Approximate controllability, exact controllability, and conical eigenvalue intersections for quantum mechanical systems

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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. Such spectral condition is structurally stable in the case of three controls or in the case of two controls when the Hamiltonian is real. 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. We conclude the article by proving that approximate and exact controllability are equivalent properties for general finite-dimensional quantum systems.

1 Introduction

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

$$i\dot{\psi}(t) = H(u(t))\psi(t) = (H_0 + u_1(t)H_1 + \cdots + u_m(t)H_m)\psi(t), \tag{1}$$

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

When the dimension of $\mathcal{H}$ is finite, the exact controllability of (1) has been characterized in [2] in terms of the Lie algebra generated by $\{H(u) \mid u \in U\}$. In the infinite-dimensional case, if the controlled Hamiltonians $H_1, \ldots, H_m$ are bounded, exact controllability can be ruled out by functional analysis arguments ([3, 30]). Sufficient conditions for approximate controllability have been obtained by proving exact controllability of restrictions of (1) to spaces where the controlled Hamiltonians are unbounded ([5, 6, 7]). Other sufficient conditions for approximate controllability have been obtained by control-Lyapunov arguments ([8, 23, 24, 25]) and Lie–Galerkin techniques ([10, 11, 13, 14, 15]).

Both in the finite- and the infinite-dimensional case, checking the above-mentioned controllability criteria is not an easy task. Typical conditions require that the eigenvalues of H_0 are non-resonant (e.g., all gaps are different or rationally independent) and that the controlled Hamiltonians "sufficiently couple" the eigenstates of H_0. Hence many efforts were made to find easily checkable sufficient conditions for controllability of (1).

It should be mentioned that most of the conditions mentioned above are obtained for single-input systems ($m = 1$). An alternative technique fully exploiting the multi-input framework uses adiabatic theory to obtain approximate descriptions of the evolution of (1) for slowly varying control functions $u(\cdot)$ [1, 12, 20]. Adiabatic methods work when the spectrum exhibits eigenvalue intersections. In [12], in the case $m = 2$, it is shown how to exploit the existence of *conical intersections* (see Figure 1 and Definition 5) 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 [12].

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

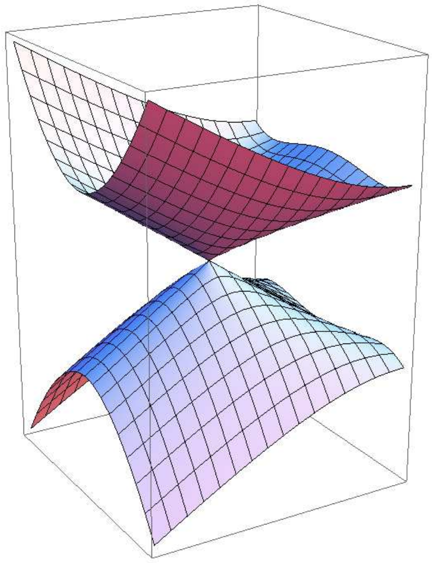

Figure 1: A conical intersection when $m = 2$: the surfaces represent two eigenvalues of $H(u_1, u_2)$ as functions of u_1 and u_2.

for $m = 3$ or for $m = 2$, when restricted to real Hamiltonians. This structural stability dates back to the 1920s ([9, 31]) and is discussed in more details in Section 2.1 (see Remark 6).

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 $\mathrm{Lie}\{H(u) \mid u \in U\}$ is equal to $\mathrm{u}(n)$ or $\mathrm{su}(n)$. In particular (1) is exactly controllable and the same is true for its lift in $\mathrm{U}(n)$ or $\mathrm{SU}(n)$;

- if $\mathcal{H}$ is infinite-dimensional and the spectrum of $H(\cdot)$ is conically connected then (1) is approximately controllable. (For a counterpart of the finite-dimensional lifted-system controllability, see Remark 16.)

Motivated by the exact/approximate dichotomy in the controllability of finite-/infinite-dimensional systems, we investigate in the last part of the paper the equivalence between exact and approximate controllability. We have already seen that exact controllability cannot hold when $\dim(\mathcal{H}) = \infty$, since we assume H_1 and H_2 to be bounded. When $\dim(\mathcal{H}) < \infty$ we prove that exact and approximate controllability are indeed equivalent, both for (1) and its lift on $\mathrm{U}(n)$. This last result holds in the more general setting where $H(u)$ depends on u in a possibly nonlinear way.

The structure of the paper is the following. In Section 2 we introduce the basic definitions related to controllability and conical intersections and we prove the finite-dimensional exact controllability of a system exhibiting a conically connected spectrum and of its lift in $\mathrm{U}(n)$ or $\mathrm{SU}(n)$ (Theorem 8). In Section 3 we prove that an infinite-dimensional system having a conically connected spectrum is approximately controllable (Theorem 13). Finally, in Section 4 we prove the equivalence between approximate and exact controllability for finite-dimensional closed quantum mechanical systems.

2 Conical intersections and exact controllability in finite dimension

2.1 Basic definitions and facts

In this section we introduce some definitions and recall some basic facts about control systems evolving on finite-dimensional manifolds.

