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A weak spectral condition for the controllability of the bilinear Schrödinger equation with application to the control of a rotating planar molecule

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Abstract

In this paper we prove an approximate controllability result for the bilinear Schrödinger equation. This result requires less restrictive non-resonance hypotheses on the spectrum of the uncontrolled Schrödinger operator than those present in the literature. The control operator is not required to be bounded and we are able to extend the controllability result to the density matrices. The proof is based on fine controllability properties of the finite dimensional Galerkin approximations and allows to get estimates for the L^1 norm of the control. The general controllability result is applied to the problem of controlling the rotation of a bipolar rigid molecule confined on a plane by means of two orthogonal external fields.

1 Introduction

In this paper we are concerned with the controllability problem for the Schrödinger equation

$$i\frac{d\psi}{dt} = (H_0 + u(t)H_1)\psi. \quad (1.1)$$

Here ψ belongs to the Hilbert sphere of a complex Hilbert space \mathcal{H} and H_0, H_1 are self-adjoint operators on \mathcal{H} . The control u is scalar-valued and represents the action of an external field. The reference model is the one in which $H_0 = -\Delta + V(x)$, $H_1 = W(x)$, where x belongs to a domain $D \subset \mathbf{R}^n$ with suitable boundary conditions and V, W are real-valued functions (identified with the corresponding multiplicative operators) characterizing respectively the autonomous dynamics and the coupling of the system with the control u . However, equation (1.1) can be used to describe more general controlled dynamics. For instance, a quantum particle on a Riemannian manifold subject to an external field (in this case Δ is the Laplace–Beltrami operator) or a two-level ion trapped in a harmonic potential (the so-called Eberly and Law model [18, 9, 14]). In the last case, as in many others relevant physical situations, the operator H_0 cannot be written as the sum of a Laplacian plus a potential.

Equation (1.1) is usually named *bilinear Schrödinger equation* in the control community, the term *bilinear* referring to the linear dependence with respect to ψ and the affine dependence with respect to u . (The term linear is reserved for systems of the form $\dot{x} = Ax + Bu(t)$.) The operator H_0 is usually called the *drift*.

The controllability problem consists in establishing whether, for every pair of states ψ_0 and ψ_1 , there exist a control $u(\cdot)$ and a time T such that the solution of (1.1) with initial condition $\psi(0) = \psi_0$ satisfies $\psi(T) = \psi_1$. Unfortunately the answer to this problem is negative when \mathcal{H} is infinite dimensional. Indeed, Ball, Marsden, and Slemrod proved in [3] a result which implies (see [28]) that equation (1.1) is not controllable in (the Hilbert sphere of) \mathcal{H} . Moreover, they proved that in the case in which H_0 is the sum of the Laplacian and a potential in a domain D of \mathbf{R}^n , equation (1.1) is neither controllable in the Hilbert sphere \mathbf{S} of $L^2(D, \mathbf{C})$ nor in the natural functional space where the problem is formulated, namely the intersection of \mathbf{S} with the Sobolev spaces $H^2(D, \mathbf{C})$ and $H_0^1(D, \mathbf{C})$. Hence one has to look for weaker controllability properties as, for instance, approximate controllability or controllability between the eigenstates of H_0 (which are the most relevant physical states).

However, in certain cases one can describe quite precisely the set of states that can be connected by admissible paths. Indeed in [4, 5] the authors prove that, in the case in which H_0 is the Laplacian on the interval $[-1, 1]$, with Dirichlet boundary conditions, and H_1 is the operator of multiplication by x , the system is exactly controllable near the eigenstates in $H^7(D, \mathbf{C}) \cap \mathbf{S}$ (with suitable boundary conditions). This result was then refined in [6], where the authors proved that the exact controllability holds in $H^3(D, \mathbf{C}) \cap \mathbf{S}$, for a large class of control potentials (see also [23]).

In dimension larger than one (for H_0 equal to the sum of the Laplacian and a potential) or for more general situations, the exact description of the reachable set appears to be more difficult and at the moment only approximate controllability results are available.

In [11] an approximate controllability result for (1.1) was proved via finite dimensional geometric control techniques applied to the Galerkin approximations. The main hypothesis is that the spectrum of H_0 is discrete and without rational resonances, which means that the gaps between the eigenvalues of H_0 are \mathbf{Q} -linearly independent. Another crucial hypothesis appearing naturally is that the operator H_1 couples all eigenvectors of H_0 .

The main advantages of that result with respect to those previously known are that: **i)** it does not need H_0 to be of the form $-\Delta + V$; **ii)** it can be applied to the case in which H_1 is an unbounded operator; **iii)** the control is a bounded function with arbitrarily small bound; **iv)** it allows to prove controllability for density matrices and it can be generalized to prove approximate controllability results for a system of Schrödinger equations controlled by the same control (see [10]).

The biggest difficulty in order to apply the results given in [11] to academic examples is that in most of the cases the spectrum is described as a simple numerical series (and hence \mathbf{Q} -linearly dependent). However, it has been proved that the hypotheses under which the approximate controllability results holds are generic [19, 24]. Notice that writing $H_0 + u(t)H_1 = (H_0 + \varepsilon H_1) + (u(t) - \varepsilon)H_1$ and redefining $(u(t) - \varepsilon)$ as new control may be useful. As a matter of fact, perturbation theory permits often to prove the \mathbf{Q} -linearly independence of the eigenvalues of $(H_0 + \varepsilon H_1)$ for most values of ε . This idea was used in [11] to prove the approximate controllability of the harmonic oscillator and the 3D potential well with a Gaussian control potential.

Results similar to those presented in [11] have been obtained, with different techniques,

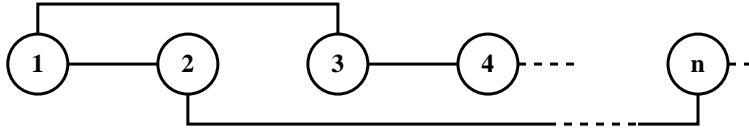


Figure 1: Each vertex of the graph represents an eigenstate of H_0 (when the spectrum is not simple, several nodes may be attached to the same eigenvalue). An edge links two vertices if and only if H_1 connects the corresponding eigenstates. In this example, $\langle \phi_1, H_1 \phi_2 \rangle$ and $\langle \phi_1, H_1 \phi_3 \rangle$ are not zero, while $\langle \phi_1, H_1 \phi_4 \rangle = \langle \phi_2, H_1 \phi_3 \rangle = \langle \phi_2, H_1 \phi_4 \rangle = 0$.

in [22] (see also [15, 8, 21, 23]). They require less restrictive hypotheses on the spectrum of H_0 (which is still assumed to be discrete) but they do not admit H_1 unbounded and do not apply to the density matrices. However, it should be noticed that [22] proves approximate controllability with respect to some Sobolev norm H^s , while the results given in [11] permit to get approximate controllability in the weaker norm L^2 . As it happens for the results in [11], the sufficient conditions for controllability obtained in [22] are generic.

Fewer controllability results are known in the case in which the spectrum of H_0 is not discrete. Let us mention the paper [20], in which approximate controllability is proved between wave functions corresponding to the discrete part of the spectrum (in the 1D case), and [15].

In this paper we prove the approximate controllability of (1.1) under less restrictive hypotheses than those in [11]. More precisely, assume that H_0 has discrete spectrum $(\lambda_k)_{k \in \mathbf{N}}$ (possibly not simple) and denote by ϕ_k an eigenvector of H_0 corresponding to λ_k in such a way that $(\phi_k)_{k \in \mathbf{N}}$ is an orthonormal basis of \mathcal{H} . Let Ξ be the subset of \mathbf{N}^2 given by all (k_1, k_2) such that $\langle \phi_{k_1}, H_1 \phi_{k_2} \rangle \neq 0$. Assume that, for every $(j, k) \in \Xi$ such that $j \neq k$, we have $\lambda_j \neq \lambda_k$ (that is, degenerate energy levels are not directly coupled by H_1). We prove that the system is approximately controllable if there exists a subset S of Ξ such that the graph whose vertices are the elements of \mathbf{N} and whose edges are the elements of S is connected (see Figure 1) and, moreover, for every $(j_1, j_2) \in S$ and every $(k_1, k_2) \in \Xi$ different from (j_1, j_2) and (j_2, j_1) ,

$$|\lambda_{j_1} - \lambda_{j_2}| \neq |\lambda_{k_1} - \lambda_{k_2}|. \quad (1.2)$$

As in [11], H_1 is not required to be bounded and we are able to extend the controllability result to the density matrices and to simultaneous controllability (see Section 2.2 for precise definitions). This extension is interesting in the perspective of getting controllability results for open systems.

Interesting features of our result are that it permits to get L^1 estimates for the control laws and that it does not require the spectrum of A to be simple. Moreover, beside requiring less restrictive hypotheses, this new result works better in academic examples where very often one has a spectrum which is resonant, but a lot of products $\langle \phi_{k_1}, H_1 \phi_{k_2} \rangle$ which vanish. The consequence of the presence of these vanishing elements (i.e., of the smallness of Ξ) is that less conditions of the type (1.2) need being verified.

The condition on the spectrum given above is still generic and it is less restrictive than the one given in [22], which corresponds to the case $S = \{(k_0, k) \mid k \in \mathbf{N}, k \neq k_0\}$ for some $k_0 \in \mathbf{N}$ and where condition (1.2) is required for every $(k_1, k_2) \in \mathbf{N}^2 \setminus \{(j_1, j_2), (j_2, j_1)\}$. Notice however that the approximate controllability result given in [22] is still in a stronger norm.

The idea of the proof is the following. We recover approximate controllability for the

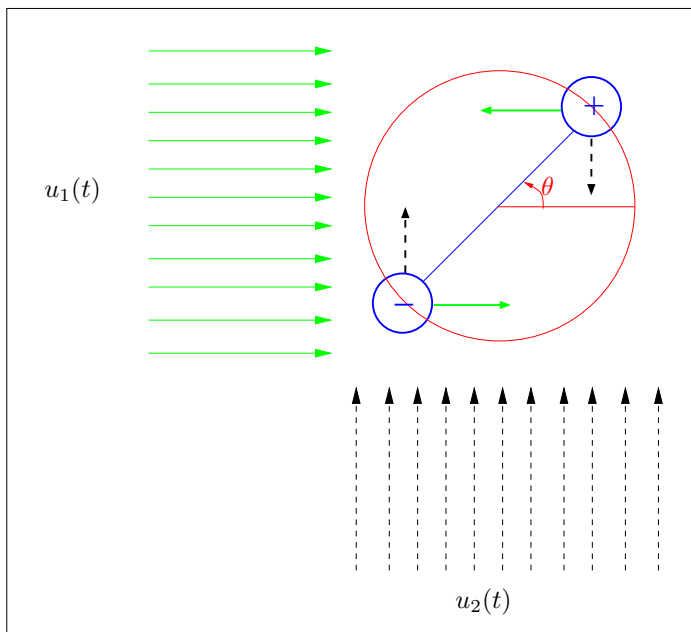


Figure 2: The bipolar rigid molecule confined to a plane.

system defined on an infinite dimensional Hilbert space through fine controllability properties of the N -dimensional Galerkin approximations, $N \in \mathbf{N}$, which allow us to pass to the limit as $N \rightarrow \infty$. More precisely, we prove that, for $n, N \in \mathbf{N}$ with $N \gg n \gg 1$, for given initial and final conditions ψ_0, ψ_1 in the Hilbert sphere of \mathcal{H} which are linear combinations of the first n eigenvectors of H_0 , it is possible to steer ψ_0 to ψ_1 in the Galerkin approximation of order N in such a way that the projection on the components $n + 1, \dots, N$ has arbitrarily small norm along the trajectory. This kind of controllability for the Galerkin approximation of order N is proved in two steps: firstly, thanks to a time-dependent change of variables we transform the system in a driftless one, nonlinear in the control, and we prove the result up to phases. The change of variables was already introduced in [1, 11]; the technical novelty of this paper is the convexification analysis for the transformed system, which allows to conclude the controllability with less restrictive non-resonance hypotheses. Secondly, the control of phases is obtained via a classical method, using as pivot an eigenstate of H_0 and exploiting the controllability (up to phases) of the time-reversed Schrödinger equation. This last step requires some further arguments in the case of simultaneous controllability.

In the second part of the paper we apply our result to the problem of controlling a bipolar rigid molecule confined on a plane by means of two electric fields constant in space and controlled in time, oriented along two orthogonal directions (see Figure 2). The corresponding Schrödinger equation can be written as

$$i \frac{\partial \psi(\theta, t)}{\partial t} = \left(-\frac{\partial^2}{\partial \theta^2} + u_1(t) \cos(\theta) + u_2(t) \sin(\theta) \right) \psi(\theta, t), \quad \theta \in \mathbb{S}^1, \quad (1.3)$$

where $\mathbb{S}^1 = \mathbf{R}/2\pi\mathbf{Z}$. Notice that a controlled rotating molecule is the most relevant physical application for which the spectrum of H_0 is discrete.

The system described by (1.3) is not controllable if we fix one control to zero. Indeed by

parity reasons the potential $\cos(\theta)$ does not couple an odd wave function with an even one and the potential $\sin(\theta)$ does not couple wave functions with the same parity.

Up to our knowledge, the controllability result presented in this paper is the only one which can be directly applied to system (1.3). Indeed, both the results obtained in [11] and [22] seem to require sophisticated perturbation arguments in order to conclude the approximate controllability of (1.3).

The proof of the controllability of (1.3) by means of the controllability result obtained in this paper is not immediate since we have to use in a suitable way the two controls. The idea is to prove that, given an initial condition ψ_0 which is even with respect to some $\bar{\theta} \in \mathbb{S}^1$, by varying the control $u = (u_1, u_2) \in \mathbf{R}^2$ along the line $\mathbf{R}(\cos(\bar{\theta}), \sin(\bar{\theta}))$, it is possible to steer it (approximately) towards any other wave function even with respect to $\bar{\theta}$. In particular, it is possible to steer any eigenfunction (which is necessarily even with respect to some $\bar{\theta}$) to the ground state (that is, the constant function $1/\sqrt{2\pi}$), which can, in turn, be steered towards any other eigenfunction. The argument can be refined to prove approximate controllability among any pair of wave functions on the Hilbert sphere.

The structure of the paper is the following. In Section 2 we introduce the class of systems under consideration and we discuss their well-posedness. Then, we state the main results contained in the paper. Section 3 is devoted to the case in which \mathcal{H} is finite dimensional. Sections 4, 5, and 6 contain the proof of the main results and in Section 5.6 we present estimates on the L^1 norm of the control. Section 7 contains an application to the infinite potential well, showing controllability and establishing L^1 estimates of the control. Section 8 provides the application to the bipolar planar molecule evolving on the plane.

2 Framework and main results

2.1 Settings and notations

As in [11], we use an abstract framework instead of a presentation in terms of partial differential equations. The advantage of this presentation is that it is very versatile and applies without modification for Schrödinger equation on a (possibly unbounded) domain of \mathbf{R}^n or on a manifold such as \mathbb{S}^1 (see Section 8). To avoid confusion, let us stress that H_0 and H_1 , introduced in the introduction, are self-adjoint operators while $A = -iH_0$ and $B = -iH_1$, used in what follows, are skew-adjoint. Hereafter \mathbf{N} denotes the set of strictly positive integers. We also denote by $\mathbf{U}(\mathcal{H})$ the space of unitary operators on \mathcal{H} .

