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On the controllability in projections for linear quantum systems

Nabile Boussaïd, Marco Caponigro, and Thomas Chambrion

Abstract We present sufficient conditions for the exact controllability in projection of the linear Schrödinger equations in the case where the spectrum of the free Hamiltonian is pure point. We consider the general case in which the Hamiltonian may be nonlinear with respect to the control. The controllability result applies, in particular, to Schrödinger equations with a polarizability term.

1 Introduction

1.1 Control of linear quantum systems

In a complex Hilbert space \mathcal{H} with hermitian product $\langle \cdot, \cdot \rangle$, we consider the linear Schrödinger equation

$$\begin{cases} \partial_t \psi = -iH(u)\psi, \\ \psi(0) = \psi_0, \end{cases} \quad (\text{LS})$$

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where $\psi(t)$ is the state of the system at time t , $\psi_0 \in \mathcal{H}$ is the given initial datum, $H(u)$ is a self-adjoint linear operator in \mathcal{H} depending on a real-valued function u . The operator $H(u)$ is usually called *Hamiltonian*. The parameter u is a control representing our ability to influence the system and accounts for an external, appropriately shaped, electromagnetic field. Equation (LS) models many quantum systems under the assumptions that the interaction with the external environment (i.e. decoherence) is negligible and that the control u can be treated as a classical field.

The aim of quantum control is to design a (open-loop) *control* $u : [0, T] \rightarrow \mathbf{R}$ such that the solution of (LS) satisfies desirable properties, for instance: the final point $\psi(T)$ is close, in some sense, to a given target.

The controllability of system (LS) is a well-established topic when the state space \mathcal{H} is finite-dimensional, i.e. when the quantum mechanical system under consideration can be adequately approximated as a system having a finite number of energy levels, see, for instance [D'A08] or [BCS17] and references therein. Many controllability results in the finite-dimensional framework rely on general controllability methods for left-invariant control systems on compact Lie groups ([JS72, JK81, GB82, EAGK96]).

When the state space \mathcal{H} is infinite-dimensional the situation is complicated by the subtleties of the evolution in Banach spaces and the consequent fragmental nature of controllability theory for PDEs. For this reason, most of the current literature focuses on closed (i.e., conservative) systems and on the dipolar approximation, i.e. when the Hamiltonian $H(u) = H_0 + uH_1$ is linear with respect to the control. For this kind of, so called, bilinear systems, one of the first known results is a negative one: indeed when H_1 is a bounded operator the bilinear Schrödinger equation is not exactly controllable, namely the attainable set has empty interior as a meagre set [BMS82, Tur00]. The obstruction to exact controllability holds even when considering very large class of controls [BCC20], as for instance L^1 controls [BCC19b] or Radon measures [BCC19a]. In certain cases, it is possible to prove exact controllability for the potential well in suitable functional spaces on a real interval (see [BC06, BL10, MN15]). The results extend to a system describing a particle confined on a radially symmetric 2D domains [Moy17]. However in higher dimension and for more general systems the exact description of the reachable set seems a difficult task. The literature hence focuses on weaker controllability properties. Approximate controllability results have been obtained with different techniques: adiabatic control ([AB05, BCMS12]), Lyapunov methods ([Mir09, Ner09, Ner10, NN12]), and Lie-algebraic methods ([CMSB09, BBR10, BCCS12, Cha12, BCS14, KZSH14, PS15, CS18]).

Although the dipolar approximation usually gives excellent results for low intensity fields, it is sometimes necessary, when dealing with stronger fields, to consider a better approximation of $H(u)$ involving more terms of its expansion in u . In the control of orientation of a rotating HCN molecule, for instance, the model involves a quadratic term [DBA⁺99, DAB99] call polarizability term, and $H(u) = H_0 + uH_1 + u^2H_2$. This question has

been tackled with Lyapunov methods for finite dimensional approximations in [CGLT09, GLT09] and in [Mor13] for the infinite dimensional version for a class of regular systems.

In this paper we study the general case when the Hamiltonian $H(u)$ is nonlinear in the control. We prove that, under generic condition, it is possible to control (LS) approximately in a very strong sense. Theorem 1 states that for every dimension n of the Galerkin approximation and every initial and target condition, there exists a control steering in finite time the infinite-dimensional control system from the initial condition to a final state having the same first n coordinates as the target (as long as the remaining coordinates do not vanish simultaneously). In quantum systems, this problem is quite natural, since in physical experiments one can measure with accuracy only the low-energy states. From the mathematical viewpoint, this kind of study is particularly interesting since the regularity of system, needed in order to define the solution, is, in fact, an obstacle to exact controllability (see, for instance [BCC20]). Exact controllability in projection has been introduced and proved using geometric techniques based on controllability result for the Galerkin approximations in [AS06] for the 2D Euler and Navier–Stokes equations (see [Shi07] for the 3D case).

Our approach is based on Lie-algebraic techniques. Lie-algebraic methods usually provide intrinsic, robust, and sometimes explicit control results for quantum mechanical systems. For these reasons, these techniques represent the main tool in the controllability of finite dimensional quantum systems. In the infinite-dimensional case, however, even the extension of the notion of Lie-bracket to infinite dimensional operators is not trivial. While there are Lie-algebraic based control results in the presence of bounded operator [BB14] when dealing with unbounded operators the notion of Lie algebra is not well-defined in general. The Lie–Galerkin condition developed in [BCS14] for bilinear systems combines a Lie-algebraic finite-dimensional condition with the Galerkin method to find sufficient conditions for approximate controllability. Indeed the underlying idea of this Lie–Galerkin technique is to choose a suitable sequence of Galerkin approximations, then to use finite-dimensional geometric control tools in order to prove strong controllability (in some suitable sense) for each Galerkin approximation, and finally to show how these controllability properties provide approximate controllability for the original infinite-dimensional system. This condition has been used to prove exact controllability in projections with piecewise constant controls for the bilinear Schrödinger equation [CS18]. In this paper we extend the notion of Lie–Galerkin condition to infinite dimensional linear systems and prove exact controllability in projections for (LS) by means of piecewise constant controls taking only two values. The main tool used in the proof is the continuity of the propagators of bilinear systems. This fact, combined with the approximation results of Section 2.1 allows to infer controllability of the bilinear system with “bang-bang” controls, i.e. piecewise constant controls

taking only two values allows, which in turns implies approximate controllability for (LS).