We first define approximate and exact controllability for a smooth control system

$$\dot{q}(t) = f(q(t), u(t)) \qquad (\Sigma)$$

defined on a connected manifold M with controls $u(\cdot)$ taking values in $U \subset \mathbb{R}^m$.

Definition 1

- *The* reachable set $\mathcal{A}_{q_0}$ *from a point* $q_0 \in M$ *for* (Σ) *is the set of points* $q_1 \in M$ *such that there exist a time* $T \geq 0$ *and a* L^∞ *control* $u : [0, T] \to U$ *for which the solution of the Cauchy problem* $\dot{q}(t) = f(q(t), u(t))$ *starting from* $q(0) = q_0$ *is well defined on* $[0, T]$ *and satisfies* $q(T) = q_1$.
- *The system* (Σ) *is said to be* exactly controllable *if for every* $q_0 \in M$ *we have* $\mathcal{A}_{q_0} = M$.
- *The system* (Σ) *is said to be* approximately controllable *if for every* $q_0 \in M$ *we have that* $\mathcal{A}_{q_0}$ *is dense in* M.

A relevant class of control systems for our discussion is given by right-invariant control systems on Lie groups, namely, systems for which M is a connected Lie group and each vector field $f(\cdot, u)$, $u \in U$, is right-invariant.

Lemma 3 below is a classical result concerning right-invariant control systems on compact Lie groups (see, e.g., [19] and [22, p. 155]).

Definition 2 *Let* (Σ) *be a right-invariant control system and denote by* e *the identity of the group* M. *Let* $\mathrm{Lie}\{f(e,u) \mid u \in U\}$ *be the* Lie algebra generated by $\{f(e,u) \mid u \in U\}$, *i.e., the smallest subalgebra of the Lie algebra of* M *containing* $\{f(e,u) \mid u \in U\}$. *The* orbit G *of* (Σ) *is the connected subgroup of* M *whose Lie algebra is* $\mathrm{Lie}\{f(e,u) \mid u \in U\}$.

Lemma 3 *Let* M *be a connected compact Lie group and consider a right-invariant control system* (Σ) *on* M. *The following conditions are equivalent:*

- (Σ) *is exactly controllable;*
- *the orbit* G *of* (Σ) *is equal to* M*;*
- $\mathrm{Lie}\{f(e,u) \mid u \in U\}$ *is the Lie algebra of* M.

The last condition is usually referred to as the *Lie-bracket generating condition.*

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

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

where $\psi : [0,T] \to S^{2n-1} \subset \mathbb{C}^n$ 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 $\mathrm{U}(n)$,

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

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.

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

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 $\mathrm{U}(n)$ onto $S^{2n-1} \subset \mathbb{C}^n$. As a consequence, system (2) is exactly controllable if and only if

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

(See [17].)

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

$$H(u) = H_0 + u_1 H_1 + \cdots + u_m H_m.$$

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

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

and its lift

$$i\dot{g}(t) = (H_0 + u_1(t)H_1 + \cdots + u_m(t)H_m)g(t), \qquad g(t) \in \mathrm{U}(n). \tag{6}$$

Remark 4 *Let us briefly discuss the role of the assumptions listed in hypotheses* **(A)**. *The affine structure of H with respect to the control is natural in quantum control ([17]) and allows the application of the controllability criteria we are using in the following (see Proposition 11). Moreover, the connectedness of U is required in order to apply adiabatic techniques in the whole set of control parameters.*

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 5 *Let* **(A)** *be satisfied. Let $\Sigma(u) = \{\lambda_1(u), \ldots, \lambda_n(u)\}$ be the spectrum of $H(u)$, where the eigenvalues $\lambda_1(u) \leq \cdots \leq \lambda_n(u)$ 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*

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

See Figure 1 for the picture of a conical intersection. Notice that the hypothesis $m \geq 2$ guarantees that conical intersections do not disconnect U. This is crucial in the arguments below (see, in particular, Lemma 9.)

Remark 6 *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 $\mathrm{sym}(n)$ be the set of all $n \times n$ symmetric real matrices. Then, generically with respect to the pair (H_1, H_2) in $\mathrm{sym}(n) \times \mathrm{sym}(n)$

(i.e., for all (H_1, H_2) in an open and dense subset of $\mathrm{sym}(n) \times \mathrm{sym}(n)$*), for each $u = (u_1, u_2) \in \mathbb{R}^2$ and $\lambda \in \mathbb{R}$ such that λ is a multiple eigenvalue of $H_0 + u_1 H_1 + u_2 H_2$, the eigenvalue intersection u is conical. Moreover, each conical intersection u is structurally stable, in the sense that small perturbations of H_0, H_1 and H_2 give rise, in a neighborhood of u, to conical intersections for the perturbed H. See Section 3 for a version of this result in infinite dimension and [12] for more details.*

In the case $m = 3$, let $\mathrm{Herm}(n)$ *be the space of $n \times n$ Hermitian matrices. Then, generically with respect to the triple (H_1, H_2, H_3) in* $\mathrm{Herm}(n)^3$*, 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 $H_0 + u_1 H_1 + u_2 H_2 + u_3 H_3$, the eigenvalue intersection u is conical. Structural stability also holds, in the same sense as above. See [16] 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 7 *Let* **(A)** *be satisfied. We say that the spectrum $\Sigma(\cdot)$ of $H(\cdot)$ is* conically connected *if all eigenvalue intersections are conical and for every $j = 1, \ldots, n-1$, 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.