Definition 2.1. Let \mathcal{H} be an Hilbert space with scalar product $\langle \cdot, \cdot \rangle$ and A, B be two (possibly unbounded) linear operators on \mathcal{H} , with domains $D(A)$ and $D(B)$. Let U be a subset of \mathbf{R} . Let us introduce the formal controlled equation

$$\frac{d\psi}{dt}(t) = (A + u(t)B)\psi(t), \quad u(t) \in U. \quad (2.1)$$

We say that (A, B, U, Φ) satisfies (\mathfrak{A}) if the following assumptions are verified:

- (A1) $\Phi = (\phi_k)_{k \in \mathbf{N}}$ is an Hilbert basis of \mathcal{H} made of eigenvectors of A associated with the family of eigenvalues $(i\lambda_k)_{k \in \mathbf{N}}$;
- (A2) $\phi_k \in D(B)$ for every $k \in \mathbf{N}$;

(A3) $A + uB : \text{span}\{\phi_k \mid k \in \mathbf{N}\} \rightarrow \mathcal{H}$ is essentially skew-adjoint for every $u \in U$;

(A4) if $j \neq k$ and $\lambda_j = \lambda_k$ then $\langle \phi_j, B\phi_k \rangle = 0$.

Remark 2.2. If A has simple spectrum then (A4) is verified. If all the eigenvalues of A have finite multiplicity, then, up to a change of basis, hypothesis (A4) is a consequence of (A1 – 2 – 3).

A crucial consequence of assumption (A3) is that, for every constant u in U , $A + uB$ generates a group of unitary transformations $e^{t(A+uB)} : \mathcal{H} \rightarrow \mathcal{H}$. The unit sphere of \mathcal{H} is invariant for all these transformations.

Definition 2.3. Let (A, B, U, Φ) satisfy (A) and $u : [0, T] \rightarrow U$ be piecewise constant. The *solution* of (2.1) with initial condition $\psi_0 \in \mathcal{H}$ is

$$\psi(t) = \Upsilon_t^u(\psi_0), \quad (2.2)$$

where $\Upsilon^u : [0, T] \rightarrow \mathbf{U}(\mathcal{H})$ is the *propagator* of (2.1) that associates, with every t in $[0, T]$, the unitary linear transformation

$$\Upsilon_t^u = e^{(t - \sum_{l=1}^{j-1} t_l)(A+u_j B)} \circ e^{t_{j-1}(A+u_{j-1} B)} \circ \dots \circ e^{t_1(A+u_1 B)},$$

where $\sum_{l=1}^{j-1} t_l \leq t < \sum_{l=1}^j t_l$ and $u(\tau) = u_j$ if $\sum_{l=1}^{j-1} t_l \leq \tau < \sum_{l=1}^j t_l$.

The notion of solution introduced above makes sense in very degenerate situations and can be enhanced when B is bounded (see [3] and references therein).

Note that, since

$$\langle \phi_n, e^{t(A+uB)} \psi_0 \rangle = \langle e^{-t(A+uB)} \phi_n, \psi_0 \rangle,$$

for every $n \in \mathbf{N}$, $\psi_0 \in \mathcal{H}$, and $u \in U$, then, for every solution $\psi(\cdot)$ of (2.1), the function $t \mapsto \langle \psi(t), \phi_n \rangle$ is absolutely continuous and satisfies, for almost every $t \in [0, T]$,

$$\frac{d}{dt} \langle \phi_n, \psi(t) \rangle = - \langle (A + u(t)B) \phi_n, \psi(t) \rangle. \quad (2.3)$$

2.2 Main results

As already recalled in the introduction, exact controllability is hopeless in general. Several relevant definitions of approximate controllability are available. The first one is the standard approximate controllability.

Definition 2.4. Let (A, B, U, Φ) satisfy (A). We say that (2.1) is *approximately controllable* if for every ψ_0, ψ_1 in the unit sphere of \mathcal{H} and every $\varepsilon > 0$ there exist a piecewise constant control function $u : [0, T] \rightarrow U$ such that $\|\psi_1 - \Upsilon_T^u(\psi_0)\| < \varepsilon$.

Recall that A has purely imaginary eigenvalues $(i\lambda_k)_{k \in \mathbf{N}}$ with associated eigenfunctions $(\phi_k)_{k \in \mathbf{N}}$. Next we introduce the notion of *connectedness chain*, whose existence is crucial for our result.

Definition 2.5. Let (A, B, U, Φ) satisfy (A). A subset S of \mathbf{N}^2 *couples* two levels j, k in \mathbf{N} , if there exists a finite sequence $((s_1^1, s_2^1), \dots, (s_1^p, s_2^p))$ in S such that

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

S is called a *connectedness chain* (respectively m -connectedness chain) for (A, B, U, Φ) if S (respectively $S \cap \{1, \dots, m\}^2$) couples every pair of levels in \mathbf{N} (respectively in $\{1, \dots, m\}$).

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 $\langle \phi_{t_2}, B\phi_{t_1} \rangle \neq 0$.

Theorem 2.6. *Let $\delta > 0$ and let $(A, B, [0, \delta], \Phi)$ satisfy (\mathfrak{A}) . If there exists a non-resonant connectedness chain for $(A, B, [0, \delta], \Phi)$ then (2.1) is approximately controllable.*

Theorem 2.6 is a particular case of Theorem 2.11, stated in the next section.

Remark 2.7. Notice that in the assumptions of Theorem 2.6 we do not require that the eigenvalues of A are simple. Take for instance $\mathcal{H} = \mathbf{C}^4$, $U = [0, 1]$, and

$$A = \begin{pmatrix} i & 0 & 0 & 0 \\ 0 & 2i & 0 & 0 \\ 0 & 0 & 4i & 0 \\ 0 & 0 & 0 & 4i \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}.$$

A connectedness chain is given by $\{(1, 2), (2, 1), (1, 3), (3, 1), (2, 4), (4, 2)\}$. The corresponding eigenvalue gaps are $|\lambda_2 - \lambda_1| = 1$, $|\lambda_3 - \lambda_1| = 3$, and $|\lambda_4 - \lambda_2| = 2$. Hence, the connectedness chain is non-resonant.

The following proposition gives an estimate of the L^1 norm of the control steering (2.1) from one eigenvector to an ε -neighborhood of another. A generalization of this proposition is given by Theorem 2.13.

Proposition 2.8. *Let $\delta > 0$. Let $(A, B, [0, \delta], \Phi)$ satisfy (\mathfrak{A}) and admit a non-resonant chain of connectedness S . Then for every $\varepsilon > 0$ and $(j, k) \in S$ there exist a piecewise constant control $u : [0, T_u] \rightarrow [0, \delta]$ and $\theta \in \mathbf{R}$ such that $\|\Upsilon_{T_u}^u(\phi_j) - e^{i\theta}\phi_k\| < \varepsilon$ and*

$$\|u\|_{L^1} \leq \frac{5\pi}{4|\langle \phi_k, B\phi_j \rangle|}.$$

2.3 Simultaneous controllability and controllability in the sense of density matrices

We define now a notion of controllability in the sense of density matrices. Recall that a density matrix ρ is a non-negative, self-adjoint operator of trace class whose trace is normalized to one. Its time evolution is determined by

$$\rho(t) = \Upsilon_t^u \rho(0) \Upsilon_t^{u*}$$

where Υ_t^{u*} is the adjoint of Υ_t^u . Notice that the spectrum of $\rho(t)$ is constant along the motion, since, for every t , $\rho(t)$ is unitarily equivalent to $\rho(0)$.

Definition 2.9. Let (A, B, U, Φ) satisfy (\mathfrak{A}) . We say that (2.1) is *approximately controllable in the sense of the density matrices* if for every pair of unitarily equivalent density matrices ρ_0, ρ_1 and every $\varepsilon > 0$ there exists a piecewise constant control $u : [0, T] \rightarrow U$ such that

$$\|\rho_1 - \Upsilon_T^u \rho_0 \Upsilon_T^{u*}\| < \varepsilon,$$

in the sense of the operator norm induced by the Hilbert norm of \mathcal{H} .

Definition 2.10. Let (A, B, U, Φ) satisfy (\mathfrak{A}) . We say that (2.1) is *approximately simultaneously controllable* if for every r in \mathbf{N} , ψ_1, \dots, ψ_r in \mathcal{H} , $\hat{\Upsilon}$ in $\mathbf{U}(\mathcal{H})$, and $\varepsilon > 0$ there exists a piecewise constant control $u : [0, T] \rightarrow U$ such that, for every $1 \leq k \leq r$,

$$\left\| \hat{\Upsilon} \psi_k - \Upsilon_T^u \psi_k \right\| < \varepsilon.$$

The following result is proved in Sections 4, 5, and 6.

Theorem 2.11. Let $\delta > 0$ and let $(A, B, [0, \delta], \Phi)$ satisfy (\mathfrak{A}) . If there exists a non-resonant connectedness chain for $(A, B, [0, \delta], \Phi)$, then (2.1) is *approximately simultaneously controllable*.

Simultaneous controllability implies controllability in the sense of density matrices (see Proposition A.1). Hence we have the following.

Corollary 2.12. Let $\delta > 0$ and let $(A, B, [0, \delta], \Phi)$ satisfy (\mathfrak{A}) . If there exists a non-resonant connectedness chain for $(A, B, [0, \delta], \Phi)$, then (2.1) is *approximately controllable in the sense of the density matrices*.

Theorem 2.13. Let (A, B, U, Φ) satisfy (\mathfrak{A}) and admit a non-resonant chain of connectedness. Then there exists a basis $\hat{\Phi} = (\hat{\phi}_k)_{k \in \mathbf{N}}$ of eigenvectors of A and a subset S of \mathbf{N}^2 such that, for every $m \in \mathbf{N}$, S is a m -connectedness chain for $(A, B, U, \hat{\Phi})$. Moreover, let $\delta > 0$ and $U = [0, \delta]$, then for every $\varepsilon > 0$ and for every permutation $\sigma : \{1, \dots, m\} \rightarrow \{1, \dots, m\}$ there exist a piecewise constant control $u : [0, T_u] \rightarrow [0, \delta]$ and $\theta_1, \dots, \theta_m$ in \mathbf{R} for which the propagator Υ^u of (2.1) satisfies $\|\Upsilon_{T_u}^u \hat{\phi}_l - e^{i\theta_l} \hat{\phi}_{\sigma(l)}\| < \varepsilon$ for every $1 \leq l \leq m$ and

$$\|u\|_{L^1} \leq \frac{5 \pi (2^{m-1} - 1)}{4 \inf\{|\langle \hat{\phi}_k, B \hat{\phi}_j \rangle| : (j, k) \in S, 1 \leq j, k \leq m\}}.$$

The proof of the first part of the statement of Theorem 2.13 is given in Section 4.4. The second part is proved in Section 5.6.

Notice that a lower bound on the L^1 norm of the control was already proved in [11] (see Proposition 5.9).

3 Finite dimensional case

Denote by $\mathfrak{u}(n)$ and $\mathfrak{su}(n)$ the Lie algebras of the group of unitary matrices $U(n)$ and its special subgroup $SU(n) = \{M \in U(n) \mid \det M = 1\}$ respectively.

Here we address the case where \mathcal{H} is of finite dimension n . Equation (2.1) then defines a bilinear control system on $U(n)$. Finite dimensional systems of the type (2.1) have been

extensively studied. A necessary and sufficient condition for controllability on $SU(n)$ (i.e. the property that every two points of $SU(n)$ can be joined by a trajectory in $U(n)$ of system (2.1)) is that the Lie algebra generated by A and B contains $\mathfrak{su}(n)$. This criterion is optimal, yet sometimes too complicated to be checked for n large. Easily verifiable sufficient conditions for controllability on $SU(n)$ have been thoroughly studied in the literature (see for instance [13] and references therein). Next proposition gives a new sufficient condition, slightly improving those in [28] and [11, Proposition 4.1]. Its proof is based on the techniques that we extend to the infinite dimensional case in the following sections.

The controllability result is obtained under a slightly weaker assumption than (\mathfrak{A}) .

Proposition 3.1. *Let $\mathcal{H} = \mathbf{C}^n$. Let (A, B, U, Φ) satisfy $(\mathfrak{A}1 - 2 - 3)$ and admit a non-resonant connectedness chain S . Assume, moreover, that $\lambda_j \neq \lambda_k$ for every $(j, k) \in S$. Then the control system (2.1) is controllable both on the unit sphere of \mathbf{C}^n and on $SU(n)$, provided that U contains at least two points. If, moreover, $\text{tr } A \neq 0$ or $\text{tr } B \neq 0$, then the control system (2.1) is controllable on $U(n)$.*

Proof. For every $1 \leq j, k \leq n$, let $e_{jk}^{(n)}$ be the $n \times n$ matrix whose entries are all zero, but the one at line j and column k which is equal to 1. We denote by a_{jk} and b_{jk} the (j, k) -th entry of A and B , respectively.

Recall that, for any two $n \times n$ matrices X and Y , $\text{ad}_X(Y) = [X, Y] = XY - YX$, and compute the iterated matrix commutator

$$\text{ad}_A^p(B) = \sum_{j,k=1}^n (a_{jj} - a_{kk})^p b_{jk} e_{jk}^{(n)}.$$

Fix (j, k) in S . By hypothesis, for every l, m in $\{1, \dots, n\}$ such that $\{l, m\} \neq \{j, k\}$, $(a_{jj} - a_{kk})^2 \neq (a_{ll} - a_{mm})^2$ or $b_{lm} = 0$. There exists some polynomial P_{jk} with real coefficients such that $P_{jk}((a_{jj} - a_{kk})^2) = 1$ and $P_{jk}((a_{ll} - a_{mm})^2) = 0$ if $(a_{jj} - a_{kk})^2 \neq (a_{ll} - a_{mm})^2$. Let $P_{jk} = \sum_{h=0}^d c_h X^h$. Then

$$\sum_{h=0}^d c_h \text{ad}_A^{2h}(B) = b_{jk} e_{jk}^{(n)} + b_{kj} e_{kj}^{(n)}.$$

As a consequence,

$$\sum_{h=0}^d c_h \text{ad}_A^{2h+1}(B) = (a_{jj} - a_{kk}) \left(b_{jk} e_{jk}^{(n)} + \overline{b_{jk}} e_{kj}^{(n)} \right) = i(\lambda_j - \lambda_k) \left(b_{jk} e_{jk}^{(n)} + \overline{b_{jk}} e_{kj}^{(n)} \right),$$

and then the two elementary Hermitian matrices $e_{jk}^{(n)} - e_{kj}^{(n)}$ and $i e_{jk}^{(n)} + i e_{kj}^{(n)}$ also belong to $\text{Lie}(A, B)$. Because of the connectedness of B and thanks to the relation

$$\left[e_{jk}^{(n)}, e_{lm}^{(n)} \right] = \delta_{kl} e_{jm}^{(n)} - \delta_{jm} e_{lk}^{(n)},$$

one deduces that $\mathfrak{su}(n) \subset \text{Lie}(A, B)$.

If $\text{tr } A = \text{tr } B = 0$, then A and B belong to $\mathfrak{su}(n)$, hence $\mathfrak{su}(n) = \text{Lie}(A, B)$. If $\text{tr } A \neq 0$ or $\text{tr } B \neq 0$, then A or B does not belong to $\mathfrak{su}(n)$ and $\mathfrak{u}(n) = \text{Lie}(A, B)$. This completes the proof of the controllability of the control system (2.1) on $SU(n)$ and $U(n)$.

It remains to prove the controllability on the unit sphere \mathbf{S}^n of \mathbf{C}^n . Fix x_0, x_1 in \mathbf{S}^n , and consider an element of $g_1 \in SU(n)$ such that $g_1 x_0 = x_1$. According to what precedes there exists a trajectory g in $U(n)$ of (2.1) from I_n to g_1 . The curve $t \mapsto g(t)x_0$ is a trajectory of (2.1) in \mathbf{S}^n that links x_0 to x_1 . \square

4 Convexification procedure

4.1 Time-reparametrization

We denote by PC the set of piecewise constant functions $u : [0, \infty) \rightarrow [0, \infty)$ such that there exist $u_1, \dots, u_p > 0$ and $0 = t_1 < \dots < t_{p+1} = T_u$ for which

$$u : t \mapsto \sum_{j=1}^p u_j \chi_{[t_j, t_{j+1})}(t).$$

Let us identify $u = \sum_{j=1}^p u_j \chi_{[t_j, t_{j+1})}$ with the finite sequence $(u_j, \tau_j)_{1 \leq j \leq p}$ where $\tau_j = t_{j+1} - t_j$ for every $1 \leq j \leq p$.