The proof of the main result, in Section 3 is based on a refined analysis on the controllability of a bilinear system presented in Section 2. The result is then applied to the controllability of systems with a polarizability term in Section 4.

1.2 Framework and definition of propagators

The well-posedness of system (LS) when $H(u)$ is an unbounded operator on a infinite-dimensional space \mathcal{H} is, in general, not trivial. In order to define the solution we assume the following condition.

Assumption 1 *The operators $H(0)$ and $H(1)$ are self-adjoint. $H(0)$ has pure point spectrum with an associated orthonormal basis Φ of eigenvectors and $H(1) - H(0)$ is bounded.*

We denote by $\Phi = (\phi_k)_{k \in \mathbf{N}}$ the complete orthonormal family of eigenvectors of $H(0)$ and by $(\lambda_k)_{k \in \mathbf{N}}$ the associated eigenvalues (that is, for all k in \mathbf{N} , $H(0)\phi_k = \lambda_k\phi_k$).

Under Assumption 1 it is possible to define the propagator \mathcal{Y}^u of $-iH(u)$ and, hence, the solution of (LS) associated with a piecewise constant control $u : [0, T] \rightarrow \{0, 1\}$. Indeed, since $H(1) - H(0)$ is bounded the domain $D(H(1))$ of the self-adjoint operator $H(1)$ contains the domain $D(H(0))$ and, in particular, every eigenvector $\phi \in \Phi$. Therefore, if

$$u = \sum_{j=1}^m u_j \mathbf{1}_{[t_{j-1}, t_j]}, \quad u_j = 0, 1,$$

for $0 = t_0 < t_1 < \dots < t_m$, then, one can define the associated propagator as

$$\mathcal{Y}_t^u = e^{-i(t-t_k)H(u_k)} \circ e^{-i(t_k-t_{k-1})H(u_{k-1})} \circ \dots \circ e^{-it_1H(u_1)}, \quad (1)$$

where $t_k \leq t < t_{k+1}$.

1.3 Notation

For $N \in \mathbf{N}$, $\mathbb{M}_N(\mathbb{C})$ is the set of $N \times N$ matrices with entries in \mathbb{C} . The identity matrix of order N is I_N . The group of special unitary matrices $SU(N)$ is

$$SU(N) = \{M \in \mathbb{M}_N(\mathbb{C}) \mid \overline{M}^T M = I_N \text{ and } \det M = 1\},$$

which is a Lie group whose Lie algebra is

$$\mathfrak{su}(N) = \{M \in \mathbb{M}_N(\mathbf{C}) \mid \overline{M}^T + M = 0 \text{ and } \text{Tr}M = 0\}.$$

This Lie algebra, seen as a real linear space, has dimension $N^2 - 1$. We denote by $U(\mathcal{H})$ the set of unitary operators on \mathcal{H} .

1.4 Main result

For every n in \mathbf{N} , we define

$$\mathcal{L}_n^\Phi = \text{span}\{\phi_1, \dots, \phi_n\},$$

and the projection of \mathcal{H} on \mathcal{L}_n^Φ , namely

$$\begin{aligned} \Pi_n^\Phi : \mathcal{H} &\rightarrow \mathcal{H} \\ \psi &\mapsto \sum_{j=1}^n \langle \phi_j, \psi \rangle \phi_j. \end{aligned} \quad (2)$$

The compression of a linear operator Q on \mathcal{H} , with $\mathcal{L}_n^\Phi \subset D(Q)$, is denoted by

$$Q^{(\Phi, n)} = \Pi_n^\Phi Q \upharpoonright_{\mathcal{L}_n^\Phi}.$$

Remark 1 The projections in (2) and, as a consequence, the compressions of operators strongly depend on the basis Φ . However, for the sake of readability we drop the mention to Φ .

Remark 2 When it does not create ambiguities we identify $\text{Im}(\Pi_n) = \mathcal{L}_n^\Phi$ with \mathbb{C}^n . Given a linear operator Q on \mathcal{H} we identify the linear operator $Q^{(n)} = \Pi_n Q \Pi_n$ preserving $\text{span}\{\phi_1, \dots, \phi_n\}$ with its $n \times n$ complex matrix representation with respect to the basis (ϕ_1, \dots, ϕ_n) .

Define

$$H_0^{(n)} = \Pi_n H(0) \Pi_n \quad \text{and} \quad H_1^{(n)} = \Pi_n H(1) \Pi_n.$$

Let us introduce the set Σ_n of spectral gaps associated with the first n eigenvalues of $H(0)$ as

$$\Sigma_n = \{|\lambda_l - \lambda_k| \mid l, k = 1, \dots, n\}.$$

For every $\sigma \geq 0$, every $m \in \mathbf{N}$, and every $m \times m$ matrix M , let

$$\mathcal{E}_\sigma(M) = (M_{l,k} \delta_{\sigma, |\lambda_l - \lambda_k|})_{l,k=1}^m,$$

where $\delta_{\cdot, \cdot}$ denotes the Kronecker symbol. The $n \times n$ matrix $\mathcal{E}_\sigma(H_1^{(n)})$, corresponds then to the “selection” in $H_1^{(n)}$ of the spectral gap σ : the (l, k) -elements such that $|\lambda_l - \lambda_k| \neq \sigma$ are set to 0.