2.2 Conical connectedness implies exact controllability

The main result of Section 2 is the following theorem.

Theorem 8 *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 $u(n)$ or $su(n)$ (in the case $H_0, \ldots, H_m \in su(n)$). Hence, system (6) is either exactly controllable in $U(n)$ or well-posed and exactly controllable in $SU(n)$.*

The proof of the theorem is based on the following lemma.

Lemma 9 *Let* **(A)** *be satisfied and assume that the spectrum $\Sigma(\cdot)$ of $H(\cdot)$ is conically connected. Then there exists $\bar{U} \subset U$ which is dense and with zero-measure complement in U such that if $\sum_{j=1}^{n} \alpha_j \lambda_j(\bar{u}) = 0$ with $(\alpha_1, \ldots, \alpha_n) \in \mathbb{Q}^n$ and $\bar{u} \in \bar{U}$ then $\alpha_1 = \alpha_2 = \cdots = \alpha_n$.*

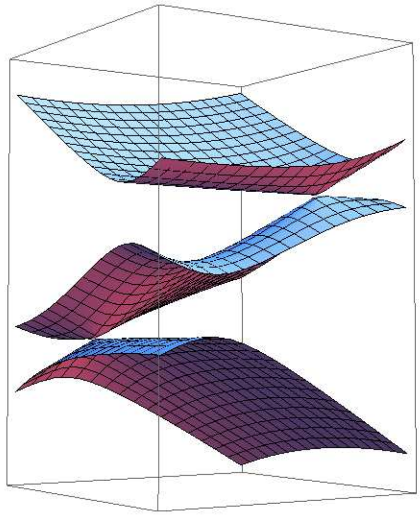

Figure 2: A conically connected spectrum in the case $m = 2$.

Proof. For every $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{Q}^n$ define

$$U_\alpha = \{u \in U \mid \sum_{j=1}^{n} \alpha_j \lambda_j(u) = 0\}.$$

Notice that, by definition of conical intersection and since $m \geq 2$, $\{u \in U \mid \Sigma(u) \text{ is simple}\}$ is connected. Thanks to the analyticity of the spectrum in $\{u \in U \mid \Sigma(u) \text{ is simple}\}$, either $U_\alpha = U$ or U_α has empty interior. The proof is completed by showing that if $U_\alpha = U$ then $\alpha_1 = \cdots = \alpha_n$.

Assume that $U_\alpha = U$. Consider $j \in \{1, \dots, n-1\}$ and an analytic path $\gamma : \mathbb{R} \to U$ such that $\gamma(0) = \bar{u}_j$, $\dot{\gamma}(0) \neq 0$, where $\bar{u}_j \in U$ is a conical intersection between the eigenvalues λ_j, and λ_{j+1}, with $\lambda_l(\bar{u}_j)$ simple if $l \neq j, j+1$.

Since $U_\alpha = U$, we have for every $t \in \mathbb{R}$,

$$\sum_{l=1}^{n} \alpha_l \lambda_l(\gamma(t)) = 0.$$

By analytic dependence of the spectrum along γ in a neighbourhood of $\gamma(0)$ [27], the functions

$$t \mapsto \begin{cases} \lambda_j(\gamma(t)) & \text{if } t < 0 \\ \lambda_{j+1}(\gamma(t)) & \text{if } t \geq 0, \end{cases} \qquad t \mapsto \begin{cases} \lambda_{j+1}(\gamma(t)) & \text{if } t < 0 \\ \lambda_j(\gamma(t)) & \text{if } t \geq 0, \end{cases}$$

and $t \mapsto \lambda_l(\gamma(t))$, $l \neq j, j+1$, are analytic in a neighborhood of 0. Hence,

$$\alpha_{j+1}\lambda_j(\gamma(t)) + \alpha_j\lambda_{j+1}(\gamma(t)) + \sum_{l\neq j,j+1} \alpha_l\lambda_l(\gamma(t)) = 0$$

for t in a neighborhood of 0. Then

$$(\alpha_j - \alpha_{j+1})(\lambda_j(\gamma(t)) - \lambda_{j+1}(\gamma(t))) = 0$$

for t in a neighborhood of 0. By definition of conical intersection it must be $\alpha_j = \alpha_{j+1}$. Since j is arbitrary, we deduce that $\alpha_1 = \cdots = \alpha_n$ concluding the proof. $\square$

Remark 10 *The lemma fails to hold if $m = 1$. Consider for instance $n = 3$, $H_0 = \mathrm{diag}(0, 1, 2)$ and $H_1 = \mathrm{diag}(1, 1, 0)$. Then the eigenvalues of $H(u)$ are $u, u+1$ and 2. The spectrum is conically connected, but clearly $\bar{U} = \emptyset$.*

Notice that $\mathrm{Lie}(iH_0, iH_1)$ is made only by diagonal matrices and therefore $\{iH_0, iH_1\}$ does not generate $u(n)$. Hence, this example also shows that Theorem 8 does not hold if we remove the hypothesis $m \geq 2$.