We define the map

$$\begin{aligned} \mathcal{P} : PC &\rightarrow PC \\ (u_j, \tau_j)_{1 \leq j \leq p} &\mapsto \left(\frac{1}{u_j}, u_j \tau_j \right), \end{aligned}$$

which satisfies the following easily verifiable properties.

Proposition 4.1. *For every $u \in PC$, $\mathcal{P} \circ \mathcal{P}(u) = u$ and $\|\mathcal{P}(u)\|_{L^1} = \sum_{i=1}^p \tau_j$.*

Assume that (A, B, U, Φ) satisfies (\mathfrak{A}) . In analogy with Definition 2.3, we define, for every $u = \sum_{j=1}^p u_j \chi_{[t_j, t_{j+1})} \in PC$ such that $u(t) \in U$ for every $t \geq 0$, the solution of

$$\frac{d\psi}{dt}(t) = (u(t)A + B)\psi(t), \quad (4.1)$$

with initial condition $\psi_0 \in \mathcal{H}$ as

$$\psi(t) = e^{(t-t_l)(u_l A + B)} \circ \dots \circ e^{t_1(u_1 A + B)}(\psi_0),$$

where $t_l \leq t \leq t_{l+1}$.

System (4.1) is the time reparametrization of system (2.1) induced by the transformation \mathcal{P} , as stated in the following proposition.

Proposition 4.2. *Let $u = (u_j, \tau_j)_{1 \leq j \leq p}$ belong to PC and ψ_0 be a point of \mathcal{H} . Let ψ be the solution of (2.1) with control u and initial condition ψ_0 , and $\tilde{\psi}$ be the solution of (4.1) with control $\mathcal{P}(u)$ and initial condition ψ_0 . Then $\psi(T_u) = \tilde{\psi}(\|u\|_{L^1})$.*

Proof. It is enough to remark that, if $u \neq 0$, for every $t \in [0, \infty)$, $e^{t(A+uB)} = e^{tu(\frac{1}{u}A+B)}$. \square

As a consequence of Proposition 4.2 it is equivalent to prove controllability for (2.1) with $U = (0, \delta]$ or to prove controllability for system (4.1) with control $u \in [1/\delta, \infty)$.

4.2 Convexification

For every positive integer N let the matrices

$$A^{(N)} = \text{diag}(i\lambda_1, \dots, i\lambda_N) \quad \text{and} \quad B^{(N)} = (\langle \phi_j, B\phi_k \rangle)_{j,k=1}^N =: (b_{jk})_{j,k=1}^N,$$

be the Galerkin approximations at order N of A and B , respectively. Let $t \mapsto \psi(t)$ be a solution of

$$\dot{\psi} = (uA^{(N)} + B^{(N)})\psi,$$

corresponding to a control function u and consider $v(t) = \int_0^t u(\tau)d\tau$. Denote by $d(B)$ the diagonal of $B^{(N)}$ and let $\hat{B}^{(N)} = B^{(N)} - d(B)$. Then $q : t \mapsto e^{-v(t)A^{(N)} - td(B)}\psi(t)$, is a solution of

$$\dot{q}(t) = e^{-v(t)A^{(N)} - td(B)} \hat{B}^{(N)} e^{v(t)A^{(N)} + td(B)} q(t). \quad (\Theta_N)$$

Let us set

$$\vartheta_N(t, v) = e^{-vA^{(N)} - td(B)} \hat{B}^{(N)} e^{vA^{(N)} + td(B)}. \quad (4.2)$$

Lemma 4.3. *Let K be a positive integer and $\gamma_1, \dots, \gamma_K \in \mathbf{R} \setminus \{0\}$ be such that $|\gamma_1| \neq |\gamma_j|$ for $j = 2, \dots, K$. Let*

$$\varphi(t) = (e^{it\gamma_1}, \dots, e^{it\gamma_K}).$$

Then, for every $t_0 \in \mathbf{R}$, we have

$$\overline{\text{conv } \varphi([t_0, \infty))} \supseteq \nu \mathbb{S}^1 \times \{(0, \dots, 0)\},$$

where $\nu = \prod_{k=2}^{\infty} \cos\left(\frac{\pi}{2k}\right) > 0$. Moreover, for every $R > 0$ and $\xi \in \mathbb{S}^1$ there exists a sequence $(t_k)_{k \in \mathbf{N}}$ such that $t_{k+1} - t_k > R$ and

$$\lim_{h \rightarrow \infty} \frac{1}{h} \sum_{k=1}^h \varphi(t_k) = (\nu\xi, 0, \dots, 0).$$

Proof. Since

$$\varphi(t - t_0) = (e^{-it_0\gamma_1} e^{it\gamma_1}, \dots, e^{-it_0\gamma_K} e^{it\gamma_K}), \quad (4.3)$$

it is enough to prove the lemma for $t_0 = 0$. We can suppose that $|\gamma_1| = 1$ and, up to a reordering of the indexes, that there exist n and \tilde{n} such that $1 \leq n \leq \tilde{n} \leq K$, $|\gamma_i| \neq |\gamma_j|$ for every $i, j \in \{1, \dots, n\}$, $\gamma_2, \dots, \gamma_{\tilde{n}} \in \mathbf{Z}$, $\gamma_{\tilde{n}+1}, \dots, \gamma_K \in \mathbf{R} \setminus \mathbf{Z}$, and $\{|\gamma_{n+1}|, \dots, |\gamma_{\tilde{n}}|\} \subset \{|\gamma_2|, \dots, |\gamma_n|\}$.

Consider the 2^{n-1} real numbers defined as follows: let

$$\bar{t}_1 = 0,$$

and for $k \in \{1, \dots, n-1\}$ and $j \in \{1, \dots, 2^{k-1}\}$,

$$\bar{t}_{2^{k-1}+j} = \bar{t}_j + \frac{\pi}{|\gamma_{k+1}|}.$$

Up to a reordering of the \bar{t}_j , we can suppose that $0 = \bar{t}_1 < \bar{t}_2 < \dots < \bar{t}_{2^{n-1}}$. Take an integer r larger than $R/2\pi$, then set $t_j = \bar{t}_j + 2\pi r(j-1)$, in such a way that $t_k - t_{k-1} > R$ for every $k = 2, \dots, 2^{n-1}$.

Now consider the arithmetic mean of the l -th (complex) coordinates of $\varphi(t_1), \dots, \varphi(t_{2^{n-1}})$. We show that this quantity is zero for $l = 2, \dots, \tilde{n}$. Indeed, from the definition of t_j , we have

$$\sum_{j=1}^{2^{n-1}} e^{it_j \gamma_l} = \prod_{k=1}^{n-1} (1 + e^{i\pi \gamma_l / |\gamma_{k+1}|}),$$

which is zero since so is the k -th factor when $|\gamma_l| = |\gamma_{k+1}|$.

On the other hand, the arithmetic mean of the first coordinate is uniformly bounded away from zero. Indeed

$$\begin{aligned} \left| \frac{1}{2^{n-1}} \sum_{j=1}^{2^{n-1}} e^{i\gamma_1 t_j} \right| &= \prod_{k=1}^{n-1} \left| \frac{1 + e^{i\pi \gamma_1 / |\gamma_{k+1}|}}{2} \right| = \prod_{k=2}^n \cos \left(\frac{\pi}{2|\gamma_k|} \right) = \exp \left(\sum_{k=2}^n \log \left(\cos \left(\frac{\pi}{2|\gamma_k|} \right) \right) \right) \\ &\geq \exp \left(\sum_{k=2}^{\infty} \log \left(\cos \left(\frac{\pi}{2k} \right) \right) \right) = \nu. \end{aligned} \quad (4.4)$$

Since $\log \left(\cos \left(\frac{\pi}{2k} \right) \right) \sim -\frac{\pi^2}{8k^2}$ as k tends to infinity, then the sum $\sum_{k \geq 2} \log \left(\cos \left(\frac{\pi}{2k} \right) \right)$ converges to a (negative) finite value l . As a consequence, $\nu = \exp(l)$ is a non-zero positive number.

Therefore we have found a sequence of numbers t_j such that the arithmetic mean of the first coordinate of $\varphi(t_1), \dots, \varphi(t_{2^{n-1}})$ is uniformly bounded away from zero and the arithmetic means of following $\tilde{n} - 1$ coordinates are zero. According to (4.3), the role of $t_1, \dots, t_{2^{n-1}}$ can equivalently be played, for every $k \in \mathbf{N}$, by the 2^{n-1} -uple

$$t_j^k = t_j + 2\pi m k, \quad j = 1, \dots, 2^{n-1},$$

where the integer m is larger than $r + t_{2^{n-1}}/2\pi$. Now, let $l \in \{\tilde{n} + 1, \dots, K\}$, so that $\gamma_l \notin \mathbf{Z}$. For every $h \in \mathbf{N}$, the arithmetic mean of the l -th coordinate of the points $\varphi(t_j^k)$ ($k = 0, \dots, h$, $j = 1, \dots, 2^{n-1}$) is

$$\begin{aligned} \frac{1}{2^{n-1}(h+1)} \sum_{j=1}^{2^{n-1}} \sum_{k=0}^h e^{it_j^k \gamma_l} &= \frac{1}{2^{n-1}(h+1)} \sum_{j=1}^{2^{n-1}} e^{it_j \gamma_l} \sum_{k=0}^h e^{i2\pi m k \gamma_l} \\ &= \left(\frac{1}{2^{n-1}} \sum_{j=1}^{2^{n-1}} e^{it_j \gamma_l} \right) \frac{1}{(h+1)} \frac{1 - e^{i2\pi m(h+1)\gamma_l}}{1 - e^{i2\pi m \gamma_l}} \xrightarrow{h \rightarrow \infty} 0. \end{aligned}$$

Therefore, we found a sequence of points in the convex hull of $\varphi([0, \infty))$ converging to $(2^{1-n} \sum_{j=1}^{2^{n-1}} e^{i\gamma_1 t_j}, 0, \dots, 0)$. The lemma follows from (4.4) and by rotation invariance (see (4.3)). \square

Remark 4.4. In order to estimate ν , notice that, for every x in $(-1, 1)$, $-\frac{x^2}{2} - \frac{x^4}{11} \leq \log(\cos(x))$. Hence, taking $x = \frac{\pi}{2k}$ for $k \geq 2$,

$$\sum_{k=2}^{\infty} \log \left(\cos \left(\frac{\pi}{2k} \right) \right) > -\frac{\pi^2}{8} \sum_{k=2}^{\infty} \frac{1}{k^2} - \frac{\pi^4}{176} \sum_{k=2}^{\infty} \frac{1}{k^4} = -\frac{\pi^8 + 240\pi^4 - 1980\pi^2}{15840}$$

from which one deduces $\nu > \exp \left(-\frac{\pi^8 + 240\pi^4 - 1980\pi^2}{15840} \right) > \frac{2}{5}$. Numerically, one finds $\nu \approx 0.430$.

4.3 An auxiliary system

Let (A, B, U, Φ) satisfy (\mathfrak{A}) . With every non-resonant connectedness chain S for (A, B, U, Φ) and every $n \in \mathbf{N}$ we associate the subset

$$S_n = \{(j, k) \in S \mid 1 \leq j, k \leq n, j \neq k\}$$

of S and the control system on \mathbf{C}^n

$$\dot{x} = \nu |b_{jk}| \left(e^{i\theta} e_{jk}^{(n)} - e^{-i\theta} e_{kj}^{(n)} \right) x, \quad (\Sigma_n)$$

where $\theta = \theta(t) \in \mathbb{S}^1$ and $(j, k) = (j(t), k(t)) \in S_n$ are piecewise constant controls. Recall that $e_{jk}^{(n)}$ is the $n \times n$ matrix whose entries are all zero but the one of index (j, k) which is equal to 1 and that $\nu = \prod_{k=2}^{\infty} \cos\left(\frac{\pi}{2k}\right)$ (see Lemma 4.3).

The control system (Σ_n) is linear in x . For every θ in \mathbb{S}^1 and every $1 \leq j, k \leq n, j \neq k$, the matrix $e^{i\theta} e_{jk}^{(n)} - e^{-i\theta} e_{kj}^{(n)}$ is skew-adjoint with zero trace. Hence the control system (Σ_n) leaves the unit sphere \mathbf{S}^n of \mathbf{C}^n invariant. In order to take advantage of the rich Lie group structure of group of matrices, it is also possible to lift this system in the group $SU(n)$, considering x as a matrix.

4.4 Existence of a n -connectedness chain

Notice that system (Σ_n) cannot be controllable if S is not a n -connectedness chain (see [11, Remark 4.2]). This motivates the following proposition.

Proposition 4.5. *Let (A, B, U, Φ) satisfy (\mathfrak{A}) . If there exists a connectedness chain for (A, B, U, Φ) , then there exists a bijection $\sigma : \mathbf{N} \rightarrow \mathbf{N}$ such that, setting $\hat{\Phi} = (\phi_{\sigma(k)})_{k \in \mathbf{N}}$ and $\hat{S} = \{(\sigma(j), \sigma(k)) : (j, k) \in S\}$, $(A, B, U, \hat{\Phi})$ satisfies (\mathfrak{A}) and \hat{S} is a n -connectedness chain for $(A, B, U, \hat{\Phi})$ for every n in \mathbf{N} .*

Proof. Following [19, Proof of Theorem 4.2], σ can be constructed recursively by setting $\sigma(1) = 1$ and $\sigma(n+1) = \min \alpha(\{\sigma(1), \dots, \sigma(n)\})$, where, for every subset J of \mathbf{N} , $\alpha(J) = \{k \in \mathbf{N} \setminus J \mid \langle \phi_j, B\phi_k \rangle \neq 0 \text{ for some } j \text{ in } J\}$. \square

Proposition 4.5 proves the first part of the statement of Theorem 2.13.

5 Modulus tracking

The aim of this section is to prove the following proposition, which is the main step in the proof of Theorem 2.6.

Proposition 5.1. *Let $\delta > 0$. Let $(A, B, [0, \delta], \Phi)$ satisfy (\mathfrak{A}) and admit a non-resonant connectedness chain. Then, for every continuous curve $\hat{\Upsilon} : [0, T] \rightarrow \mathbf{U}(\mathcal{H})$, \mathfrak{r} in \mathbf{N} , and $\varepsilon > 0$, there exist $T_u > 0$, a continuous increasing bijection $s : [0, T] \rightarrow [0, T_u]$, and a piecewise constant control function $u : [0, T_u] \rightarrow [0, \delta]$ such that the propagator Υ^u of equation (2.1) satisfies*

$$\left| |\langle \phi_j, \hat{\Upsilon}_t \phi \rangle| - |\langle \phi_j, \Upsilon_{s(t)}^u \phi \rangle| \right| < \varepsilon \quad \text{for every } t \in [0, T], j \in \mathbf{N},$$

for every $\phi \in \text{span}\{\phi_1, \dots, \phi_{\mathfrak{r}}\}$ with $\|\phi\| = 1$.

The proof of Proposition 5.1 splits in several steps. In Section 5.1 we recall some classical results of finite dimensional control theory, which, in Section 5.2, are applied to system (Σ_n) introduced in Section 4.3. In Section 5.3 we prove that system (Θ_N) can track in projection the trajectories of system (Σ_n) . Then we prove tracking for the original infinite dimensional system in Section 5.4. The proof of Proposition 5.1 is completed in Section 5.5.