Define

$$\begin{aligned} \Xi_n = \{ \sigma \in \Sigma_n \mid (H_1)_{k,l} \delta_{\sigma, |\lambda_l - \lambda_k|} = 0, \\ \text{for every } k = 1, \dots, n \text{ and } l > n \}. \end{aligned} \quad (3)$$

The set Ξ_n can be seen as follows: If $\sigma \in \Xi_n$ then the matrix $M = \mathcal{E}_\sigma(H_1^{(n)})$ is such that

$$\mathcal{E}_\sigma(H_1^{(N)}) = \begin{pmatrix} M & 0 \\ 0 & * \end{pmatrix} \text{ for every } N > n,$$

or, which is equivalent,

$$[\Pi_n, \mathcal{E}_\sigma(H_1^{(N)})] = 0 \quad \text{for every } N > n. \quad (4)$$

In particular $\text{span}\{\phi_1, \dots, \phi_n\}$ is invariant for the evolution of $\mathcal{E}_\sigma(H_1^{(N)})$ for every $N > n$. The spectral gaps $\sigma \in \Xi_n$ are, therefore, those for which the selections $\mathcal{E}_\sigma(H_1^{(n)})$ define finite dimensional dynamics of order n decoupled from the infinite dimensional evolution.

The main assumption of this paper, introduced in the definition below, is the extension of the Lie–Galerkin condition [BCS14] to system (LS).

Definition 1 For every $n \in \mathbf{N}$ define

$$\mathcal{M}_n = \{iH_0^{(n)}\} \cup \{i\mathcal{E}_\sigma(H_1^{(n)}) \mid \sigma \in \Xi_n\}.$$

We say that the *Lie–Galerkin condition* holds for system (LS) if for every $n_0 \in \mathbf{N}$ there exists $n > n_0$ such that $0 \in \Xi_n$ and

$$\text{Lie}\mathcal{M}_n \supseteq \mathfrak{su}(n). \quad (5)$$

We can now state the main result of exact controllability in projections.

Theorem 1 *Let system (LS) satisfy Assumption 1 and the Lie–Galerkin condition. Then, for every $N \in \mathbf{N}$, $\psi_0, \psi_1 \in \text{span}(\Phi)$, with $\|\psi_0\| = \|\psi_1\| = 1$ and $\|\Pi_N(\psi_1)\| < 1$ there exists a piecewise constant control $u : [0, T] \rightarrow \{0, 1\}$ such that*

$$\Pi_N(\mathcal{Y}_T^u(\psi_0)) = \Pi_N(\psi_1).$$

2 The Bilinear Schrödinger Equation

In this section we focus on the case $H(u) = iA + uiB$, that is when H is linear with respect to the control u . The corresponding system is usually called bilinear because it is linear with respect to the state and with respect to the control. We aim at proving that the bilinear case is exactly controllable in projection by means of bang-bang controls, i.e. piecewise constant controls

taking value 0 and 1. We will prove in Section 3 that this result implies Theorem 1.

Consider the system

$$\begin{cases} \partial_t \psi = A\psi + u(t)B\psi, \\ \psi(0) = \phi_0 \in \mathcal{H}, \end{cases} \quad (\text{BSE})$$

satisfying the following assumption.

Assumption 2 *The pair of operators (A, B) is such that*

- *The skew-adjoint operator A has pure point spectrum with an associated complete orthonormal basis Ψ of eigenvectors ;*
- *The operator B is skew-symmetric and bounded.*

By Assumption 2 for every $u \in \mathbf{R}$, $A + uB$ defined on $\text{Span}(\Psi) \subset D(A)$ is essentially skew-adjoint. We can, therefore, define the solution of (BSE) associated with a piecewise constant control

$$u = \sum_{j=1}^m u_j \mathbf{1}_{[t_{j-1}, t_j)}$$

with $u_j \in [0, \delta]$, for $j = 1, \dots, m$, $0 = t_0 < t_1 < \dots < t_m$ as the concatenation

$$\Upsilon_t^u = e^{(t-t_k)(A+u_k B)} \circ e^{(t_k-t_{k-1})(A+u_{k-1} B)} \circ \dots \circ e^{t_1(A+u_1 B)},$$

where $t_k \leq t < t_{k+1}$. In analogy with the definition of solution associated with a bang-bang control (1).

Remark 3 One of the main advantages of dealing with bilinear control systems is that, when the control operator B is bounded on \mathcal{H} , then the propagator Υ of the system is continuous with respect to the control (see [BMS82, BCC20]) in the sense: If $(u_k)_{k \in \mathbf{N}}$ is a sequence of piecewise constant controls, $u_n : [0, T] \rightarrow [0, \delta]$, converging in $L^1([0, T])$ to a piecewise constant control $u : [0, T] \rightarrow [0, \delta]$ then

$$\Upsilon_t^{u_k} \psi \rightarrow \Upsilon_t^u \psi \quad \text{as } k \rightarrow \infty,$$

uniformly in $t \in [0, T]$ for every $\psi \in \Psi$.

We say that system (BSE) satisfies the Lie–Galerkin condition if the system (LS) with $H(0) = iA$ and $H(1)$ as the closure of $i(A + B)$ satisfies the Lie–Galerkin condition.