The proof of Theorem 8 is based on the following adaptation of a controllability criteria for single-input quantum control systems appeared in [10, Proposition 3.1]. The proof can be obtained following exactly the same arguments as in [10].

Proposition 11 *Let $A_0, A_1, \ldots, A_m$ be skew-Hermitian $n \times n$ matrices. Denote by $\lambda_1, \ldots, \lambda_n$ the eigenvalues of A_0, repeated according to their multiplicities and let $\phi_1, \ldots, \phi_n$ be an orthonormal basis of associated eigenvectors. Let*

$$S_0 = \{(j, k) \in \{1, \ldots, n\}^2 \mid \exists\, l \in \{1, \ldots, m\} \text{ such that } \langle \phi_j, A_l\phi_k\rangle \neq 0\}.$$

Assume that there exists $S \subseteq S_0$ such that the graph having $1, \ldots, n$ as nodes and S as set of edges is connected. Assume, moreover, that for every $(j, k) \in S$ and $(r, s) \in S_0 \setminus \{(j, k)\}$ we have $\lambda_j - \lambda_k \neq \lambda_r - \lambda_s$. Then Lie$(A_0, \ldots, A_m) = su(n)$ if $A_0, \ldots, A_m \in su(n)$ and Lie$(A_0, \ldots, A_m) = u(n)$ otherwise.

Proof of Theorem 8. Applying Lemma 9 we deduce the existence of $u_0 \in U$ such that if $\sum_{j=1}^{n} \alpha_j\lambda_j(u_0) = 0$ with $(\alpha_1, \ldots, \alpha_n) \in \mathbb{Q}^n$ then $\alpha_1 = \cdots = \alpha_n$. In particular, the spectrum of $H(u_0)$ is simple and two spectral gaps $\lambda_j(u_0) - \lambda_k(u_0)$ and $\lambda_r(u_0) - \lambda_s(u_0)$ are different if $(j, k) \neq (r, s)$ and $j \neq k$, $r \neq s$. Let $\phi_1, \ldots, \phi_n$ be an orthonormal basis of eigenvectors of $H(u_0)$.

Let us conclude the proof by applying Proposition 11 to $A_0 = iH(u_0)$, $A_j = iH_j$ for $j = 1, \ldots, m$: to this purpose, we are left to prove that the graph having $1, \ldots, n$ as nodes and

$$S_0 = \{(j, k) \in \{1, \ldots, n\}^2 \mid \langle \phi_j, H_l\phi_k\rangle \neq 0 \text{ for some } l = 1, \ldots, m\}$$

as set of edges is connected.

Assume by contradiction that such graph is not connected. Then there exists a proper subspace V of $\mathbb{C}^n$ generated by eigenvectors of $H(u_0)$ which is invariant for the evolution of (5). Without loss of generality $V = \mathrm{span}\{\phi_1, \dots, \phi_r\}$ with $r < n$.

Since the spectrum is conically connected, we can apply [29, Corollary 2.5] and deduce that there exists an admissible trajectory of (5) steering ϕ_1 to an arbitrary small neighbourhood of $\{e^{i\theta}\phi_n \mid \theta \in \mathbb{R}\}$. (See also [12, Proposition 3.4] for a rephrasing in control terms of [29, Corollary 2.5], which deals with general adiabatic evolutions through conical intersections. The result is stated in [12] in the case $m = 2$ for symmetric Hamiltonians but actualy holds in the general case.) The contradiction is reached, since $V \cap \{e^{i\theta}\phi_n \mid \theta \in \mathbb{R}\} = \emptyset$. □

3 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:

($\mathbf{A}^\infty$) 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

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

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 **($\mathbf{A}^\infty$)** we can associated the control system

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

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 [26]).

A typical case for which **($\mathbf{A}^\infty$)** 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.

3.1 Conical connectedness implies approximate controllability in infinite dimension

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 $(\mathbf{A}^\infty)$ and $(\mathbf{B})$ 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 $\lambda_j(\cdot)$ continuos on U. In analogy with Definition 7, 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 12 *Recall from [12] that conical intersections are generic in the case $m = 2$ in the reference case where $\mathcal{H} = L^2(\Omega,\mathbb{C})$, $H_0 = -\Delta + V_0 : D(H_0) = H^2(\Omega,\mathbb{C}) \cap H^1_0(\Omega,\mathbb{C}) \to L^2(\Omega,\mathbb{C})$, $H_1 = V_1$, $H_2 = V_2$, with Ω a bounded domain of $\mathbb{R}^d$ and $V_j \in \mathcal{C}^0(\Omega,\mathbb{R})$ for $j = 0, 1, 2$. Indeed, generically with respect to the pair (V_1, V_2) in $\mathcal{C}^0(\Omega,\mathbb{R}) \times \mathcal{C}^0(\Omega,\mathbb{R})$ (i.e., for all (V_1, V_2) in a countable intersection of open and dense subsets of $\mathcal{C}^0(\Omega,\mathbb{R}) \times \mathcal{C}^0(\Omega,\mathbb{R})$), for each $u \in \mathbb{R}^2$ and $\lambda \in \mathbb{R}$ such that λ is a multiple eigenvalue of $H_0 + u_1H_1 + u_2H_2$, the eigenvalue intersection u is conical. Moreover, each conical intersection u is structurally stable, in the sense that small perturbations of 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 8 to the infinite-dimensional case, as follows.