5.1 Tracking: definitions and general facts

Let M be a smooth manifold, U be a subset of \mathbf{R} , and $f : M \times U \rightarrow TM$ be such that, for every x in M and every u in U , $f(x, u)$ belongs to T_xM and $f(\cdot, u)$ is smooth. Consider the control system

$$\dot{x} = f(x, u), \quad (5.1)$$

whose admissible controls are piecewise constant functions $u : \mathbf{R} \rightarrow U$. For a fixed u in U , we denote by f_u the vector field $x \mapsto f(x, u)$.

Definition 5.2 (Tracking). Given a continuous curve $\mathbf{c} : [0, T] \rightarrow M$ we say that system (5.1) can *track up to time reparametrization* the curve \mathbf{c} if for every $\varepsilon > 0$ there exist $T_u > 0$, an increasing bijection $s : [0, T] \rightarrow [0, T_u]$, and a piecewise constant control $u : [0, T_u] \rightarrow U$ such that the solution $x : [0, T_u] \rightarrow M$ of (5.1) with control u and initial condition $x(0) = \mathbf{c}(0)$ satisfies $\text{dist}(x(s(t)), \mathbf{c}(t)) < \varepsilon$ for every $t \in [0, T]$, where $\text{dist}(\cdot, \cdot)$ is a fixed distance compatible with the topology of M . If s can be chosen to be the identity then we say that system (5.1) can track \mathbf{c} *without time reparametrization*.

Notice that this definition is independent of the choice of the distance $\text{dist}(\cdot, \cdot)$. Next proposition gives well-known sufficient conditions for tracking. It is a simple consequence of small-time local controllability (see for instance [12, Proposition 4.3] and [16]).

Proposition 5.3. *If, for every x in M , $\{f(x, u) \mid u \in U\} = \{-f(x, u) \mid u \in U\}$ and $\text{Lie}_x(\{f_u \mid u \in U\}) = T_xM$, then system (5.1) can track up to time reparametrization any continuous curve in M .*

5.2 Tracking in (Σ_n)

We now proceed with the first step of the proof of Proposition 5.1. Using Proposition 5.3 we can prove the following.

Proposition 5.4. *Let (A, B, U, Φ) satisfy (\mathfrak{A}) . Let S be a non-resonant connectedness chain for (A, B, U, Φ) such that, for every n in \mathbf{N} , S is a n -connectedness chain. Then, for every n in \mathbf{N} , the finite dimensional control system (Σ_n) can track up to time reparametrization any curve in $SU(n)$.*

Proof. Recall that $S_n = \{(j, k) \in S \mid 1 \leq j, k \leq n, j \neq k\}$. In order to apply Proposition 5.3 we notice that the set

$$\mathcal{V}(x) = \left\{ \nu |b_{jk}| \left(e^{i\theta} e_{jk}^{(n)} - e^{-i\theta} e_{kj}^{(n)} \right) x : \theta \in \mathbb{S}^1, (j, k) \in S_n \right\}$$

is symmetric with respect to 0 and we are left to prove that the Lie algebra generated by the linear vector fields $x \mapsto \nu |b_{jk}| (e^{i\theta} e_{jk} - e^{-i\theta} e_{kj}) x$ contains the whole tangent space $\mathfrak{su}(n)x$ of the state manifold $SU(n)$. The latter condition is verified if and only if $B^{(n)}$ is connected, as shown in the proof of Proposition 3.1. \square

5.3 Tracking trajectories of (Σ_n) in (Θ_N)

Next proposition states that, for every $N \geq n$, system (Θ_N) , defined in Section 4, can track without time reparametrization, in projection on the first n components, every trajectory of system (Σ_n) .

Hereafter we denote by $\Pi_n^{(N)}$ the projection mapping a $N \times N$ complex matrix to the $n \times n$ matrix obtained by removing the last $N - n$ columns and the last $N - n$ rows.

Proposition 5.5. *Let $\delta > 0$. Let $(A, B, [0, \delta], \Phi)$ satisfy (\mathfrak{A}) and admit a non-resonant connectedness chain S . For every $n, N \in \mathbf{N}$, $N \geq n$, $\varepsilon > 0$ and for every trajectory $x : [0, T] \rightarrow SU(n)$ of system (Σ_n) with initial condition $x(0) = I_n$ there exists a piecewise constant control $u : [0, T] \rightarrow [1/\delta, +\infty)$ such that the solution $y : [0, T] \rightarrow SU(N)$ of system (Θ_N) with initial condition I_N satisfies*

$$\|x(t) - \Pi_n^{(N)}(y(t))\| < \varepsilon \quad \text{for every } t \in [0, T].$$

Proof. Given a trajectory $x(t)$ of system (Σ_n) with initial condition $x(0) = I_n$, denote by $(j, k) = (j(t), k(t)) \in S_n$ and $\theta = \theta(t) \in \mathbb{S}^1$ its corresponding control functions. Being these functions piecewise constant, it is possible to write $[0, T] = \bigcup_{p=0}^q [t_p, t_{p+1}]$ in such a way that j, k , and θ are constant on $[t_p, t_{p+1}]$ for every $p = 0, \dots, q$.

We are going to construct the control u by applying recursively Lemma 4.3. Let $\bar{\delta} > 1/\delta$. Fix $p \in \{0, \dots, q\}$ and j, k, θ such that $(j(t), k(t)) = (j, k)$ and $\theta(t) = \theta$ on $[t_p, t_{p+1}]$. Apply Lemma 4.3 with $\gamma_1 = \lambda_j - \lambda_k$, $\{\gamma_2, \dots, \gamma_K\} = \{\lambda_l - \lambda_m \mid l, m \in \{1, \dots, N\}, b_{lm} \neq 0, \{l, m\} \neq \{j, k\}, \text{ and } l \neq m\}$, $R = \max_{(l,m) \in S_n} \frac{|b_{lm} - b_{mm}|}{|\lambda_l - \lambda_m|} T + \bar{\delta} T$, and $t_0 = t_0(p)$ to be fixed later depending on p . Then, for every $\eta > 0$, there exist $h = h(p) > 1/\eta$ and a sequence $(w_\alpha^p)_{\alpha=1}^h$ such that $w_1^p \geq t_0$, $w_\alpha^p - w_{\alpha-1}^p > R$, and such that

$$\left| \frac{1}{h} \sum_{\alpha=1}^h e^{i(\lambda_k - \lambda_j)w_\alpha^p} - \nu \frac{\bar{b}_{jk}}{|b_{jk}|} e^{i\theta} \right| < \eta,$$

and

$$\left| \frac{1}{h} \sum_{\alpha=1}^h e^{i(\lambda_l - \lambda_m)w_\alpha^p} \right| < \eta,$$

for every $l, m \in \{1, \dots, N\}$ such that $b_{lm} \neq 0$, $\{l, m\} \neq \{j, k\}$, and $l \neq m$.

Set $\tau_\alpha^p = t_p + (t_{p+1} - t_p)\alpha/h$, $\alpha = 0, \dots, h$, and define the piecewise constant function

$$v_\eta(t) = \sum_{p=0}^q \sum_{\alpha=1}^h \left(w_\alpha^p + \tau_\alpha^p \frac{b_{jj} - b_{kk}}{\lambda_k - \lambda_j} \right) \chi_{[\tau_{\alpha-1}^p, \tau_\alpha^p)}(t). \quad (5.2)$$

Note that by choosing $t_0(p) = w_{h(p-1)}^{p-1} + R$ for $p = 1, \dots, q$ and $t_0(0) = R$ we have that $v_\eta(t)$ is non-decreasing.

Set $M(t) = \nu |b_{j(t)k(t)}| \left(e^{i\theta(t)} e_{j(t)k(t)}^{(N)} - e^{-i\theta(t)} e_{k(t)j(t)}^{(N)} \right)$. From the construction of v_η we have

$$\int_0^t \vartheta_N(s, v_\eta(s)) ds \xrightarrow{\eta \rightarrow 0} \int_0^t M(s) ds, \quad (5.3)$$

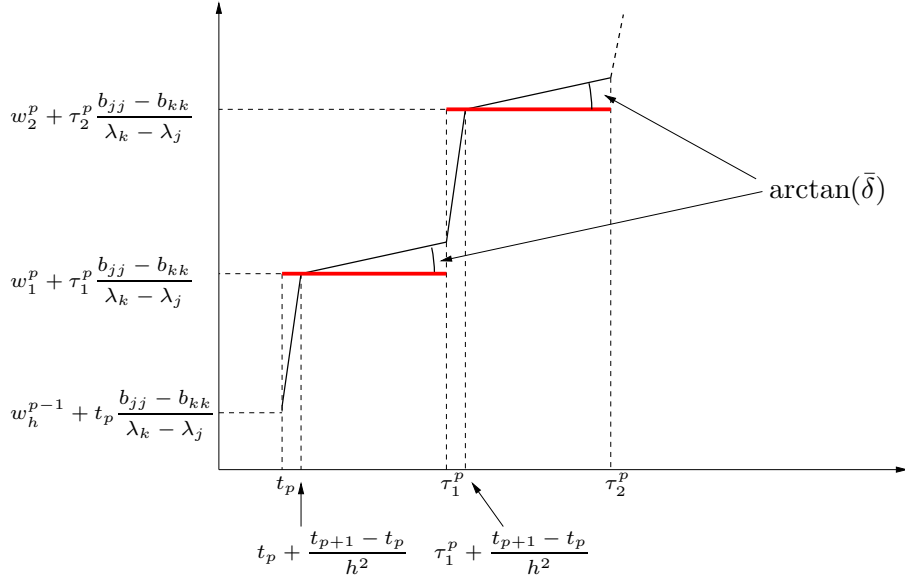


Figure 3: The piecewise constant function v_η (in bold) and the piecewise linear approximation \check{v}_η with slope greater than $\bar{\delta}$.

uniformly with respect to $t \in [0, T]$, where ϑ_N is defined as in (4.2). This convergence guarantees (see for example [2, Lemma 8.2]) that, denoting by $y_\eta(t)$ the solution of system (Θ_N) with control v_η and initial condition I_N , $\Pi_n^{(N)}(y_\eta(t))$ converges to $x(t)$ as η tends to 0 uniformly with respect to $t \in [0, T]$. Hence, for every η sufficiently small,

$$\|\Pi_n^{(N)} \circ y_\eta(t) - x(t)\| < \frac{\varepsilon}{2} \quad \text{for every } t \in [0, T].$$

If the functions v_η were of the type $t \mapsto \int_0^t u(s)ds$ for some $u : [0, T] \rightarrow [1/\delta, \infty)$ piecewise constant, then we would be done. For every $\eta > 0$ consider the piecewise linear continuous function \check{v}_η uniquely defined on every interval $[t_p, t_{p+1})$ by

$$\left\{ \begin{array}{ll} \check{v}_\eta(t_p) = w_h^{p-1} \\ \check{v}_\eta(t) = 0 & \text{if } t \in \bigcup_{\alpha=1}^h [\tau_{\alpha-1}^p, \tau_{\alpha-1}^p + \frac{(t_{p+1}-t_p)}{h^2}), \\ \check{v}_\eta(\tau_{\alpha-1}^p + \frac{(t_{p+1}-t_p)}{h^2}) = w_\alpha^p & \text{for } \alpha = 1, \dots, h, \\ \check{v}_\eta(t) = \bar{\delta} & \text{if } t \in \bigcup_{\alpha=1}^h [\tau_{\alpha-1}^p + \frac{(t_{p+1}-t_p)}{h^2}, \tau_\alpha^p), \end{array} \right.$$

where we set $w_h^{-1} = 0$ (see Figure 5.3). On each interval $[\tau_{l-1}^p + \frac{(t_{p+1}-t_p)}{h^2}, \tau_l^p)$ the difference between v_η and \check{v}_η is bounded in absolute value by $\bar{\delta}(t_{p+1} - t_p)/h$. Therefore,

$$\sup \left\{ \|\vartheta_N(t, v_\eta(t)) - \vartheta_N(t, \check{v}_\eta(t))\| \mid t \in \bigcup_{l,p} \left[\tau_{l-1}^p + \frac{(t_{p+1}-t_p)}{h^2}, \tau_l^p \right) \right\}$$

tends to zero as η tends to 0.

Since $\|\vartheta_N(t, v)\|$ is uniformly bounded with respect to $(t, v) \in [0, T] \times \mathbf{R}$ and the measure of $\bigcup_{l,p} [\tau_{l-1}^p, \tau_{l-1}^p + \frac{(t_{p+1}-t_p)}{h^2})$ goes to 0 as η goes to 0, we have

$$\int_0^t (\vartheta_N(\tau, v_\eta(\tau)) - \vartheta_N(\tau, \check{v}_\eta(\tau))) d\tau \xrightarrow{\eta \rightarrow 0} 0 \quad \text{uniformly with respect to } t \in [0, T].$$

In particular, for η sufficiently small, if \check{y}_η denotes the solution of system (Θ_N) with control \check{v}_η and initial condition I_N , then

$$\|y_\eta(t) - \check{y}_\eta(t)\| < \frac{\varepsilon}{2} \quad \text{for every } t \in [0, T].$$

Finally, u can be taken as the derivative of \check{v}_η , which is defined almost everywhere. \square

5.4 Tracking trajectories of (Σ_n) in the original system

Next proposition extends the tracking property obtained in the previous section from the system (Θ_N) to the infinite dimensional system (4.1). We denote by $\Pi_n : \mathcal{H} \rightarrow \mathbf{C}^n$ the projection mapping $\psi \in \mathcal{H}$ to $(\langle \phi_1, \psi \rangle, \dots, \langle \phi_n, \psi \rangle) \in \mathbf{C}^n$ and we write $\phi_k^{(n)}$ for $\Pi_n \phi_k$.

Proposition 5.6. *Let $\delta > 0$ and let $(A, B, [0, \delta], \Phi)$ satisfy (\mathfrak{A}) . For every $\varepsilon > 0$, $n \in \mathbf{N}$, and for every trajectory $x : [0, T] \rightarrow SU(n)$ of system (Σ_n) with initial condition I_n there exists a piecewise constant function $u : [0, T] \rightarrow [1/\delta, +\infty)$ such that the propagator Υ^u of (4.1) satisfies*

$$\left| |\langle \phi_j^{(n)}, x(t) \Pi_n \phi \rangle| - |\langle \phi_j, \Upsilon_t^u(\phi) \rangle| \right| < \varepsilon$$

for every $\phi \in \text{span}\{\phi_1, \dots, \phi_n\}$ with $\|\phi\| = 1$ and every t in $[0, T]$ and j in \mathbf{N} .