Theorem 2 *Let (A, B) satisfy Assumption 2 and let system (BSE) satisfy the Lie–Galerkin condition. Then, for every $N \in \mathbf{N}$, $\psi_0, \psi_1 \in \text{span}(\Phi)$, with $\|\psi_0\| = \|\psi_1\| = 1$ and $\|\Pi_N(\psi_1)\| < 1$ there exists a piecewise constant control $u : [0, T] \rightarrow \{0, 1\}$ such that*

$$\Pi_N(\Upsilon_T^u(\psi_0)) = \Pi_N(\psi_1).$$

2.1 Bang-bang approximation of piecewise constant functions

In this section we prove that it is possible to approximate the propagator of a particular finite dimensional system associated with piecewise constant controls with the one associated with suitable controls taking only two values. As mentioned, this approximation, together with the continuity of the propagators is crucial in the extension of the controllability results from bilinear systems to linear ones.

Lemma 1 *Let $u : [0, T] \rightarrow [0, \delta]$, $\delta > 0$ be a piecewise constant function and let $a > \delta$. There exists a sequence $(w_k)_{k \in \mathbf{N}}$ of piecewise constant functions $w_k : [0, T] \rightarrow \{0, a\}$ uniformly bounded in $L^1([0, T], \mathbf{R})$ by $\|u\|_{L^1}$, and continuously depending on u for the L^1 topology, such that*

$$\int_0^t w_k(s) ds \rightarrow \int_0^t u(s) ds, \quad \text{as } k \rightarrow \infty,$$

uniformly for t in $[0, T]$.

Proof We prove the convergence on $[0, T]$. Lemma 1 follows on $[0, T]$ by continuity. Let k in \mathbf{N} and let us divide the interval $[0, T]$ in k intervals $I_h := [hT/k, (h+1)T/k)$ for $h = 0, \dots, k-1$. Let

$$U_h = \int_{I_h} u(s) ds.$$

We define the piecewise constant function $w_k : [0, T] \rightarrow \{0, a\}$ as follows

$$w_k(t) = \begin{cases} 0 & \text{for } t \in \left[\frac{hT}{k}, \frac{(h+1)T}{k} - \frac{U_h}{a} \right), \\ a & \text{for } t \in \left[\frac{(h+1)T}{k} - \frac{U_h}{a}, \frac{(h+1)T}{k} \right), \\ 0 & \text{for } t \notin I_h. \end{cases}$$

Hence, for every $h = 0, \dots, k-1$, we have

$$\int_{I_h} w_k(s) ds = U_h = \int_{I_h} u(s) ds.$$

Now for every $t \in [0, T]$ let h_t be the smallest integer such that $(h_t+1)T \geq tk$, then

$$\begin{aligned} \left| \int_0^t w_k(s) ds - \int_0^t u(s) ds \right| &= \left| \int_{\frac{h_t T}{k}}^t (w_k(s) - u(s)) ds \right| \\ &\leq (\delta + a) \frac{T}{k}. \end{aligned}$$

Finally, notice that

$$\begin{aligned} \int_0^T |w_k(s)| ds &= \sum_{h=0}^{k-1} \int_{I_h} |w_k(s)| ds \\ &= \sum_{h=0}^{k-1} \left| \int_{I_h} u(s) ds \right| \\ &\leq \sum_{h=0}^{k-1} \int_{I_h} |u(s)| ds = \int_0^T |u(s)| ds, \end{aligned}$$

which ensures the boundedness in L^1 and concludes the proof. \square

Let $\Theta(t) = e^{-tA} B e^{tA}$. For every $N \in \mathbf{N}$ consider

$$\Theta^{(N)}(t) = \Pi_N \Theta(t) \Pi_N = e^{-tA^{(N)}} B^{(N)} e^{tA^{(N)}}.$$

Then, for every piecewise constant function v let us denote by $X_{t,s}^{(N)}(v)$, the propagator of $v(\cdot) \Theta^{(N)}(\cdot)$.

Lemma 2 *Let $u : [0, T] \rightarrow [0, \delta]$, $\delta > 0$ be a piecewise constant function and let $a > \delta$. There exists a sequence $(w_k)_{k \in \mathbf{N}}$ of piecewise constant functions $w_k : [0, T] \rightarrow \{0, a\}$ uniformly bounded in $L^1([0, T], \mathbf{R})$ by $\|u\|_{L^1}$, such that, for every $N \in \mathbf{N}$,*

$$X_{t,s}^{(N)}(w_k) \rightarrow X_{t,s}^{(N)}(u), \quad \text{as } k \rightarrow \infty,$$

uniformly for s, t in $[0, T]$.

Proof Let $(w_k)_{K \in \mathbf{N}}$ be the sequence of controls whose existence is given by Lemma 1. For every $N \in \mathbf{N}$ and for every $t > 0$, by integration by parts,

$$\begin{aligned} &\left\| \int_0^t u(s) \Theta^{(N)}(s) ds - \int_0^t w_k(s) \Theta^{(N)}(s) ds \right\| \\ &\leq \left\| \left(\int_{\tau=0}^t (u(\tau) - w_k(\tau)) d\tau \right) \Theta^{(N)}(t) \right\| \\ &\quad + \left\| \int_{s=0}^t \left(\int_{\tau=0}^s (u(\tau) - w_k(\tau)) d\tau \right) e^{-sA^{(N)}} [B^{(N)}, A^{(N)}] e^{sA^{(N)}} ds \right\|. \end{aligned}$$