Theorem 13 *Let hypotheses* $(\mathbf{A}^\infty)$ *and* $(\mathbf{B})$ *be satisfied. If the spectrum $\Sigma(\cdot)$ is conically connected then (8) is approximately controllable.*

The proof of Theorem 13 follows the same pattern as the one of Theorem 8. The first step is the following straightforward generalisation of Lemma 9.

Lemma 14 *Let hypotheses* $(\mathbf{A}^\infty)$ *and* $(\mathbf{B})$ *be satisfied and assume that the spectrum $\Sigma(\cdot)$ is conically connected. Then there exists $\bar{U} \subset U$ which is dense and with zero-measure complement in U such that for each $N \in \mathbb{N}$, $\sum_{j=1}^N \alpha_j\lambda_j(\bar{u}) = 0$ with $(\alpha_1, \ldots, \alpha_N) \in \mathbb{Q}^N$ and $\bar{u} \in \bar{U}$ implies $\alpha_1 = \alpha_2 = \cdots = \alpha_N = 0$.*

In particular the spectrum of $H(\bar{u})$ for $\bar{u} \in \bar{U}$ as in Lemma 14 is such that two spectral gaps $\lambda_k(\bar{u}) - \lambda_j(\bar{u})$ and $\lambda_r(\bar{u}) - \lambda_s(\bar{u})$ are different if $(k, j) \neq (r, s)$ and $k \neq j$, $r \neq s$.

In the infinite-dimensional case, the role of Proposition 11 is played by the following corollary of [10, Theorem 2.6].

Proposition 15 *Let hypotheses* $(\mathbf{A}^\infty)$ *and* $(\mathbf{B})$ *be satisfied. Assume that there exists* $\bar{u} \in U$ *such that* $\lambda_k(\bar{u}) - \lambda_j(\bar{u}) \neq \lambda_r(\bar{u}) - \lambda_s(\bar{u})$ *if* $(k, j) \neq (r, s)$, $(k, j), (r, s) \in \mathbb{N}^2 \setminus \{(l, l) \mid l \in \mathbb{N}\}$. *Denote by* $(\phi_j(\bar{u}))_{j\in\mathbb{N}}$ *a Hilbert basis of eigenvectors of* $H(\bar{u})$ *and let*

$$S = \{(j, k) \in \mathbb{N}^2 \mid \langle \phi_j(\bar{u}), H_l \phi_k(\bar{u}) \rangle \neq 0 \text{ for some } l = 1, \dots, m\}.$$

If the graph having $\mathbb{N}$ *as set of nodes and* S *as set of edges is connected then* (8) *is approximately controllable in* $\mathcal{S}$.

The proof of Theorem 13 is then concluded as follows: Lemma 14 guarantees the existence of $\bar{u}$ such that the spectral gaps of $\Sigma(\bar{u})$ are all different; this allows to deduce the conclusion from Proposition 15 provided that no proper linear subspace of $\mathcal{H}$ spanned by eigenvectors of $H(\bar{u})$ is invariant for (8). As in the finite-dimensional case, this can be be proved by adiabatic methods, deducing from [29, Corollary 2.5] (or [12, Proposition 3.4]) that for every pair of eigenvectors of $H(\bar{u})$ there exists and admissible trajectory of (8) connecting them with arbitrary precision.

Remark 16 *Following [11] a stronger version of Proposition 15, and hence of Theorem 13, could be stated, namely: under the same hypotheses, for every* $l \in \mathbb{N}$, $\psi_1, \dots, \psi_l \in \mathcal{S}$, $\varepsilon > 0$, *and every unitary transformation* Υ *of* $\mathcal{H}$, *there exists a control function* $u : [0, T] \to U$ *such that, for every* $j = 1, \dots, l$ *the solution of* (8) *having* ψ_j *as initial conditions arrives in a* ε*-neighborhood of* $\Upsilon(\psi_j)$ *at time* T. *Notice that this is the natural counterpart of controllability of the lift of* (5) *in the group of unitary transformations proved in Section 2.*

4 Equivalence between exact and approximate controllability for finite-dimensional systems

In the previous sections we have seen several sufficient conditions for controllability, which is exact in the finite-dimensional case and approximate in the infinite-dimensional one.

In this section we discuss the relation between approximate and exact controllability. It is well known that exact controllability of a control-affine system in an infinite-dimensional Hilbert space cannot be expected if the control operators are bounded (see [3, 21, 30]).