Proof. Consider $\mu > 0$. For every $j \in \mathbf{N}$ the hypothesis that ϕ_j belongs to $D(B)$ implies that the sequence $(b_{jk})_{k \in \mathbf{N}}$ is in ℓ^2 . It is therefore possible to choose $N \geq n$ such that $\sum_{k > N} |b_{jk}|^2 < \mu$ for every $j = 1, \dots, n$. By Proposition 5.5, for every $\eta > 0$ and for every trajectory $x : [0, T] \rightarrow SU(n)$ of system (Σ_n) with initial condition I_n , there exists a piecewise constant control $u^\eta : [0, T] \rightarrow [1/\delta, +\infty)$ such that the solution y^η of system (Θ_N) with initial condition I_N satisfies

$$\|x(t) - \Pi_n^{(N)}(y^\eta(t))\| < \eta.$$

Denote by $R^\eta(t, s) : \mathbf{C}^N \rightarrow \mathbf{C}^N$, $0 \leq s, t \leq T$, the resolvent of system (Θ_N) associated with the control $v^\eta(t) = \int_0^t u^\eta(\tau) d\tau$, so that $y^\eta(t) = R^\eta(t, 0)$. Fix $\phi \in \text{span}\{\phi_1, \dots, \phi_n\}$ with $\|\phi\| = 1$ and set

$$Q^\eta(t) = e^{-v^\eta(t)A - t d(B)} \Upsilon_t^{u^\eta}(\phi).$$

The components of $Q^\eta(t)$, say

$$q_j^\eta(t) = e^{-i\lambda_j v^\eta(t) - t b_{jj}} \langle \phi_j, \Upsilon_t^{u^\eta}(\phi) \rangle, \quad j \in \mathbf{N},$$

satisfy, for almost every $t \in [0, T]$,

$$\dot{q}_j^\eta(t) = \sum_{k=1}^{\infty} b_{jk} e^{i(\lambda_k - \lambda_j) v^\eta(t) + t(b_{kk} - b_{jj})} q_k^\eta(t). \quad (5.4)$$

Therefore $Q_N^\eta(t) = \Pi_N Q^\eta(t) = (q_1^\eta(t), \dots, q_N^\eta(t))^T$ satisfies the time-dependent linear equation

$$\dot{Q}_N^\eta(t) = \vartheta_N(t, v^\eta(t)) Q_N^\eta(t) + P_N^\eta(t),$$

where $P_N^\eta(t) = (\sum_{k > N} b_{1k} e^{i(\lambda_k - \lambda_1) v^\eta(t) + t(b_{kk} - b_{11})} q_k^\eta, \dots, \sum_{k > N} b_{Nk} e^{i(\lambda_k - \lambda_N) v^\eta(t) + t(b_{kk} - b_{NN})} q_k^\eta)^T$. Hence

$$Q_N^\eta(t) = R^\eta(t, 0) \Pi_N \phi + \int_0^t R^\eta(s, t) P_N^\eta(s) ds.$$

Consider the projection of the equality above on the first n coordinates. Notice that, because of the choice of N , the norm of the first n components of $P_N^\eta(t)$ is smaller than $\sqrt{\mu n}$. By (5.3), $R^\eta(s, t)$ converges uniformly, as η tends to 0, to a time-dependent operator from \mathbf{C}^N into itself which preserves the norm of the first n components. Then, there exists η sufficiently small such that

$$\left\| \Pi_n^{(N)} \left(\int_0^t R^\eta(s, t) P_N^\eta(s) ds \right) \right\| < 2T\sqrt{\mu n}.$$

Hence

$$\begin{aligned} \|\Pi_n Q^\eta(t) - x(t)\Pi_n \phi\| &\leq \|\Pi_n Q^\eta(t) - \Pi_n^{(N)}(R^\eta(t, 0))\Pi_n \phi\| + \|\Pi_n^{(N)}(R^\eta(t, 0))\Pi_n \phi - x(t)\Pi_n \phi\| \\ &\leq 2T\sqrt{\mu n} + \eta < \frac{\varepsilon}{2}, \end{aligned} \quad (5.5)$$

if $\mu < \varepsilon^2/(32nT^2)$ and $\eta < T\sqrt{\mu n}$. In particular, for $j = 1, \dots, n$,

$$|\langle \phi_j^{(n)}, x(t)\Pi_n \phi \rangle| - |\langle \phi_j, \Upsilon_t^{u^\eta}(\phi) \rangle| < \frac{\varepsilon}{2}.$$

It remains to prove the statement for $j > n$. From (5.5) it follows

$$\sum_{j=1}^n |q_j^\eta(t)|^2 > \left(1 - \frac{\varepsilon}{2}\right)^2,$$

then, since $\Upsilon_t^{u^\eta}$ is a unitary operator for every t , we have

$$\sum_{j>n} |q_j^\eta(t)|^2 < 1 - \left(1 - \frac{\varepsilon}{2}\right)^2 < \varepsilon. \quad \square$$

5.5 Proof of modulus tracking

The following proposition allows to reduce the tracking problem stated in Proposition 5.1 to the tracking of a curve in $SU(n)$.

Proposition 5.7. *For every continuous curve $\hat{\Upsilon} : [0, T] \rightarrow \mathbf{U}(\mathcal{H})$, $\varepsilon > 0$, and $\mathfrak{r} \in \mathbf{N}$, there exist $n \geq \mathfrak{r}$ and a continuous curve $\mathbf{F}^n : [0, T] \rightarrow SU(n)$ such that $|\langle \phi_j, \hat{\Upsilon}_t \phi_k \rangle - \langle \phi_j^{(n)}, \mathbf{F}^n(t) \phi_k^{(n)} \rangle| < \varepsilon$ for every t in $[0, T]$, $1 \leq k \leq \mathfrak{r}$, and $j \in \mathbf{N}$.*

Proof. For every n in \mathbf{N} , define the function $g_n : t \mapsto \sum_{k=1}^{\mathfrak{r}} \sum_{l=1}^n |\langle \phi_l, \hat{\Upsilon}_t \phi_k \rangle|^2$. The functions g_n are continuous and $g_n(t)$ converges monotonically to \mathfrak{r} as n tends to infinity for every $t \in [0, T]$. Hence g_n converges to the constant function \mathfrak{r} uniformly with respect to $t \in [0, T]$. Therefore, for every $1 \leq k \leq \mathfrak{r}$, $\psi_k^n(t) = \sum_{l=1}^n \langle \phi_l, \hat{\Upsilon}_t \phi_k \rangle \phi_l$ converges to $\hat{\Upsilon}_t \phi_k$ uniformly with respect to $t \in [0, T]$. In particular, the matrix $(\langle \psi_k^n(t), \psi_j^n(t) \rangle)_{j,k=1}^{\mathfrak{r}}$ converges to $I_{\mathfrak{r}}$ uniformly with respect to $t \in [0, T]$.

For every n large enough, the vectors $\psi_1^n(t), \dots, \psi_{\mathfrak{r}}^n(t)$ are linearly independent and can be completed to a basis $\mathcal{B}^n(t) = (\psi_1^n(t), \dots, \psi_{\mathfrak{r}}^n(t), \varphi_{\mathfrak{r}+1}^n(t), \dots, \varphi_n^n(t))$ of $\text{span}\{\phi_1, \dots, \phi_n\}$ depending continuously on $t \in [0, T]$. Let $M^n(t)$ be the $n \times n$ matrix of the components of $\mathcal{B}^n(t)$ with respect to the basis (ϕ_1, \dots, ϕ_n) . Denote by $\mathbf{F}^n(t)$ the matrix whose columns are the Gram–Schmidt transform of the columns of $M^n(t)$. Then, for every n large enough, \mathbf{F}^n satisfies the statement of the proposition. \square

We are now ready to prove Proposition 5.1.

Proof of Proposition 5.1. Thanks to Proposition 4.2, it is sufficient to prove that, for every $\mathbf{r} \in \mathbf{N}$, $\varepsilon > 0$, and every continuous curve $\hat{\Upsilon} : [0, T] \rightarrow \mathbf{U}(\mathcal{H})$, there exist $T_u > 0$, a continuous increasing bijection $s : [0, T] \rightarrow [0, T_u]$, and a piecewise constant control function $u : [0, T_u] \rightarrow [1/\delta, +\infty)$ such that the propagator Υ^u of system (4.1) satisfies

$$|\langle \phi_j, \hat{\Upsilon}_t \phi \rangle - \langle \phi_j, \Upsilon_{s(t)}^u \phi \rangle| < \varepsilon,$$

for every $\phi \in \text{span}\{\phi_1, \dots, \phi_{\mathbf{r}}\}$ with $\|\phi\| = 1$ and every $t \in [0, T]$, $j \in \mathbf{N}$.

By Proposition 5.7 there exist $n \geq \mathbf{r}$ and a continuous curve $\mathbf{F}^n : [0, T] \rightarrow SU(n)$ such that $|\langle \phi_j, \hat{\Upsilon}_t \phi_k \rangle - \langle \phi_j^{(n)}, \mathbf{F}^n(t) \phi_k^{(n)} \rangle| < \varepsilon/3$ for every t in $[0, T]$, $1 \leq k \leq \mathbf{r}$, and $j \in \mathbf{N}$.

By Proposition 5.4, there exists an admissible trajectory $x : [0, T_\Sigma] \rightarrow SU(n)$ of system (Σ_n) with initial condition I_n satisfying

$$\|x(s(t)) - \mathbf{F}^n(t)\| < \frac{\varepsilon}{3} \quad \text{for every } t \in [0, T].$$

Finally, by Proposition 5.6, there exists a piecewise constant function $u : [0, T_\Sigma] \rightarrow [1/\delta, +\infty)$ such that the propagator Υ^u of (4.1) satisfies

$$|\langle \phi_j^{(n)}, x(t) \Pi_n \phi \rangle - \langle \phi_j, \Upsilon_t^u(\phi) \rangle| < \frac{\varepsilon}{3}$$

for every $\phi \in \text{span}\{\phi_1, \dots, \phi_{\mathbf{r}}\}$ with $\|\phi\| = 1$ and every $t \in [0, T_\Sigma]$, $j \in \mathbf{N}$. □

5.6 Estimates of the L^1 norm of the control

We derive now estimates of the minimal L^1 norm of the control u whose existence is asserted in Proposition 5.1. We focus here on the physically relevant transitions inducing permutations between eigenvectors of A .

The strategy to get L^1 estimates is the following. Recall that, instead of considering the control system $\dot{x} = (A + uB)x$ driven by a piecewise continuous function $u : [0, T_u] \rightarrow [0, \delta]$, we have defined the function $\mathcal{P}(u) : [0, \|u\|_{L^1}] \rightarrow [1/\delta, \infty)$ and considered the control system $\dot{x} = (\mathcal{P}(u)A + B)x$. By Propositions 4.1 and 4.2, in order to estimate the L^1 norm of u , it is enough to estimate the time needed to transfer the system $\dot{x} = (uA + B)x$ from a given source to an ε -neighborhood of a given target. We observe that the time needed to transfer $\dot{x} = (uA + B)x$ from one state to an ε -neighborhood of another is smaller than or equal to the time needed to transfer system (Σ_n) between the n -Galerkin approximations of the initial and the final condition for n large enough.

We proceed to the proofs of Proposition 2.8 and Theorem 2.13.

Proof of Proposition 2.8. Let S be a non-resonant chain of connectedness for $(A, B, [0, \delta], \Phi)$. Choose (j, k) in S and let m in \mathbf{N} be such that $m \geq j, k$. The solution $x : \mathbf{R} \rightarrow SU(m)$ of the Cauchy problem

$$\dot{x} = \nu |b_{jk}| \left(e_{jk}^{(m)} - e_{kj}^{(m)} \right) x, \quad x(0) = I_m$$

is a trajectory of (Σ_m) and has the form $x(t) = \exp \left(t\nu |b_{jk}| \left(e_{jk}^{(m)} - e_{kj}^{(m)} \right) \right)$. The matrix $M := x \left(\frac{\pi}{2\nu |b_{jk}|} \right)$ satisfies $M\phi_l^{(m)} = \phi_l^{(m)}$ if $l \neq j, k$, $M\phi_j^{(m)} = -\phi_k^{(m)}$, $M\phi_k^{(m)} = \phi_j^{(m)}$. In other

words, the control system (Σ_m) can exchange (up to a phase factor) the eigenstates j and k of $A^{(m)}$, leaving all the others eigenstates invariant, in time $\frac{\pi}{2\nu|b_{jk}|}$. \square

Proof of Theorem 2.13. Using Proposition 4.5 one may assume that S is a m -connectedness chain for every $m \in \mathbf{N}$. Let us prove by induction that every permutation of $\{1, \dots, m\}$ is a product of at most $2^{m-1} - 1$ transpositions of the form $(j k)$ with $(j, k) \in S \cap \{1, \dots, m\}^2$. Let $h(n)$ be the minimal integer such that every permutation of $\{1, \dots, n\}$ is the product of at most $h(n)$ transpositions of the form $(j k)$ with $(j, k) \in S_m$. For every permutation σ of $\{1, \dots, n+1\}$, either $\sigma(n+1) = n+1$, and σ is generated by at most $h(n)$ transpositions, or $\sigma(n+1) < n+1$. In this case, there exists $1 \leq k \leq n$ such that $(k, n+1) \in S$. Since the product $(k n+1)(k \sigma(n+1))\sigma$ leaves $n+1$ invariant, it is a product of at most $h(n)$ permutations. As a conclusion, $h(n+1) \leq 2h(n) + 1$ and since $h(2) = 1$, we find $h(m) \leq 2^{m-1} - 1$.

The time needed for each of the transpositions $(j k)$ with $(j, k) \in S$ has been computed in Proposition 2.8. The conclusion follows from the estimate $\nu > 2/5$ proved in Remark 4.4. \square

Remark 5.8. The bound given in Theorem 2.13 does not depend on ε . However, it is possible that the time T_u needed to achieve the transfer of system (2.1) grows to infinity as ε tends to zero. When $S = \mathbf{N}^2$ and some $|b_{jk}|$ are much smaller than the others, the bound given by Theorem 2.13 may be too conservative. It is possible to find other estimates by comparing the time needed to steer a permutation with (Σ_m) with ad-hoc metrics on $SU(n)$. The resulting expressions are rather intricate and can be found in [1, Section 5]. In [1] time estimates have been given also for general propagators (i.e., that do not necessarily steer an eigenstate of A to another). This result could be generalized to the case under consideration. It is, however, rather technical and involves advanced notions of Lie group theory.

Following the method of [11, Section 4.5], one can also give a lower bound for the L^1 norm of the control.

Proposition 5.9. *Let (A, B, U, Φ) satisfy (\mathfrak{A}) . For every $\hat{\Upsilon}$ in $\mathbf{U}(\mathcal{H})$, m in \mathbf{N} , $\varepsilon > 0$, $\theta_1, \dots, \theta_n \in \mathbf{R}$, and every piecewise constant function $u : [0, T_u] \rightarrow U$ such that the propagator Υ^u of (2.1) satisfies $\|e^{i\theta_k} \hat{\Upsilon}(\phi_k) - \Upsilon_{T_u}^u(\phi_k)\| \leq \varepsilon$ for $1 \leq k \leq m$, one has*

$$\|u\|_{L^1} \geq \sup_{1 \leq k \leq m} \sup_{j \in \mathbf{N}} \frac{|\langle \phi_j, \phi_k \rangle - |\langle \phi_j, \hat{\Upsilon} \phi_k \rangle| - \varepsilon}{\|B\phi_j\|}.$$

Notice that while some strong assumptions about the existence of connectedness chains are needed in Theorem 2.13, Proposition 5.9 is valid even if (2.1) is not approximately controllable.

6 Phase tuning

Based on Proposition 5.1, we shall now complete the proof of Theorem 2.6, proving approximate simultaneous controllability.

In order to outline the mechanism of the proof, we treat in a first time the case of a single wave function (proving directly the first part of Corollary 2.12) and we then turn, in Section 6.2, to the general case.

6.1 Phase tuning for the control of a single wave function

Simultaneous controllability is obtained from Proposition 5.1 applied both to (2.1) and to its time-reversed version. If $(A, B, [0, \delta], \Phi)$ satisfies (\mathfrak{A}) and admits a non-resonant connectedness chain, then the same is true for $(-A, -B, [0, \delta], \Phi)$. Notice, moreover, that, by unitarity of the evolution of the Schrödinger equation, if $u : [0, T] \rightarrow [0, \delta]$ steers ψ_0 to a ε -neighborhood of ψ_1 for the time-reversed control system

$$\frac{d\psi}{dt}(t) = -(A + u(t)B)\psi(t), \quad u(t) \in [0, \delta], \quad (6.1)$$

then $u(T - \cdot) : [0, T] \rightarrow [0, \delta]$ steers ψ_1 ε -close to ψ_0 for the original system (2.1).

Take any eigenvector $\phi_{\bar{k}}$ such that $\lambda_{\bar{k}} \neq 0$ (its existence clearly follows from the existence of a non-resonant connectedness chain) and consider the control $u : [0, T] \rightarrow [0, \delta]$ steering ψ_0 to a ε -neighborhood of $e^{i\theta}\phi_{\bar{k}}$ for some $\theta \in [0, 2\pi)$. The existence of such a u follows from Proposition 5.1, with $\hat{\Upsilon}$ any continuous curve in $\mathbf{U}(\mathcal{H})$ from the identity to a unitary operator sending ψ_0 into $\phi_{\bar{k}}$ and \mathfrak{r} sufficiently large.

