(H_0) = H^2(\Omega, \mathbb{C}) \cap H_0^1(\Omega, \mathbb{C}) \rightarrow L^2(\Omega, \mathbb{C})$, $H_1 = V_1$, $H_2 = V_2$, with Ω a bounded domain of \mathbb{R}^d and $V_j \in C^0(\Omega, \mathbb{R})$ for $j = 0, 1, 2$. Indeed,

generically with respect to the pair (V_1, V_2) in $C^0(\Omega, \mathbb{R}) \times C^0(\Omega, \mathbb{R})$ (i.e., for all (V_1, V_2) in a countable intersection of open and dense subsets of $C^0(\Omega, \mathbb{R}) \times C^0(\Omega, \mathbb{R})$), for each $u \in \mathbb{R}^2$ and $\lambda \in \mathbb{R}$ such that λ is a multiple eigenvalue of $H_0 + u_1 H_1 + u_2 H_2$, the eigenvalue intersection u is conical. Moreover, each conical intersection u is structurally stable, in the sense that small perturbations of V_0, V_1 and V_2 give rise, in a neighbourhood of u , to conical intersections for the perturbed H .

The main purpose of this section is to extend Theorem 4 to the infinite-dimensional case, as follows.

Theorem 6: Let hypotheses (A[∞]) and (B) be satisfied. If the spectrum $\Sigma(\cdot)$ is conically connected then (8) is approximately controllable.

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