Our aim is to show that in the finite-dimensional case approximate controllability always yields exact controllability for systems of the type

$$i\dot{\psi}(t) = H(u(t))\psi(t), \qquad \psi(t) \in S^{2n-1},\ u(t) \in U \subset \mathbb{R}^m, \tag{9}$$

or

$$i\dot{g}(t) = H(u(t))g(t), \qquad g(t) \in \mathscr{G},\ u(t) \in U \subset \mathbb{R}^m, \tag{10}$$

where $\mathscr{G}$ denotes the group $\mathrm{SU}(n)$ if the trace of $H(u)$ is zero for every $u \in U$ and $\mathrm{U}(n)$ otherwise.

More precisely, we have the following.

Theorem 17 *System (9) is approximately controllable if and only it is exactly controllable. The same holds for system* (10)*.*

For the control problem on S^{2n-1} the proof is based on some results in representation theory, recalled in the following section. For the lifted problem in $\mathrm{U}(n)$ (or $\mathrm{SU}(n)$) the proof directly follows from results from a 1942 result by Smith [28], as detailed in Section 4.3.

4.1 Some facts from group-representation theory

In this section, we recall the two basic main facts from representation theory that are needed in order to prove Theorem 17. We consider a finite-dimensional representation of a Lie group G, $\mathfrak{X} :\ G \to L(h)$, where h is a finite dimensional complex Hilbert space and $L(h)$ denotes the space of endomorphisms of h.

Theorem 18 below is stated by Dixmier in [18]. We need it for Lie groups, although it holds more generally for locally compact topological groups.

We recall that the intersection of the kernels of all unitary irreducible finite-dimensional representations of a group G is a subgroup of G. Then, G is said to be *injectable in a compact group*[1] if this subgroup is reduced to the identity of G.

Theorem 18 ([18] 16.4.8) *Let G be a connected, locally compact group. Then G is injectable in a compact group if and only if $G = \mathbb{R}^p \times K$ with K a compact group.*

[1]The definition given here is not the most natural, since injectability in a compact group is related to the notion of *compact group associated with a topological group* that is defined via an universal property: For each topological group G there exists a compact group Σ and a continuous morphism $\alpha : G \to \Sigma$ such that for any compact group Σ' and continuous morphism $\alpha' : G \to \Sigma'$ it exists a continuous morphism $\beta : \Sigma \to \Sigma'$ such that $\alpha' = \beta \circ \alpha$. We give here only the definition that fits better with our purposes. For such beautiful theory, see [18, 16.4].

The second key fact that we need is due to Weil (see [32, p. 66]).

Proposition 19 ([18] 13.1.8) *Let $G = G_1 \times G_2$ be the Cartesian product of two locally compact topological groups, and let $\mathfrak{X}$ be an irreducible representation of G. Define the representation $\mathfrak{X}_1'$ of G_1 as $\mathfrak{X}_1'(g_1) := \mathfrak{X}(g_1, e)$ and the representation $\mathfrak{X}_2'$ of G_2 as $\mathfrak{X}_2'(g_2) := \mathfrak{X}(e, g_2)$. If $\mathfrak{X}_1'$ and $\mathfrak{X}_2'$ lie in a semisimple class of representations, then $\mathfrak{X}$ is equivalent to the tensor product $\mathfrak{X}_1 \otimes \mathfrak{X}_2$ with $\mathfrak{X}_1, \mathfrak{X}_2$ irreducible representations of G_1, G_2, respectively.*

We would need to specify what a semisimple class of representations is, see [32, p. 65]. For our purpose, however, it is enough to recall that any class of bounded representation is semisimple (see, e.g., [32, p. 70]).

We finally recall some elementary properties for unitary representations of $\mathbb{R}^p$. First recall that each irreducible unitary representation is equivalent to a representation of the type $\chi_\xi(x) := e^{i\xi\cdot x}$ for some $\xi \in \mathbb{R}^p$, called *character* (see, e.g., [4, 6.1]). As a consequence we have:

Lemma 20 *If $\mathbb{R}^p$ admits an irreducible unitary faithful representation, then $p = 0$.*

4.2 Proof of the first part of Theorem 17

In this section we prove the part of Theorem 17 dealing with system (9). It is clear that its exact controllability implies approximate controllability. We now prove that approximate controllability implies exact controllability for systems of type (9).

Assume that system (9) is approximately controllable. Let G be the orbit of (10), i.e., the subgroup of $\mathscr{G}$ whose Lie algebra is generated by $\{iH(u) \mid u \in U\}$ (see Definition 2).

We now prove that G is compact, in four steps.

1. Observe that the inclusion $\jmath : G \hookrightarrow \mathscr{G}$ is a faithful (by definition) representation of G over $\mathbb{C}^n$, since $\mathscr{G} \subset L(\mathbb{C}^n) = gl(n, \mathbb{C})$. Then, the kernel of $\jmath$ is reduced to $\{e\}$, and thus G is injectable in a compact group.

   Applying Theorem 18, we have that $G = \mathbb{R}^p \times K$.

2. We claim that $\jmath$ is an irreducible representation of G. We prove it by contradiction. Assume that the inclusion is not irreducible so that there exists a proper subspace H_1 of $\mathbb{C}^n$ which is invariant with respect to the action of G. Now take $z_0 \in H_1 \cap S^{2n-1}$ and observe that $Gz_0 \subset H_1 \cap S^{2n-1}$. Clearly the reachable set $\mathcal{A}(z_0)$ is contained in Gz_0. Thus $\mathcal{A}(z_0)$ is not dense. Hence the system is not approximately controllable. Contradiction.