Similarly, there exist $\tilde{u} : [0, \tilde{T}] \rightarrow [0, \delta]$ and $\tilde{\theta} \in [0, 2\pi)$ such that \tilde{u} steers ψ_1 ε -close to $e^{i\tilde{\theta}}\phi_{\bar{k}}$ for (6.1). Let $\tau > 0$ be such that

$$e^{\tau A}(e^{i\theta}\phi_{\bar{k}}) = e^{i\tilde{\theta}}\phi_{\bar{k}}.$$

Hence, the concatenation of u , of the control constantly equal to zero for a time τ , and of $\tilde{u}(\tilde{T} - \cdot)$, steers ψ_0 2ε -close to ψ_1 .

6.2 Phase tuning for simultaneous control

Let r be the number of equations that we would like to control simultaneously, as in Definition 2.10. The scheme of the argument is similar to the one above. The pivotal role of the orbit of $\{e^{tA}\phi_{\bar{k}} \mid t\}$ is now played by a torus of dimension r .

The crucial point is to ensure that an orbit of A “fills” the torus densely enough. This is formally stated in the proposition below. Recall that a subset Ω_1 is ε -dense in a metric space Ω_2 if any point of Ω_2 is at distance smaller than ε from every point of Ω_1 . For every $m \in \mathbf{N}$ and $k_1, \dots, k_m \in \mathbf{N}$, define

$$\begin{aligned} \mathcal{T}(k_1, \dots, k_m) &= \{e^{\theta_1 A}\phi_{k_1} + \dots + e^{\theta_m A}\phi_{k_m} \mid \theta_1, \dots, \theta_m \in \mathbf{R}\} \\ \mathcal{C}(k_1, \dots, k_m) &= \{e^{tA}\phi_{k_1} + \dots + e^{tA}\phi_{k_m} \mid t \in \mathbf{R}\}. \end{aligned}$$

Notice that, if k_1, \dots, k_m are distinct, $\mathcal{T}(k_1, \dots, k_m)$ is diffeomorphic to the torus \mathbb{T}^m .

Proposition 6.1. *Let $(A, B, [0, \delta], \Phi)$ satisfy (\mathfrak{A}) and admit a non-resonant connectedness chain. Assume that, for every $\eta > 0$, there exist r pairwise distinct positive integers $\bar{k}_1, \dots, \bar{k}_r$ such that $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_r)$ is η -dense in $\mathcal{T}(\bar{k}_1, \dots, \bar{k}_r)$. Then (2.1) is simultaneously approximately controllable.*

Proof. Take r orthonormal initial conditions $\psi_0^1, \dots, \psi_0^r$ and r orthonormal final conditions $\psi_1^1, \dots, \psi_1^r$. Fix a tolerance $\eta > 0$. Take $\bar{k}_1, \dots, \bar{k}_r$ as in the statement of the proposition.

According to Proposition 5.1 (with \mathfrak{r} sufficiently large and $\hat{\Upsilon}$ a continuous curve in $\mathbf{U}(\mathcal{H})$ from the identity to a unitary operator sending ψ_0^j to $\phi_{\bar{k}_j}$ for each $j = 1, \dots, r$), there exists

a control $u(\cdot)$ steering simultaneously each ψ_0^j , for $j = 1, \dots, r$, η -close to $e^{\theta_j A} \phi_{\bar{k}_j}$ for some $\theta_1, \dots, \theta_r \in \mathbf{R}$. Similarly, applying Proposition 5.1 to the triple $(-A, -B, [0, \delta], \Phi)$, there exists a control $\tilde{u} : [0, \tilde{T}] \rightarrow [0, \delta]$ steering simultaneously ψ_1^j η -close to $e^{\tilde{\theta}_j A} \phi_{\bar{k}_j}$ for (6.1), for $j = 1, \dots, r$ and for some $\tilde{\theta}_1, \dots, \tilde{\theta}_r \in \mathbf{R}$.

Since the positive orbit of A passing through $\sum_{j=1}^r e^{\theta_j A} \phi_{\bar{k}_j}$ is η -close to $\sum_{j=1}^r e^{\tilde{\theta}_j A} \phi_{\bar{k}_j} \in \mathcal{T}(\bar{k}_1, \dots, \bar{k}_r)$, then the concatenation of $u(\cdot)$, a control constantly equal to zero on a time interval of suitable length, and $\tilde{u}(\tilde{T} - \cdot)$ steers each ψ_0^j 3η -close to ψ_1^j for $j = 1, \dots, r$. \square

We are left to prove that

(P) for every $\eta > 0$, there exist r distinct positive integers $\bar{k}_1, \dots, \bar{k}_r$ such that $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_r)$ is η -dense in $\mathcal{T}(\bar{k}_1, \dots, \bar{k}_r)$.

We split the proof in four cases.

6.2.1 $\dim_{\mathbf{Q}}(\text{span}_{\mathbf{Q}}(\lambda_k)_{k \in \mathbf{N}}) = \infty$

This case is trivial: it is enough to take $\bar{k}_1, \dots, \bar{k}_r$ in such a way that $\lambda_{\bar{k}_1}, \dots, \lambda_{\bar{k}_r}$ are \mathbf{Q} -linearly independent. Then $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_r)$ is dense (hence, η -dense for every $\eta > 0$) in $\mathcal{T}(\bar{k}_1, \dots, \bar{k}_r)$.

6.2.2 The spectrum of A is unbounded

The most physically relevant case is the one in which the sequence $(\lambda_k)_{k \in \mathbf{N}}$ is unbounded.

Fix \bar{k}_1 such that $\lambda_{\bar{k}_1} \neq 0$. Take then \bar{k}_2 such that $|\lambda_{\bar{k}_2}| \gg |\lambda_{\bar{k}_1}|$ in such a way that the orbit $\mathcal{C}(\bar{k}_1, \bar{k}_2)$ is η -dense in $\mathcal{T}(\bar{k}_1, \bar{k}_2)$. By recurrence, taking $|\lambda_{\bar{k}_m}| \gg |\lambda_{\bar{k}_{m-1}}|$ for $m = 2, \dots, r$ we have that $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_m)$ is η -dense in $\mathcal{T}(\bar{k}_1, \dots, \bar{k}_m)$. Indeed, by the recurrence hypothesis, $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_{m-1}) + \mathcal{T}(\bar{k}_m)$ is η -dense in $\mathcal{T}(\bar{k}_1, \dots, \bar{k}_m) = \mathcal{T}(\bar{k}_1, \dots, \bar{k}_{m-1}) + \mathcal{T}(\bar{k}_m)$ and the choice of $\lambda_{\bar{k}_m}$ is such that $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_m)$ is η' -dense in $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_{m-1}) + \mathcal{T}(\bar{k}_m)$ for η' arbitrarily small.

6.2.3 The spectrum of A is bounded and $\dim_{\mathbf{Q}}(\text{span}_{\mathbf{Q}}(\lambda_k)_{k \in \mathbf{N}}) = 1$

The existence of a connectedness chain implies that there exist infinitely many pairwise distinct gaps between eigenvalues of A . Hence, the set of eigenvalues of A has infinite cardinality.

Since all the eigenvalues of A are \mathbf{Q} -linearly dependent, we may assume, without loss of generality, that λ_j is rational for every $j \in \mathbf{N}$. Up to removing the eigenvalues equal to zero, if they exist, and changing the sign of some eigenvalues (which does not affect property **(P)**), we can also assume that

$$\lambda_j = \frac{a_j}{b_j}, \quad \gcd(a_j, b_j) = 1, \quad a_j, b_j > 0$$

for every $j \in \mathbf{N}$. The boundedness and the infinite cardinality of the spectrum of A imply that the sequence $(b_j)_{j \in \mathbf{N}}$ is unbounded.

In order to prove **(P)**, let us make some preliminary considerations. For every $m \in \mathbf{N}$ and $k_1, \dots, k_m \in \mathbf{N}$, denote by $\tau(k_1, \dots, k_m)$ the minimum of all $t > 0$ such that $t\lambda_{k_j}$ belongs to \mathbf{N} for every $j = 1, \dots, m$. Equivalently said, $2\pi\tau(k_1, \dots, k_m)$ is the period of the curve

$s \mapsto e^{sA}\phi_{k_1} + \dots + e^{sA}\phi_{k_m}$. Notice that, if $\lambda_{k_1}, \dots, \lambda_{k_m}$ are integers, then $\tau(k_1, \dots, k_m) = 1/\gcd(a_{k_1}, \dots, a_{k_m})$. In general,

$$\tau(k_1, \dots, k_m) = \frac{b_{k_1} \cdots b_{k_m}}{\gcd(a_{k_l} \prod_{j=1}^{l-1} b_{k_j} \prod_{j=l+1}^m b_{k_j})_{1 \leq l \leq m}}. \quad (6.2)$$

The following lemma guarantees that, for any choice of k_1, \dots, k_{m-1} , we can select k_m in such a way that $\tau(k_1, \dots, k_m) \gg \tau(k_1, \dots, k_{m-1})$.

Lemma 6.2. *Let $m \in \mathbf{N}$. For every $k_1, \dots, k_m \in \mathbf{N}$, there exists $c = c(k_1, \dots, k_m) > 0$ such that, for every $k_{m+1} \in \mathbf{N}$,*

$$\frac{\tau(k_1, \dots, k_{m+1})}{\tau(k_1, \dots, k_m)} \geq \frac{b_{k_{m+1}}}{c}.$$

Proof. From equation (6.2),

$$\frac{\tau(k_1, \dots, k_{m+1})}{\tau(k_1, \dots, k_m)} = b_{k_{m+1}} \frac{\gcd(a_{k_l} \prod_{j=1}^{l-1} b_{k_j} \prod_{j=l+1}^m b_{k_j})_{1 \leq l \leq m}}{\gcd(a_{k_l} \prod_{j=1}^{l-1} b_{k_j} \prod_{j=l+1}^{m+1} b_{k_j})_{1 \leq l \leq m+1}}.$$

The proof consists, then, in showing that $\gcd(a_{k_l} \prod_{j=1}^{l-1} b_{k_j} \prod_{j=l+1}^{m+1} b_{k_j})_{1 \leq l \leq m+1}$ is bounded from above by a constant independent of k_{m+1} . First, notice that

$$\gcd(a_{k_l} \prod_{j=1}^{l-1} b_{k_j} \prod_{j=l+1}^{m+1} b_{k_j})_{1 \leq l \leq m+1} \leq \gcd(a_{k_1} \prod_{j=2}^{m+1} b_{k_j}, a_{k_{m+1}} \prod_{j=1}^m b_{k_j}) =: \Gamma.$$

Set $c_1 = a_{k_1} \prod_{j=2}^m b_{k_j}$ and $c_2 = \prod_{j=1}^m b_{k_j}$ and notice that they do not depend on k_{m+1} .

Write Γ as

$$\gamma_1 \beta_{m+1} = \Gamma = \gamma_2 \alpha_{m+1}$$

where γ_1 and γ_2 divide c_1 and c_2 , respectively, while α_{m+1} and β_{m+1} divide $a_{k_{m+1}}$ and $b_{k_{m+1}}$, respectively. Since $a_{k_{m+1}}$ and $b_{k_{m+1}}$ are relatively prime, then the same is true for α_{m+1} and β_{m+1} . Therefore, α_{m+1} divides γ_1 . Hence, $\Gamma = \alpha_{m+1} \gamma_2 \leq \gamma_1 \gamma_2 \leq c_1 c_2$. \square

We show now how to choose $\bar{k}_1, \dots, \bar{k}_r$ satisfying property **(P)**. We proceed by induction on r . The case $r = 1$ has already been treated in Section 6.1. Assume that $\bar{k}_1, \dots, \bar{k}_{r-1}$ are such that $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_{r-1})$ is η -dense in $\mathcal{T}(\bar{k}_1, \dots, \bar{k}_{r-1})$. Hence, for every choice of \bar{k}_r , the set $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_{r-1}) + \mathcal{T}(\bar{k}_r)$ is η -dense in $\mathcal{T}(\bar{k}_1, \dots, \bar{k}_r)$.

We are left to show that, for a suitable choice of $\bar{k}_r \in \mathbf{N} \setminus \{\bar{k}_1, \dots, \bar{k}_{r-1}\}$, the set $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_r)$ is η' -dense in $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_{r-1}) + \mathcal{T}(\bar{k}_r)$ for η' arbitrarily small. Recall that $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_m)$ is the support of the curve $s \mapsto e^{sA}\phi_{\bar{k}_1} + \dots + e^{sA}\phi_{\bar{k}_m}$, whose period equals $2\pi\tau(\bar{k}_1, \dots, \bar{k}_m)$. Therefore, $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_{r-1})$ is the projection of $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_r)$ along $\phi_{\bar{k}_r}$ on $\phi_{\bar{k}_r}^\perp$. Hence, for every $\psi \in \mathcal{C}(\bar{k}_1, \dots, \bar{k}_{r-1})$ the cardinality of the set $(\psi + \mathcal{T}(\bar{k}_r)) \cap \mathcal{C}(\bar{k}_1, \dots, \bar{k}_r)$ is equal to $\tau(\bar{k}_1, \dots, \bar{k}_r)/\tau(\bar{k}_1, \dots, \bar{k}_{r-1})$. In particular, $(\psi + \mathcal{T}(\bar{k}_r)) \cap \mathcal{C}(\bar{k}_1, \dots, \bar{k}_r)$, which is regularly distributed, is $2\pi\tau(\bar{k}_1, \dots, \bar{k}_{r-1})/\tau(\bar{k}_1, \dots, \bar{k}_r)$ -dense in $\psi + \mathcal{T}(\bar{k}_r)$.

Lemma 6.2 and the unboundedness of the sequence $(b_j)_{j \in \mathbf{N}}$ allow to conclude.

6.2.4 The spectrum of A is bounded and $1 < \dim_{\mathbf{Q}}(\text{span}_{\mathbf{Q}}(\lambda_k)_{k \in \mathbf{N}}) < \infty$

Let $m = \dim_{\mathbf{Q}}(\text{span}_{\mathbf{Q}}(\lambda_k)_{k \in \mathbf{N}})$ and fix a \mathbf{Q} -basis μ_1, \dots, μ_m of $\text{span}_{\mathbf{Q}}(\lambda_k)_{k \in \mathbf{N}}$.

Let

$$\lambda_j = \sum_{l=1}^m \alpha_j^l \mu_l, \quad \alpha_j^1, \dots, \alpha_j^m \in \mathbf{Q}.$$

There exists $l \in \{1, \dots, m\}$ such that the cardinality of $\{\alpha_j^l \mid j \in \mathbf{N}\}$ is infinite. (Otherwise, the set of eigenvalues of A would be finite.) Without loss of generality, $l = 1$.

The results of Sections 6.2.2 and 6.2.3 imply that, for every $\eta > 0$, there exist $\bar{k}_1, \dots, \bar{k}_r \in \mathbf{N}$ such that $\{(e^{it\mu_1 \alpha_{\bar{k}_1}^1}, \dots, e^{it\mu_1 \alpha_{\bar{k}_r}^1}) \mid t \in \mathbf{R}\}$ is η -dense in \mathbb{T}^r . We are going to show that $\mathcal{C}(\bar{k}_1, \dots, \bar{k}_r)$ is $rm\eta$ -dense in $\mathcal{T}(\bar{k}_1, \dots, \bar{k}_r)$ or, equivalently, that $\{(e^{it\lambda_{\bar{k}_1}}, \dots, e^{it\lambda_{\bar{k}_r}}) \mid t \in \mathbf{R}\}$ is $rm\eta$ -dense in \mathbb{T}^r .