Hence, by Lebesgue Dominated Convergence Theorem, since $(\int_0^t w_k(s) ds)_{k \in \mathbf{N}}$ converges to $\int_0^t u(s) ds$ uniformly for t in $[0, T]$, then

$$\int_0^t w_k(s) \Theta^{(N)}(s) ds \rightarrow \int_0^t u(s) \Theta^{(N)}(s) ds, \quad \text{as } k \rightarrow \infty,$$

which, in turn, implies (see, for instance, [AS04, Lemma 8.2]) that

$$X_{t,s}^{(N)}(w_k) \rightarrow X_{t,s}^{(N)}(u), \quad \text{as } k \rightarrow \infty,$$

uniformly for s, t in $[0, T]$. \square

Lemma 3 *Let (A, B) satisfy Assumption 2. Let $u : \mathbf{R} \rightarrow \mathbf{R}$ be a piecewise constant function and $\phi \in \mathcal{H}$. Then*

$$\frac{d}{dt} \langle \psi, e^{-tA} \Upsilon_t^u(\phi) \rangle = -\langle u(t) \Theta(t) \psi, e^{-tA} \Upsilon_t^u(\phi) \rangle,$$

for every $\psi \in \Psi$ and for almost every $t \in \mathbf{R}$.

Proof Let

$$y(t) = e^{-tA} \Upsilon_t^u(\psi).$$

Let $i\lambda$ be the eigenvalue of A associated with $\psi \in \Psi$, namely $A\psi = i\lambda\psi$. Then

$$\begin{aligned} \frac{d}{dt} \langle \psi, y(t) \rangle &= \frac{d}{dt} e^{it\lambda} \langle \psi, \Upsilon_t^u(\phi) \rangle \\ &= i\lambda e^{it\lambda} \langle \psi, \Upsilon_t^u(\phi) \rangle + e^{it\lambda} \frac{d}{dt} \langle \psi, \Upsilon_t^u(\phi) \rangle \\ &= i\lambda e^{it\lambda} \langle \psi, \Upsilon_t^u(\phi) \rangle - e^{it\lambda} \langle (A + u(t)B) \psi, \Upsilon_t^u(\phi) \rangle \\ &= -e^{it\lambda} \langle u(t)B \psi, e^{tA} y(t) \rangle \\ &= -\langle u(t) \Theta(t) \psi, y(t) \rangle, \end{aligned}$$

for almost every $t \in \mathbf{R}$. \square

2.2 Tracking of admissible matrices

Recall that system (BSE) satisfies the Lie–Galerkin condition. For $n_0 \in \mathbf{N}$ let $n > n_0$ be given by the Lie–Galerkin condition. Consider the collection of matrices

$$\begin{aligned} \mathcal{W}_n &= \left\{ A^{(n)} \right\} \cup \left\{ \mathcal{E}_0(B^{(n)}) \right\} \\ &\cup \left\{ \mathcal{E}_0(B^{(n)}) + \nu \mathcal{E}_\sigma(B^{(n)}) \mid \sigma \in \Xi_n, \sigma \neq 0, \nu \in (-1/2, 1/2) \right\}, \end{aligned}$$

where Ξ_n is defined in (3). Notice that for every $\sigma \in \Xi_n$ (4) holds true for the operator $\mathcal{E}_\sigma(B^{(N)})$, namely, $[\Pi_n, \mathcal{E}_\sigma(B^{(N)})] = 0$ for every $N > n$ and for every σ in Ξ_n .

Proposition 1 *Let (A, B) satisfy Assumption 2. Let $q \in \mathbf{N}$, $a, b \in \mathbf{R}$ with $0 < a < b$, and $M_1, \dots, M_q \in \mathcal{W}_n$. For every $\varepsilon > 0$ and $\tau_1, \dots, \tau_q \in [a, b]$ there exist $w : [0, T] \rightarrow \{0, 1\}$ piecewise constant and $\gamma \geq 0$ such that*

$$\| \Pi_n \Upsilon_T^w - e^{\tau_q M_q} \circ \dots \circ e^{\tau_1 M_1} \|_{L(\Pi_n(\mathcal{H}), \mathcal{H})} < \varepsilon.$$

Moreover, w can be taken continuously depending on $\tau_1, \dots, \tau_q \in [a, b]$.

Proof Following [CS18, Proposition 4.1] we have, for every $\eta, \delta > 0$, that there exist $u : [0, T_u] \rightarrow [0, \delta]$ piecewise constant and $\gamma \geq 0$ such that

$$\| \Upsilon_{T_u}^u - e^{\gamma A} \circ e^{\tau_q M_q} \circ \dots \circ e^{\tau_1 M_1} \|_{L(\Pi_n(\mathcal{H}), \mathcal{H})} < \eta, \quad (6)$$

where u depends continuously on $\tau_1, \dots, \tau_q \in [a, b]$ and γ is independent on $\tau_1, \dots, \tau_q \in [a, b]$. Moreover the L^1 -norm of u is independent on η (see [CS18, Section 3.1] and [Cha12]). Let $\delta < 1$, then there exists $K > 0$ such that every u in (6) satisfies $\|u\|_{L^1} \leq K$.

Let $N > n$ be such that

$$\| \Pi_n B (I - \Pi_N) \| \leq \frac{\varepsilon}{10K}.$$

The existence of such a N is guaranteed by the compactness of $\Pi_n B$ (bounded with finite rank) using the fact that $\Psi \subset D(B)$ and that B is skew-symmetric. Then, call $\xi = \|\Pi_n B (I - \Pi_N)\|$, and consider the control u associated with $\eta = \varepsilon / (10 \max\{1, K\xi\})$ in (6).