3. We have that $G = \mathbb{R}^p \times K$ and $\jmath$ is an irreducible representation. Remark that $\jmath$ is also unitary, hence bounded. As already recalled, the class of bounded representations of G is semisimple. Then we can apply Proposition 19, that gives us two irreducible bounded representations $\mathfrak{X}_1 : \mathbb{R}^p \to L(\mathbb{C}^{m_1})$ and $\mathfrak{X}_2 : K \to L(\mathbb{C}^{m_2})$ such that $\jmath$ is equivalent to $\mathfrak{X}_1 \otimes \mathfrak{X}_2$.

4. We now prove that $\mathfrak{X}_1, \mathfrak{X}_2$ can be assumed to be unitary. Denote by e_K the identity of K and observe that, for every g_1 in $\mathbb{R}^p$, one has that $\jmath(g_1, e_K)$ is unitary and equivalent to $\mathfrak{X}_1(g_1) \otimes \mathfrak{X}_2(e_K) = \mathfrak{X}_1(g_1) \otimes \mathbb{1}_{\mathbb{C}^{m_2}}$. Hence, $\mathfrak{X}_1$ is equivalent to a unitary representation. A similar argument works for $\mathfrak{X}_2$.

5. Since $\jmath$ is faithful, then $\mathfrak{X}_1$ and $\mathfrak{X}_2$ are faithful too. In conclusion, $\mathfrak{X}_1$ is equivalent to a faithful irreducible unitary representation of $\mathbb{R}^p$. Then, thanks to Lemma 20, we have that $p = 0$. Then $G = K$ is compact.

Consider now system (10) restricted to G. By construction, the system satisfies the two last equivalent conditions of Lemma 3. Then the system is exactly controllable over G and the reachable set from the identity is G itself.

The reachable set from a point ψ_0 for (9) is thus the product $G \cdot \psi_0$, which is closed since G is compact. On the other hand, since (9) is approximately controllable, then $G \cdot \psi_0$ is dense in S^{2n-1}. Henceforth, $G \cdot \psi_0$ coincides with S^{2n-1} itself, i.e., system (9) is exactly controllable. □

4.3 Proof of the second part of Theorem 17 and connections with controllability on the sphere

We first prove the second part of Theorem 17, namely, that approximate and exact controllability on the group $\mathscr{G}$ are equivalent. This is a direct consequence of the following result, proved in [28, note on p. 312].

Theorem 21 *If a dense subgroup $\hat{G}$ of a simple Lie group G of dimension larger than 1 contains an analytic arc, then $\hat{G} = G$.*

Let us apply this theorem to system (10). Let (10) be approximately controllable. Then, the orbit from the identity is a dense subgroup $\hat{\mathscr{G}}$ of $\mathscr{G}$. Any trajectory of (10) with constant u is an analytic arc, contained in $\hat{\mathscr{G}}$. Then $\hat{\mathscr{G}} = \mathscr{G}$, i.e., the orbit is the whole group. Again by Lemma 3, we have that the accessible set coincides with $\mathscr{G}$, i.e., that system (10) is exactly controllable. This concludes the proof of Theorem 17.

Let us now discuss the connection between the approximate/exact controllability on the sphere S^{2n-1} (i.e., system (9)) and the approximate/exact controllability on the group $\mathscr{G}$. Notice that Theorem 17 is not a simple corollary of Theorem 21 and that approximate/exact controllability on the group and on the sphere are not equivalent. Actually we have proven that approximate controllability on S^{2n-1} is equivalent to exact controllability, and this condition is equivalent to transitivity of G on S^{2n-1} as a homogeneous space. In [17], subgroups of $\mathrm{U}(n)$ with this property are completely described (see also (4)): up to conjugacy, they are just $\mathrm{U}(n)$ itself, $\mathrm{SU}(n)$, and, for $n > 2$ even, the symplectic group $\mathrm{Sp}(n/2)$ and $U(1) \times \mathrm{Sp}(n/2)$. In particular, for n even, it is possible to have approximate/exact controllability of (9) without having approximate/exact controllability of (10).

References

[1] Riccardo Adami and Ugo Boscain. Controllability of the Schrödinger equation via intersection of eigenvalues. In *Proceedings of the 44th IEEE Conference on Decision and Control*, pages 1080–1085, 2005.

[2] Francesca Albertini and Domenico D'Alessandro. Notions of controllability for bilinear multilevel quantum systems. *IEEE Trans. Automat. Control*, 48(8):1399–1403, 2003.

[3] J. M. Ball, J. E. Marsden, and M. Slemrod. Controllability for distributed bilinear systems. *SIAM J. Control Optim.*, 20(4):575–597, 1982.

[4] Asim O. Barut and Ryszard Rączka. *Theory of group representations and applications.* World Scientific Publishing Co., Singapore, second edition, 1986.

[5] Karine Beauchard. Local controllability of a 1-D Schrödinger equation. *J. Math. Pures Appl. (9)*, 84(7):851–956, 2005.