Up to a reparameterization, we can assume that $\alpha_{\bar{k}_j}^l \in \mathbf{Z}$ for every $j = 1, \dots, r$ and $l = 1, \dots, m$.

Fix $(e^{i\theta_1}, \dots, e^{i\theta_r})$ in \mathbb{T}^r . The choice of $\bar{k}_1, \dots, \bar{k}_r \in \mathbf{N}$ guarantees the existence of $\bar{t} \in \mathbf{R}$ such that $\|(e^{i\bar{t}\mu_1 \alpha_{\bar{k}_1}^1}, \dots, e^{i\bar{t}\mu_1 \alpha_{\bar{k}_r}^1}) - (e^{i\theta_1}, \dots, e^{i\theta_r})\| < \eta$. Because of the \mathbf{Q} -linear independence of μ_1, \dots, μ_m , there exists $t \in \mathbf{R}$ such that

$$\|(e^{it\mu_1}, e^{it\mu_2}, \dots, e^{it\mu_m}) - (e^{i\bar{t}\mu_1}, 1, \dots, 1)\| < \frac{\eta}{\max\{|\alpha_{\bar{k}_j}^l| \mid j = 1, \dots, r, l = 1, \dots, m\}}.$$

In particular $|e^{it\mu_l \alpha_{\bar{k}_j}^l} - 1| < \eta$ for every $l = 2, \dots, m$ and every $j = 1, \dots, r$.

Hence

$$\begin{aligned} \|(e^{it\lambda_{\bar{k}_1}}, \dots, e^{it\lambda_{\bar{k}_r}}) - (e^{i\theta_1}, \dots, e^{i\theta_r})\| &\leq \|(e^{it\lambda_{\bar{k}_1}}, \dots, e^{it\lambda_{\bar{k}_r}}) - (e^{i\bar{t}\mu_1 \alpha_{\bar{k}_1}^1}, \dots, e^{i\bar{t}\mu_1 \alpha_{\bar{k}_r}^1})\| \\ &\quad + \|(e^{i\bar{t}\mu_1 \alpha_{\bar{k}_1}^1}, \dots, e^{i\bar{t}\mu_1 \alpha_{\bar{k}_r}^1}) - (e^{i\theta_1}, \dots, e^{i\theta_r})\| \\ &\leq \sum_{j=1}^r |e^{i\bar{t}\mu_1 \alpha_{\bar{k}_j}^1} \dots e^{i\bar{t}\mu_m \alpha_{\bar{k}_j}^m} - e^{i\theta_j}| + \eta \\ &\leq (r(m-1) + 1)\eta. \end{aligned}$$

This concludes the proof of property **(P)** and of Theorem 2.11. \square

7 Example: Infinite potential well

We consider now the case of a particle confined in $(-1/2, 1/2)$. This model has been extensively studied by several authors in the last few years and was the first quantum system for which a positive controllability result has been obtained. Beauchard proved exact controllability in some dense subsets of L^2 using Coron's return method (see [5, 7] for a precise statement). Nersesyan obtained approximate controllability results using Lyapunov techniques. In the following, we extend these controllability results to simultaneous controllability and provide some estimates of the L^1 norm of controls achieving the transfer between two density matrices.

The Schrödinger equation writes

$$i \frac{\partial \psi}{\partial t} = -\frac{1}{2} \frac{\partial^2 \psi}{\partial x^2} - u(t)x\psi(x, t) \quad (7.1)$$

with the boundary conditions $\psi(-1/2, t) = \psi(1/2, t) = 0$ for every $t \in \mathbf{R}$.

In this case $\mathcal{H} = L^2((-1/2, 1/2), \mathbf{C})$ endowed with the Hermitian product $\langle \psi_1, \psi_2 \rangle = \int_{-1/2}^{1/2} \overline{\psi_1(x)} \psi_2(x) dx$. The operators A and B are defined by $A\psi = i\frac{1}{2} \frac{\partial^2 \psi}{\partial x^2}$ for every ψ in $D(A) = (H_2 \cap H_0^1)((-1/2, 1/2), \mathbf{C})$, and $B\psi = ix\psi$.

Unfortunately, due to the numerous resonances, we are not able to apply directly our results to system (7.1). A classical approach is in this case to use perturbation theory. Indeed, consider for every η in $[0, \delta]$, the operator $A_\eta = A + \eta B$. The controllability of system (7.1) with control in $[0, \delta]$ is equivalent to the controllability of

$$\frac{d\psi}{dt} = A_\eta \psi + v B \psi$$

with controls v taking values in $[-\eta, \delta - \eta]$. Since the perturbation $\eta \mapsto A_\eta$ is analytic, the self-adjoint operator A_η admits a complete set of eigenvectors $(\phi_k(\eta))_{k \in \mathbf{N}}$ associated with the eigenvalues $(i\lambda_k(\eta))_{k \in \mathbf{N}}$, with ϕ_k and λ_k analytic (see [17]). For $\eta = 0$,

$$\phi_k(0) = \begin{cases} x \mapsto 2 \cos(k\pi x) & \text{when } k \text{ is odd} \\ x \mapsto 2 \sin(k\pi x) & \text{when } k \text{ is even} \end{cases}$$

is a complete set of eigenvectors of A associated with the eigenvalues $i\lambda_k(0) = i\frac{k^2\pi^2}{2}$. Following [7, Proposition 2.3], one can compute the 2-jet at zero of the analytic functions λ_k :

$$\lambda_k(\eta) = \frac{k^2\pi^2}{2} + \left(\frac{1}{24\pi^2 k^2} - \frac{5}{8\pi^4 k^4} \right) \eta^2 + o(\eta^2),$$

as η goes to zero. For every k_1, k_2, p_1, p_2 in \mathbf{N} , since $\frac{1}{\pi^2}$ is transcendental on \mathbf{Q} ,

$$\begin{aligned} \lambda_{k_1}''(0) - \lambda_{k_2}''(0) = \lambda_{p_1}''(0) - \lambda_{p_2}''(0) &\Leftrightarrow \begin{cases} \frac{1}{k_1^2} - \frac{1}{k_2^2} = \frac{1}{p_1^2} - \frac{1}{p_2^2} \\ \frac{1}{k_1^4} - \frac{1}{k_2^4} = \frac{1}{p_1^4} - \frac{1}{p_2^4} \end{cases} \\ \Leftrightarrow \begin{cases} \frac{1}{k_1^2} - \frac{1}{k_2^2} = \frac{1}{p_1^2} - \frac{1}{p_2^2} \\ \left(\frac{1}{k_1^2} - \frac{1}{k_2^2} \right) \left(\frac{1}{k_1^2} + \frac{1}{k_2^2} \right) = \left(\frac{1}{p_1^2} - \frac{1}{p_2^2} \right) \left(\frac{1}{p_1^2} + \frac{1}{p_2^2} \right) \end{cases} &\Leftrightarrow \begin{cases} k_1 = p_1 \\ k_2 = p_2. \end{cases} \end{aligned}$$

Hence, the 2-jets of the gaps between two eigenvalues are all different at zero. Recall that $\langle \phi_k, B\phi_{k+1} \rangle \neq 0$. An argument similar to the one in [11, Proposition 6.2] ensures that for every $\varepsilon > 0$ there exists $0 < \eta < \varepsilon$ such that $\{(j, j+1), (j+1, j) \mid j \in \mathbf{N}\}$ is a non-resonant connectedness chain for $(A_\eta, B, [-\eta, \delta - \eta], \Phi)$.

We can now apply Theorem 2.11 to obtain simultaneous approximate controllability for (7.1) and Theorem 2.13 to get L^1 estimates. For instance, for every $\varepsilon > 0$ there exist $T > 0$ and a piecewise constant function $u : [0, T] \rightarrow [0, \delta]$ such that the propagator at time T of (7.1) exchanges (up to a correction of size ε) the density matrices

$$\frac{1}{3}\phi_1(0)\phi_1(0)^* + \frac{2}{3}\phi_2(0)\phi_2(0)^* \quad \text{and} \quad \frac{1}{3}\phi_2(0)\phi_2(0)^* + \frac{2}{3}\phi_1(0)\phi_1(0)^*$$

and

$$\|u\|_{L^1} \leq \frac{\pi}{2\nu |\langle \phi_1(0), B\phi_2(0) \rangle|} = \frac{9\pi^3}{32\nu} \approx 20.2656.$$

The control time T satisfies $T \geq \frac{1}{\delta} \|u\|_{L^1}$ and, from Proposition 5.9, the control u has to satisfy

$$\|u\|_{L^1} \geq (1 - \epsilon) \max \left\{ \frac{2\sqrt{3}\pi}{\sqrt{\pi^2 - 6}}, \frac{2\sqrt{6}\pi}{\sqrt{2\pi^2 - 3}} \right\} \approx (1 - \epsilon) 5.5323.$$

8 Orientation of a bipolar molecule in the plane by means of two external fields

We present here an example of approximately controllable quantum system. (See [25, 26, 27] and references therein.) It provides a simple model for the control by two electric fields of the rotation of a bipolar rigid molecule confined to a plane (see Figure 2). Molecular orientation and alignment are well-established topics in the quantum control of molecular dynamics both from the experimental and theoretical point of view.

The model we aim to consider can be represented by a Schrödinger equation on the circle $\mathbb{S}^1 = \mathbf{R}/2\pi\mathbf{Z}$, so that $\mathcal{H} = L^2(\mathbb{S}^1, \mathbf{C})$. In this case $A = i \partial^2 / \partial \theta^2$ has discrete spectrum and its eigenvectors are trigonometric functions. The controlled Schrödinger equation is

$$i \frac{\partial \psi(\theta, t)}{\partial t} = \left(-\frac{\partial^2}{\partial \theta^2} + u_1(t) \cos(\theta) + u_2(t) \sin(\theta) \right) \psi(\theta, t). \quad (8.1)$$

We assume that both u_1 and u_2 are piecewise constant and take values in $[0, \delta]$, $\delta > 0$.

Notice that system (8.1) is not controllable if we fix one control to zero. Indeed, by parity reasons, the potential $\cos(\theta)$ does not couple an odd wave function with an even one and the potential $\sin(\theta)$ does not couple wave functions with the same parity.

For every $\alpha \in \mathbb{S}^1$, let us split \mathcal{H} as $\mathcal{H}_e^\alpha \oplus \mathcal{H}_o^\alpha$, where \mathcal{H}_e^α (respectively, \mathcal{H}_o^α) is the closed subspace of \mathcal{H} of even (respectively, odd) functions with respect to α . Notice that \mathcal{H}_e^α and \mathcal{H}_o^α are Hilbert spaces. A complete orthonormal system for \mathcal{H}_e^α (respectively, \mathcal{H}_o^α) is given by $\{\cos(k(\cdot - \alpha)) / \sqrt{\pi}\}_{k=0}^\infty$ (respectively, $\{\sin(k(\cdot - \alpha)) / \sqrt{\pi}\}_{k=1}^\infty$). Let us write $\psi = \psi_e^\alpha + \psi_o^\alpha$, where $\psi_e^\alpha \in \mathcal{H}_e^\alpha$ and $\psi_o^\alpha \in \mathcal{H}_o^\alpha$.

Our first result states that, once α is fixed, the even or the odd part of a wave function ψ can be approximately controlled, under the constraint that their L^2 -norms are preserved.

Lemma 8.1. *Let $\psi \in \mathcal{H}$ and $\alpha \in [0, \pi/2]$. Then for every $\varepsilon > 0$ and every $\tilde{\psi} \in \mathcal{H}_e^\alpha$ such that $\|\psi_e^\alpha\|_{\mathcal{H}} = \|\tilde{\psi}\|_{\mathcal{H}}$, there exists a piecewise constant control $u = (u_1, u_2)$ steering ψ to a wave function whose even part with respect to α lies in an ε -neighborhood of $\tilde{\psi}$. Similarly, for every $\varepsilon > 0$ and every $\tilde{\psi} \in \mathcal{H}_o^\alpha$ such that $\|\psi_o^\alpha\|_{\mathcal{H}} = \|\tilde{\psi}\|_{\mathcal{H}}$, there exists a piecewise constant control u steering ψ to a wave function whose odd part with respect to α lies in an ε -neighborhood of $\tilde{\psi}$.*

Proof. The idea is to apply Theorem 2.6 to a subsystem of (8.1) corresponding to the choice of a subclass of wave functions and a subclass of admissible controls.

More precisely, let

$$\mathcal{U}_\alpha = \{u : \mathbf{R} \rightarrow [0, \delta]^2 \text{ piecewise constant} \mid u(t) \text{ is proportional to } (\cos \alpha, \sin \alpha) \text{ for all } t \in \mathbf{R}\}.$$

The control system whose dynamics are described by (8.1) with admissible control functions restricted to \mathcal{U}_α can be rewritten as

$$i\frac{\partial\psi(\theta,t)}{\partial t} = \left(-\frac{\partial^2}{\partial\theta^2} + v(t)\cos(\theta-\alpha)\right)\psi(\theta,t), \quad v \in \left(0, \delta\sqrt{1 + \min\{\tan\alpha, \cotan\alpha\}^2}\right). \quad (8.2)$$

Notice that the spaces \mathcal{H}_e^α and \mathcal{H}_o^α are invariant for the evolution of (8.2), whatever the choice of $v = v(\cdot)$, since they are invariant both for $A = i\frac{\partial^2}{\partial\theta^2}$ and for the multiplicative operator $B^\alpha : \mathcal{H} \rightarrow \mathcal{H}$ defined by $(B^\alpha\phi)(\theta) = \cos(\theta-\alpha)\phi(\theta)$.

We shall consider (8.2) as a control system defined on \mathcal{H}_e^α (the second part of the statement of the lemma can be proved similarly by considering its dynamics restricted to \mathcal{H}_o^α).

Denote by A_e^α and B_e^α the restrictions of A and B^α to \mathcal{H}_e^α . Choose as orthonormal basis of eigenfunctions for A_e^α the sequence defined by $\phi_k(\theta) = \cos(k(\theta-\alpha))/\sqrt{\pi}$ for $k \in \mathbf{N}$. The eigenvalue of A associated with ϕ_k is $i\lambda_k = -ik^2$.

Then $\langle\phi_j, B_e^\alpha\phi_k\rangle \neq 0$ if and only if $|k-j|=1$. We take as connectedness chain the set $\{(k,j) \in \mathbf{N}^2 \mid |k-j|=1\}$. Since $\lambda_{k+1} - \lambda_k = -2k-1$, then the connectedness chain is non-resonant. Theorem 2.6 implies that (8.2) can be steered from ψ_e^α to an ε -neighborhood of any $\tilde{\psi} \in \mathcal{H}_e^\alpha$ such that $\|\psi_e^\alpha\| = \|\tilde{\psi}\|$ by an admissible control $v(\cdot)$. The conclusion follows by applying $u(\cdot) = (v(\cdot)\cos\alpha, v(\cdot)\sin\alpha)$ to (8.1) (since \mathcal{H}_e^α and \mathcal{H}_o^α are invariant by the flow generated by $u(\cdot)$). \square

The main result of this section states that (8.1) is approximately controllable.

Proposition 8.2. *System (8.1) is approximately controllable.*

Proof. It is enough to prove that every wave function of norm one can be steered arbitrarily close to the constant $1/\sqrt{2\pi}$. Indeed, if ψ and $\tilde{\psi}$ have norm one, if the control $u(\cdot)$ steers the initial condition ψ ε -close to the constant $1/\sqrt{2\pi}$, and if $\tilde{u}(\cdot)$ steers the conjugate of $\tilde{\psi}$ ε -close to the same constant $1/\sqrt{2\pi}$, then the concatenation of u and of the time reversed of \tilde{u} steers ψ 2ε -close to $\tilde{\psi}$.