Let $(w_k)_{k \in \mathbf{N}}$ be a piecewise constant functions $w_k : [0, T_u] \rightarrow \{0, 1\}$ associated with (and continuously depending on) u , the existence of which is given by Lemma 1. For every $\psi \in \Pi_n(\mathcal{H})$ with norm 1, let

$$y(t) = e^{-tA} \Upsilon_t^u(\psi) \quad \text{and} \quad y_k(t) = e^{-tA} \Upsilon_t^{w_k}(\psi).$$

We deduce from Lemma 3 and from variation of constants formula that for any $\psi \in \mathcal{L}_N$

$$\begin{aligned} \Pi_n e^{-tA} \Upsilon_t^v \psi &= \Pi_n X_{t,0}^{(N)}(v)(\psi) \\ &\quad + \Pi_n \int_0^t X_{t,s}^{(N)}(v) \Pi_N v(s) \Theta(s) (I - \Pi_N) e^{-sA} \Upsilon_s^v \psi ds. \end{aligned}$$

Hence

$$\begin{aligned} \| \Pi_n (y_k(t) - y(t)) \| &\leq \| \Pi_n (X_{t,0}^{(N)}(u) - X_{t,0}^{(N)}(w_k)) \psi \| \\ &\quad + \| \Pi_n \int_{s=0}^t (X_{t,s}^{(N)}(w_k) - X_{t,s}^{(N)}(u)) \Pi_N w_k(s) \Theta(s) (I - \Pi_N) y_k(s) ds \| \\ &\quad + \| \Pi_n \int_{s=0}^t X_{t,s}^{(N)}(u) \Pi_N \Theta(s) (I - \Pi_N) (u(s)y(s) - w_k(s)y_k(s)) ds \|. \end{aligned}$$

Now

$$\begin{aligned}
& \int_{s=0}^t \Pi_n X_{t,s}^{(N)}(u) \Pi_n \Theta(s) (I - \Pi_N) (u(s)y(s) - w_k(s)y_k(s)) ds = \\
& = \int_{s=0}^t X_{t,s}^{(N)}(u) \Pi_n \Theta(s) (I - \Pi_N) (u(s)y(s) - w_k(s)y_k(s)) ds \\
& \quad - \int_{s=0}^t \left[X_{t,s}^{(N)}(u), \Pi_n \right] \Pi_n \Theta(s) (I - \Pi_N) (u(s)y(s) - w_k(s)y_k(s)) ds.
\end{aligned}$$

Notice that by (6) and for the definition of the set \mathcal{W}_n and of Ξ_n in (3) we have that

$$\sup_{s < t} \left\| \left[X_{t,s}^{(N)}(u), \Pi_n \right] \right\| < \eta = \varepsilon / (10 \max\{1, K\xi\}),$$

indeed $X_{t,s}^{(N)}(u)$ is “close” (see also [CS18, (3.8)]) to the composition of exponential of matrices in \mathcal{W}_n satisfying (4).

Then, since $\Pi_n \Theta(t) (I - \Pi_N)$ is an operator uniformly bounded with respect to $t \in \mathbf{R}$,

$$\begin{aligned}
& \left\| \Pi_n \int_{s=0}^t X_{t,s}^{(N)}(u) \Pi_n \Theta(s) (I - \Pi_N) (u(s)y(s) - w_k(s)y_k(s)) ds \right\| \\
& \leq \left\| \Pi_n B (I - \Pi_N) \right\| (\|u\|_{L^1} + \|w_k\|_{L^1}) \\
& \quad + \sup_{s < t} \left\| \left[X_{t,s}^{(N)}(u), \Pi_n \right] \right\| \left\| \Pi_n B (I - \Pi_N) \right\| (\|u\|_{L^1} + \|w_k\|_{L^1}) \\
& \leq \frac{\varepsilon}{5} + \frac{\varepsilon}{5}.
\end{aligned}$$

Finally consider $k \in \mathbf{N}$ sufficiently large such that

$$\left\| \Pi_n \left(X_{t,0}^{(N)}(u) - X_{t,0}^{(N)}(w_k) \right) \psi \right\| < \frac{\varepsilon}{5 \max\{K\xi, 1\}}.$$

Hence

$$\left\| \Pi_n \int_{s=0}^t \left(X_{t,s}^{(N)}(w_k) - X_{t,s}^{(N)}(u) \right) \Pi_n w_k(s) \Theta(s) (I - \Pi_N) y_k(s) ds \right\| \leq \frac{\varepsilon}{5}.$$

In conclusion

$$\left\| \Pi_n (y_k(t) - y(t)) \right\| < \frac{4}{5} \varepsilon.$$

uniformly with respect to $t \in [0, T_u]$. Since e^{tA} is unitary and ψ arbitrary we have that

$$\left\| \Pi_n (\Upsilon_t^{w_k} - \Upsilon_t^u) \Pi_n \right\| < \frac{4}{5} \varepsilon.$$

Hence

$$\begin{aligned}
& \|\Pi_n \Upsilon_{T_u}^w - e^{\gamma A} \circ e^{\tau_k M_k} \circ \dots \circ e^{\tau_1 M_1}\|_{L(\Pi_n(\mathcal{H}), \mathcal{H})} \leq \\
& \leq \|\Pi_n(\Upsilon_{T_u}^{w_k} - \Upsilon_{T_u}^u)\|_{L(\Pi_n(\mathcal{H}), \mathcal{H})} + \\
& \quad + \|\Pi_n \Upsilon_{T_u}^u - e^{\gamma A} \circ e^{\tau_q M_q} \circ \dots \circ e^{\tau_1 M_1}\|_{L(\Pi_n(\mathcal{H}), \mathcal{H})} \\
& \leq \frac{4}{5}\varepsilon + \frac{1}{5}\varepsilon = \varepsilon.
\end{aligned}$$

By Poincaré Recurrence Theorem (see [CS18, Lemma 4.2]) it is then sufficient to consider as control w the concatenation of the control w_k on $[0, T_u]$ with a function constantly equal to 0 for a certain time $T - T_u$. \square

2.3 A degree argument

Lemma 4 *Let $X \subset \mathbf{R}^n$ be open and bounded and let $F \in C(X, \mathbf{R}^n)$ be a homeomorphism between X and $F(X)$. Let $G \in C(X, \mathbf{R}^n)$ and $\varepsilon := \max_{x \in \partial X} |F(x) - G(x)|$. If y_0 is in $F(X)$ and such that $\varepsilon < \text{dist}(y_0, F(\partial X))$ then $y_0 \in \text{int}(G(X))$.*

Last result is standard in degree theory. The proof for the statement in this form can be found in [CS18, Lemma 5.2] or [AC10, Lemma 7].