[6] Karine Beauchard and Jean-Michel Coron. Controllability of a quantum particle in a moving potential well. *J. Funct. Anal.*, 232(2):328–389, 2006.

[7] Karine Beauchard and Camille Laurent. Local controllability of 1D linear and nonlinear Schrödinger equations with bilinear control. *J. Math. Pures Appl.*, 94(5):520–554, 2010.

[8] Karine Beauchard and Vahagn Nersesyan. Semi-global weak stabilization of bilinear Schrödinger equations. *C. R. Math. Acad. Sci. Paris*, 348(19-20):1073–1078, 2010.

[9] M. Born and V. Fock. Beweis des adiabatensatzes. *Zeitschrift für Physik A Hadrons and Nuclei*, 51(3–4):165–180, 1928.

[10] U. Boscain, M. Caponigro, T. Chambrion, and M. Sigalotti. A weak spectral condition for the controllability of the bilinear Schrödinger equation with application to the control of a rotating planar molecule. *Comm. Math. Phys.*, 311(2):423–455, 2012.

[11] Ugo Boscain, Marco Caponigro, and Mario Sigalotti. Multi-input schrdinger equation: controllability, tracking, and application to the quantum angular momentum. To appear on Journal of differential equations.

[12] Ugo Boscain, Francesca Chittaro, Paolo Mason, and Mario Sigalotti. Adiabatic control of the Schroedinger equation via conical intersections of the eigenvalues. *IEEE Trans. Automat. Control*, 57(8):1970–1983, 2012.

[13] N. Boussaid, M. Caponigro, and T. Chambrion. Weakly-coupled systems in quantum control. To appear on IEEE Trans. Automat. Control.

[14] Thomas Chambrion. Periodic excitations of bilinear quantum systems. *Automatica*, 48(9):2040–2046, September 2012.

[15] Thomas Chambrion, Paolo Mason, Mario Sigalotti, and Ugo Boscain. Controllability of the discrete-spectrum Schrödinger equation driven by an external field. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 26(1):329–349, 2009.

[16] F. Chittaro and P. Mason. Adiabatic control of quantum control systems with three inputs. Preprint.

[17] Domenico D'Alessandro. *Introduction to quantum control and dynamics.* Applied Mathematics and Nonlinear Science Series. Boca Raton, FL: Chapman, Hall/CRC., 2008.

[18] Jacques Dixmier. *Les C^*-algèbres et leurs représentations*. Cahiers Scientifiques, Fasc. XXIX. Gauthier-Villars & Cie, Éditeur-Imprimeur, Paris, 1964.

[19] R. El Assoudi, J. P. Gauthier, and I. A. K. Kupka. On subsemigroups of semisimple Lie groups. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 13(1):117–133, 1996.

[20] S. Guérin and H.R. Jauslin. Control of quantum dynamics by laser pulses: Adiabatic Floquet theory. In *Advances in Chemical Physics*, volume 125, 2003.

[21] Reinhard Illner, Horst Lange, and Holger Teismann. Limitations on the control of Schrödinger equations. *ESAIM Control Optim. Calc. Var.*, 12(4):615–635, 2006.

[22] V. Jurdjevic and I. Kupka. Control systems on semisimple Lie groups and their homogeneous spaces. *Ann. Inst. Fourier (Grenoble)*, 31(4):vi, 151–179, 1981.

[23] Mazyar Mirrahimi. Lyapunov control of a quantum particle in a decaying potential. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 26(5):1743–1765, 2009.

[24] Vahagn Nersesyan. Global approximate controllability for Schrödinger equation in higher Sobolev norms and applications. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 27(3):901–915, 2010.

[25] Vahagn Nersesyan and Hayk Nersisyan. Global exact controllability in infinite time of Schrödinger equation. *J. Math. Pures Appl. (9)*, 97(4):295–317, 2012.

[26] A. Pazy. *Semigroups Of Linear Operators And Applications To Partial Differential Equations*. Applied Mathematical Sciences Series, Springer-Verlag, New York, 1983.

[27] Franz Rellich. *Perturbation theory of eigenvalue problems*. Assisted by J. Berkowitz. With a preface by Jacob T. Schwartz. Gordon and Breach Science Publishers, New York, 1969.

[28] P. A. Smith. Everywhere dense subgroups of Lie groups. *Bull. Amer. Math. Soc.*, 48:309–312, 1942.

[29] S. Teufel. *Adiabatic perturbation theory in quantum dynamics*, volume 1821 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin, 2003.

[30] Gabriel Turinici. On the controllability of bilinear quantum systems. In M. Defranceschi and C. Le Bris, editors, *Mathematical models and methods for ab initio Quantum Chemistry*, volume 74 of *Lecture Notes in Chemistry*. Springer, 2000.

[31] J. von Neumann and E. Wigner. überdas Verhalten von Eigenwerten bei Adiabatischen Prozessen. *Z. Phys.*, 30:467–470, 1929.

[32] André Weil. *L'intégration dans les groupes topologiques et ses applications*. Actual. Sci. Ind., no. 869. Hermann et Cie., Paris, 1940. [This book has been republished by the author at Princeton, N. J., 1941.].