Fix $\psi \in \mathcal{H}$ of norm one, a tolerance $\varepsilon > 0$, and choose $\alpha \in (0, \pi/2)$. Fix $\bar{\varepsilon} = \varepsilon(1 - 1/\sqrt{2})$. Then, according to Lemma 8.1, ψ can be steered to a wave function ψ_1 such that $\|\psi - \psi_1\| < \bar{\varepsilon}$, where ψ_1 is of the form

$$\psi_1 = \frac{\|\psi_e^\alpha\|}{\sqrt{2\pi}} + \phi_1, \quad \text{with } \phi_1 \in \mathcal{H}_o^\alpha.$$

If $\|\phi_1\|$ is smaller than $\varepsilon/2$ then we are done. Indeed, ϕ_1 has L^2 -norm equal to $\sqrt{1 - \|\psi_e^\alpha\|^2}$, which implies that $1 - \|\psi_e^\alpha\| < \varepsilon^2/4$. Then

$$\begin{aligned} \left\|\tilde{\psi} - \frac{1}{\sqrt{2\pi}}\right\| &\leq \|\tilde{\psi} - \psi_1\| + \left\|\psi_1 - \frac{1}{\sqrt{2\pi}}\right\| < \bar{\varepsilon} + \sqrt{(\|\psi_e^\alpha\| - 1)^2 + \|\phi_1\|^2} \\ &= \bar{\varepsilon} + \sqrt{2}\sqrt{1 - \|\psi_e^\alpha\|} < \bar{\varepsilon} + \frac{1}{\sqrt{2}}\varepsilon = \varepsilon. \end{aligned}$$

Assume then that $\|\phi_1\| \geq \varepsilon/2$ and consider, for every $\beta \in \mathbb{S}^1$, $\tau_\beta = \|(\phi_1)_e^\beta\|^2$. We can characterize τ_β in terms of the coefficients a_k of the representation

$$\phi_1(\cdot) = \sum_{k=1}^{\infty} a_k \frac{\sin(k(\cdot - \alpha))}{\sqrt{\pi}}.$$

Indeed,

$$\begin{aligned}\tau_\beta^2 &= \sum_{k=1}^{\infty} \left| \langle \phi_1(\cdot), \cos(k(\cdot - \beta))/\sqrt{\pi} \rangle \right|^2 = \sum_{k=1}^{\infty} \left| \langle a_k \sin(k(\cdot - \alpha))/\sqrt{\pi}, \cos(k(\cdot - \beta))/\sqrt{\pi} \rangle \right|^2 \\ &= \sum_{k=1}^{\infty} |a_k \sin((\beta - \alpha)k)|^2.\end{aligned}$$

There exists $c > 0$ independent of k and α such that

$$\int_0^{\frac{\pi}{2}} \sin^2((\beta - \alpha)k) d\beta \geq c,$$

hence,

$$\int_0^{\frac{\pi}{2}} \sum_{k=1}^{\infty} |a_k|^2 \sin^2((\beta - \alpha)k) d\beta \geq c \sum_{k=1}^{\infty} |a_k|^2 = c \|\phi_1\|^2,$$

from which we conclude that there exists $\beta \in (0, \pi/2)$ such that

$$\tau_\beta \geq \frac{2c}{\pi} \|\phi_1\|^2 \geq \frac{c}{2\pi} \varepsilon^2.$$

Notice now that the even part of ψ_1 with respect to β has norm

$$\|(\psi_1)_e^\beta\| = \sqrt{\|\psi_e^\alpha\|^2 + \tau_\beta} \geq \sqrt{\|\psi_e^\alpha\|^2 + \frac{c\varepsilon^2}{2\pi}}.$$

Repeating the same argument as above replacing ψ by ψ_1 we conclude that it is then possible to steer ψ at a distance smaller than $\bar{\varepsilon}$ from the sum ψ_2 of a positive constant function of norm larger than $\sqrt{\|\psi_e^\alpha\|^2 + \frac{c\varepsilon^2}{2\pi}}$ and a function $\phi_2 \in \mathcal{H}_o^\beta$ of norm $\|\phi_2\| < \|\phi_1\|$. If $\|\phi_2\| < \varepsilon/2$ then we are done. Otherwise, since the improvement in the size of the constant is bounded from below by a quantity that does not depend on ϕ_1 , we can iterate the procedure finitely many times up to guaranteeing that the final wave function is ε -close to the constant $1/\sqrt{2\pi}$. \square

A Appendix: relations between controllability notions

Proposition A.1. *Let (A, B, U, Φ) satisfy (\mathfrak{A}) . Then*

- (i) *for every r in \mathbf{N} , $\varepsilon > 0$, and $\hat{\Upsilon}$ in $\mathbf{U}(\mathcal{H})$ there exists a piecewise constant control $u : [0, T] \rightarrow U$ such that $\|\hat{\Upsilon}\phi_k - \Upsilon_T^u\phi_k\| < \varepsilon$ for every $1 \leq k \leq r$,*

implies

- (ii) *(2.1) is controllable in the sense of densities matrices*

which implies

- (iii) *for every r in \mathbf{N} , $\varepsilon > 0$, and $\hat{\Upsilon}$ in $\mathbf{U}(\mathcal{H})$ there exist $\theta_1, \dots, \theta_r \in \mathbf{R}$ and a piecewise constant control $u : [0, T] \rightarrow U$ such that $\|e^{i\theta_k}\hat{\Upsilon}(\phi_k) - \Upsilon_T^u(\phi_k)\| < \varepsilon$ for every $1 \leq k \leq r$.*

Proof. Let us prove that (i) implies (ii). Fix two unitarily equivalent density matrices ρ_0 and ρ_1 . Write $\rho_0 = \sum_{k \in \mathbf{N}} P_k v_k v_k^*$ with $(v_k)_{k \in \mathbf{N}}$ an orthonormal sequence in \mathcal{H} and $(P_k)_{k \in \mathbf{N}}$ a sequence in $\ell^1([0, 1])$ such that $\sum_k P_k = 1$. By assumption, there exists $\hat{\Upsilon}$ in $\mathbf{U}(\mathcal{H})$ such that $\rho_1 = \hat{\Upsilon} \rho_0 \hat{\Upsilon}^* = \sum_{k \in \mathbf{N}} P_k \hat{\Upsilon}(v_k) \hat{\Upsilon}(v_k)^*$.

Let m in \mathbf{N} be such that $\sum_{k > m} P_k < \varepsilon$ and r in \mathbf{N} be such that $\|v_j - \sum_{k=1}^r \langle \phi_k, v_j \rangle \phi_k\| < \varepsilon$ for every $j = 1, \dots, m$. By hypothesis, there exists a piecewise constant function $u : [0, T] \rightarrow U$ such that $\|\hat{\Upsilon}(\phi_k) - \Upsilon_T^u(\phi_k)\| < \varepsilon/r$ for every $1 \leq k \leq r$. Hence, for $j = 1, \dots, m$,

$$\begin{aligned} \|\hat{\Upsilon}(v_j) - \Upsilon_T^u(v_j)\| &= \left\| \sum_{k=1}^{\infty} \langle \phi_k, v_j \rangle (\hat{\Upsilon}(\phi_k) - \Upsilon_T^u(\phi_k)) \right\| \\ &\leq \sum_{k=1}^r \|\langle \phi_k, v_j \rangle (\hat{\Upsilon}(\phi_k) - \Upsilon_T^u(\phi_k))\| + \left\| \hat{\Upsilon} \left(\sum_{k=r+1}^{\infty} \langle \phi_k, v_j \rangle \phi_k \right) \right\| \\ &\quad + \left\| \Upsilon_T^u \left(\sum_{k=r+1}^{\infty} \langle \phi_k, v_j \rangle \phi_k \right) \right\| \\ &\leq \varepsilon + 2 \left\| v_j - \sum_{k=1}^r \langle \phi_k, v_j \rangle \phi_k \right\| \leq 3\varepsilon. \end{aligned}$$

Then, recalling that for every θ in \mathbf{R} , a, b in \mathcal{H} , $\|aa^* - bb^*\| \leq \|aa^* - e^{i\theta}ba^* + e^{i\theta}ba^* - bb^*\| \leq \|a\| \|a - e^{i\theta}b\| + \|b\| \|e^{i\theta}a^* - b^*\| \leq (\|a\| + \|b\|) \|a - e^{i\theta}b\|$, we get

$$\begin{aligned} \|\Upsilon_T^u \rho_0 \Upsilon_T^{u*} - \rho_1\| &\leq \sum_{j=1}^m P_j \|\Upsilon_T^u(v_j) \Upsilon_T^u(v_j)^* - \hat{\Upsilon}(v_j) \hat{\Upsilon}(v_j)^*\| + 2\varepsilon \\ &\leq \sum_{j=1}^m P_j (\|\Upsilon_T^u(v_j)\| + \|\hat{\Upsilon}(v_j)\|) \|\Upsilon_T^u(v_j) - \hat{\Upsilon}(v_j)\| + 2\varepsilon \\ &\leq 6\varepsilon + 2\varepsilon = 8\varepsilon, \end{aligned}$$

which concludes the first part of the proof.

Assume now that (ii) holds true. Fix $\varepsilon, r \in \mathbf{N}$, and $\hat{\Upsilon}$ as in the hypotheses. Choose $a_1, \dots, a_r \in \mathbf{R}$ such that $0 < a_1 < a_2 < \dots < a_r$ and $\sum_{k=1}^r a_k = 1$. Define the two unitarily equivalent density matrices

$$\rho_0 = \sum_{k=1}^r a_k \phi_k \phi_k^* \quad \text{and} \quad \rho_1 = \sum_{k=1}^r a_k \hat{\Upsilon}(\phi_k) \hat{\Upsilon}(\phi_k)^*.$$

By assumption, there exists a piecewise constant $u : [0, T] \rightarrow U$ such that

$$\|\rho_1 - \Upsilon_T^u \rho_0 \Upsilon_T^{u*}\| < C\varepsilon, \tag{A.1}$$

where $C = \min\{a_j, |a_k - a_l| \mid 1 \leq j, k, l \leq r, k \neq l\}/2$. Choose $1 \leq k_0 \leq r$ and test (A.1) on $\Upsilon_T^u \phi_{k_0}$

$$\left\| a_{k_0} \Upsilon_T^u \phi_{k_0} - \sum_{k=1}^r a_k \langle \hat{\Upsilon}(\phi_k), \Upsilon_T^u \phi_{k_0} \rangle \hat{\Upsilon}(\phi_k) \right\| < C\varepsilon.$$

Since $(\hat{\Upsilon}(\phi_k))_k$ is an Hilbert basis of \mathcal{H} , then

$$\Upsilon_T^u \phi_{k_0} = \sum_{k=1}^{\infty} \langle \hat{\Upsilon}(\phi_k), \Upsilon_T^u \phi_{k_0} \rangle \hat{\Upsilon}(\phi_k),$$

and hence

$$\left\| \sum_{k=1}^r (a_{k_0} - a_k) \langle \hat{\Upsilon}(\phi_k), \Upsilon_T^u \phi_{k_0} \rangle \hat{\Upsilon}(\phi_k) + a_{k_0} \sum_{k>r} \langle \hat{\Upsilon}(\phi_k), \Upsilon_T^u \phi_{k_0} \rangle \hat{\Upsilon}(\phi_k) \right\| < C\varepsilon.$$

In particular we have

$$\left\| \sum_{k \neq k_0} \langle \hat{\Upsilon}(\phi_k), \Upsilon_T^u \phi_{k_0} \rangle \hat{\Upsilon}(\phi_k) \right\| < \frac{\varepsilon}{2}.$$

For ε small enough, this leads to $|\langle \hat{\Upsilon}(\phi_{k_0}), \Upsilon_T^u \phi_{k_0} \rangle| > \sqrt{1 - \varepsilon^2/4} > 1 - \varepsilon/2$. Hence, there exists $\theta_{k_0} \in \mathbf{R}$ such that $\|e^{i\theta_{k_0}} \hat{\Upsilon}(\phi_{k_0}) - \Upsilon_T^u(\phi_{k_0})\| < \varepsilon$. \square

Proposition A.2. *Under the hypotheses of Proposition A.1 and if, moreover, $\langle \phi_j, B\phi_k \rangle$ is purely imaginary for every $j, k \in \mathbf{N}$, then (iii) implies (ii).*

Proof. First of all, because of the hypotheses on B , system (2.1) satisfies the following time-reversibility property: If $\psi : [0, T] \rightarrow \mathcal{H}$ is a solution of (2.1) with control $u(\cdot)$, then $\varphi(t) = \sum_{k=1}^{\infty} \overline{\langle \phi_k, \psi(T-t) \rangle} \phi_k$ is a solution of (2.1) with control $u(T - \cdot)$.

Fix two unitarily equivalent density matrices ρ_0 and ρ_1 . Write $\rho_0 = \sum_{k \in \mathbf{N}} P_k v_k v_k^*$ with $(v_k)_{k \in \mathbf{N}}$ an orthonormal sequence in \mathcal{H} and $(P_k)_{k \in \mathbf{N}}$ a sequence in $\ell^1([0, 1])$ such that $\sum_{k \in \mathbf{N}} P_k = 1$. Let $\hat{\Upsilon}$ in $\mathbf{U}(\mathcal{H})$ be such that $\rho_1 = \hat{\Upsilon} \rho_0 \hat{\Upsilon}^* = \sum_{k \in \mathbf{N}} P_k \hat{\Upsilon}(v_k) \hat{\Upsilon}(v_k)^*$.

Let $r \in \mathbf{N}$ be such that $\sum_{k>r} P_k < \varepsilon$. By hypothesis there exist a control $u : [0, T_u] \rightarrow [0, \delta]$ and $\theta_1, \dots, \theta_r \in \mathbf{R}$ such that $\|e^{i\theta_k} \sum_{j=1}^{\infty} \overline{\langle \phi_j, v_k \rangle} \phi_j - \Upsilon_{T_u}^u(\phi_k)\| < \varepsilon$ for every $1 \leq k \leq r$. By time reversibility the control $u(T_u - \cdot)$ steers $e^{-i\theta_k} v_k$ ε -close to ϕ_k . Now, there exist a control $w : [0, T_w] \rightarrow [0, \delta]$ and $\hat{\theta}_1, \dots, \hat{\theta}_r$ such that

$$\|e^{i\hat{\theta}_k} \hat{\Upsilon}(v_k) - \Upsilon_{T_w}^w(\phi_k)\|.$$

Let \tilde{u} be the concatenation of the controls $u(T_u - \cdot)$ and w . Then

$$\|e^{i\hat{\theta}_k} \hat{\Upsilon}(v_k) - \Upsilon_{T_{\tilde{u}}}^{\tilde{u}}(e^{-i\theta_k} v_k)\| < 2\varepsilon.$$

Finally,

$$\begin{aligned} \|\Upsilon_{T_{\tilde{u}}}^{\tilde{u}} \rho_0 \Upsilon_{T_{\tilde{u}}}^{\tilde{u}*} - \rho_1\| &\leq \sum_{k=1}^r P_k \|\Upsilon_{T_{\tilde{u}}}^{\tilde{u}}(e^{-i\theta_k} v_k) \Upsilon_{T_{\tilde{u}}}^{\tilde{u}*}(e^{-i\theta_k} v_k)^* - \hat{\Upsilon}(v_k) \hat{\Upsilon}(v_k)^*\| + \\ &\quad + \sum_{k=r+1}^{\infty} P_k \|\Upsilon_{T_{\tilde{u}}}^{\tilde{u}}(v_k) \Upsilon_{T_{\tilde{u}}}^{\tilde{u}*}(v_k)^* - \hat{\Upsilon}(v_k) \hat{\Upsilon}(v_k)^*\| \\ &\leq 4\varepsilon \sum_{k=1}^r P_k + 2\varepsilon \leq 6\varepsilon. \end{aligned}$$

This concludes the proof. \square

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