2.4 Normal controllability

Let $\psi_0, \psi_1 \in \text{span}(\Phi)$ and with $\|\Pi_N(\psi_1)\| < 1$ and consider $U \in U(\mathcal{H})$ be such that $U\psi_0 = \psi_1$. Let $n > N$ be such that the Lie–Galerkin condition holds. Let now $M \in SU(n)$ be such that $M^{(N)} := \Pi_N M \Pi_N = \Pi_N U \Pi_N =: U^{(N)}$. Since, by the Lie–Galerkin condition

$$\text{Lie}\mathcal{W}_n \supset \mathfrak{su}(N),$$

we have classical results of *normal controllability* (see [JS72] and [Sus76, Theorem 4.3]) implying the existence of $M_1, \dots, M_k \in \mathcal{W}_n$ and $t_1, \dots, t_k > 0$ such that the map

$$E : (s_1, \dots, s_k) \mapsto e^{s_k M_k} \circ \dots \circ e^{s_1 M_1}, \quad (7)$$

has rank $n^2 - 1$ at (t_1, \dots, t_k) and

$$E(t_1, \dots, t_k) = M.$$

Let us call, for simplicity, $\nu = n^2 - 1$. By linear extraction there exist $j_1, \dots, j_\nu \in \{1, \dots, k\}$ such that the map F defined by

$(s_{j_1}, \dots, s_{j_\nu}) \mapsto (E(t_1, \dots, t_{j_1-1}, s_{j_1}, t_{j_1+1}, \dots, t_{j_\nu-1}, s_{j_\nu}, t_{j_\nu+1}, \dots, t_k)) \Pi_N \psi_0$,

has rank ν at $(t_{j_1}, \dots, t_{j_\nu})$ and

$$F(t_{j_1}, \dots, t_{j_\nu}) = M^{(N)} \Pi_N \psi_0 \quad (= \Pi_N \psi_1). \quad (8)$$

Now let $\varepsilon > 0$ be such that

$$X := B_\varepsilon(t_{j_1}, \dots, t_{j_\nu}) \subset (0, +\infty)^\nu,$$

where $B_\varepsilon(\mathbf{t})$ (resp. $\overline{B_\varepsilon(\mathbf{t})}$) is the open (resp. closed) ball of radius ε centered at $\mathbf{t} \in \mathbf{R}^\nu$. Then F is a diffeomorphism between X and $F(X)$. Let

$$\eta = \inf_{(s_1, \dots, s_\nu) \in \partial X} \|F(s_1, \dots, s_\nu) - \Pi_N \psi_1\|, \quad (9)$$

and note that $\eta > 0$.

Lemma 5 *There exists a map associating with every $(s_1, \dots, s_\nu) \in \bar{X}$ a piecewise constant control $w : [0, \infty) \rightarrow \{0, 1\}$ and $T > 0$ such that if $G = \Pi_N \mathcal{Y}_T^w \Pi_N \psi_0$ then*

$$\Pi_N \psi_1 \in \text{int}(G(X)).$$

Proof Let η be as in (9). By Proposition 1 applied with $\varepsilon < \eta$ there exists $w \in PC([0, \infty), \{0, 1\})$ such that

$$\sup_{(s_1, \dots, s_\nu) \in \partial X} |F(s_1, \dots, s_\nu) - G(s_1, \dots, s_\nu)| < \eta.$$

The continuity of the control w on (s_1, \dots, s_ν) is given by Proposition 1 while the continuity of the propagator \mathcal{Y}_T^w on the control w is given by [BCC20, Corollary 9] (see also Remark 3). The conclusion then follows from Lemma 4. \square

3 Proof of the main result

We are now ready to prove the main result that is a consequence of Theorem 2.

Proof (Proof of Theorem 2) Notice that, if

$$\mathcal{V}_n = \left\{ A^{(n)} \right\} \cup \left\{ \mathcal{E}_\sigma(B^{(n)}) \mid \sigma \in \Xi_n \right\},$$

then

$$\text{Lie}(\mathcal{V}_n) = \text{Lie}(\mathcal{M}_n).$$

Indeed for every $\sigma \in \Sigma_n$,

$$[A^{(n)}, \mathcal{E}_\sigma(B^{(n)})] = [-iH_0^{(n)}, \mathcal{E}_\sigma(-iH_1^{(n)} + iH_0^{(n)})] = [iH_0^{(n)}, \mathcal{E}_\sigma(iH_1^{(n)})].$$

Moreover if $0 \in \Xi_n$ then $\text{Lie}(\mathcal{W}_n) = \text{Lie}(\mathcal{V}_n)$. In particular by the Lie–Galerkin condition, $\text{Lie}(\mathcal{W}_n) \supseteq \mathfrak{su}(n)$ and the result follows from Lemma 5. \square

Proof (Proof of Theorem 1) Consider $A = -iH(0)$ and $B = -i(H(1) - H(0))$. Then the pair of operators (A, B) satisfies Assumption 2. Moreover if (LS) satisfies the Lie–Galerkin condition then so does (BSE) by definition. Theorem 1 then follows directly from Theorem 2 since

$$\mathcal{X}_t^u = \mathcal{Y}_t^u,$$

for every control $u : \mathbf{R} \rightarrow \{0, 1\}$ and for every $t \geq 0$. \square

4 Control of the Schrödinger Equation with a polarizability term

4.1 Non-resonance condition

A simple assumption implying the Lie–Galerkin condition is the existence of a non-resonant chain of connectedness. This notion, presented in [BCCS12] as a sufficient condition for approximate controllability for bilinear systems can be extended to (LS) under Assumption 1 as follows.

Definition 2 We say that $S \subset \mathbf{N}^2$ couples two levels l, k in \mathbf{N} , if there exists a finite sequence $((s_1^1, s_2^1), \dots, (s_1^q, s_2^q))$ in S such that

- (i) $s_1^1 = l$ and $s_2^q = k$;
- (ii) $s_2^j = s_1^{j+1}$ for every $1 \leq j \leq q - 1$;
- (iii) $\langle \phi_{s_1^j}, H(1)\phi_{s_2^j} \rangle \neq 0$ for $1 \leq j \leq q$.

S is called a *connectedness chain* if S couples every pair of levels in \mathbf{N} .

A connectedness chain is said to be *non-resonant* if for every (s_1, s_2) in S , $|\lambda_{s_1} - \lambda_{s_2}| \neq |\lambda_{t_1} - \lambda_{t_2}|$ for every (t_1, t_2) in $\mathbf{N}^2 \setminus \{(s_1, s_2), (s_2, s_1)\}$ such that $\langle \phi_{t_2}, B\phi_{t_1} \rangle \neq 0$.

A system admitting a non-resonant chain of connectedness satisfies the Lie–Galerkin condition as the following Lemma states.

Lemma 6 Assume that $\langle \phi_l, H(1)\phi_k \rangle = 0$ whenever $l \neq k$ and $\lambda_l = \lambda_k$. If there exists a non-resonant connectedness chain coupling every pair of levels of $H(0)$ then system (LS) satisfies the Lie–Galerkin condition.

Proof The first assumption in the statement of the proposition implies that $0 \in \Xi_n$ for every n . The non-resonance condition on the eigenvalues implies that, for every n , $\Xi_n = \Sigma_n$. Since, moreover, $\mathcal{E}_{|\lambda_l - \lambda_k|}(H_1^{(n)})$ has at most two nonzero entries, the Lie–Galerkin condition follows from the existence of a connectedness chain (see, for instance the proof of [BCCS12, Proposition 3.1] for details). \square

4.2 Generic bounded coupling potentials

Let Ω be a compact Riemannian manifold or a bounded domain in \mathbf{R}^n . Let $V, W_1, W_2 : \Omega \rightarrow \mathbf{R}$ be three measurable bounded functions. We consider the system

$$\begin{aligned} i\frac{\partial\psi}{\partial t}(x, t) &= (-\Delta + V(x))\psi(x, t) + u(t)W_1(x)\psi(x, t) \\ &\quad + u^2(t)W_2(x)\psi(x, t), \end{aligned} \tag{10}$$

with x in Ω and t in \mathbf{R} . Here $\mathcal{H} = L^2(\Omega, \mathbf{C})$, and $H(0) = -\Delta + V(x)$. By Kato-Rellich theorem, the domain $D(H(0))$ of $H(0)$ is equal to the domain of the Laplacian $H_{(0)}^2 = \{\psi \in H^2(\Omega, \mathbf{C}) \mid \psi|_{\partial\Omega} = \Delta\psi|_{\partial\Omega} = 0\}$ if Ω is a bounded domain of \mathbf{R}^n and it is equal to $H^2(\Omega, \mathbf{C})$ if Ω is compact manifold. The operator $H(1) - H(0) = W_1(x) + W_2(x)$ is bounded from \mathcal{H} to \mathcal{H} .

The existence of a nonresonant chain of connectedness is a generic property [MS10, Theorem 3.4] for systems of the form (10). By Lemma 6 system (10) is exactly controllable in projections for generic control potential W_1 and W_2 .

5 Conclusions and perspectives

We presented a sufficient condition for the exact controllability in projections of the linear Schrödinger equation with an Hamiltonian that is a bounded perturbation of a free Hamiltonian with pure point spectrum. Most of the results in literature focus on the bilinear case and, indeed, there are several technical challenges arising from the nonlinearity of the Hamiltonian $H(u)$ with respect to the control u .

The condition that $H(1) - H(0) = iB$ is bounded is a quite strong technical assumption. Indeed, this assumption is needed mainly to infer continuity of the propagators, see Remark 3, which is crucial in the application of the topological degree argument of Lemma 4. Sufficient conditions for the continuity of the propagator of linear systems are technically involved and may be hard to check in practice on physical examples (see for instance [BCC20]).

A natural extension of the controllability result in this paper is the analysis of the controllability with several controls. In many examples controllability cannot be achieved with a single scalar control as a consequence of the symmetries of the system. This happens, for instance, for a planar rotating molecule controlled by one external field only [BCC12], which is not controllable. The Lie–Galerkin condition has been introduced in [BCS14] exactly to tackle this challenge in the bilinear case.

Finally a challenging perspective is the case in which the free Hamiltonian presents also a continuous spectrum. The Lie–Galerkin methods, indeed, re-

lies on the lack of coupling between the first n eigenstates and the rest of the spectrum which ensures the invariance of the evolution on a suitable Galerkin approximation. In order to tackle such a challenge one has to adapt the Lie-Galerkin condition to Hamiltonians having finitely many distinct eigenvalues and estimate the loss of population to the continuous part of the spectrum.

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