On some open questions in bilinear quantum control

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***Abstract*— The aim of this paper is to provide a short introduction to modern issues in the control of infinite dimensional closed quantum systems, driven by the bilinear Schrödinger equation.**

The first part is a quick presentation of some of the numerous recent developments in the fields. This short summary is intended to demonstrate the variety of tools and approaches used by various teams in the last decade. In a second part, we present four examples of bilinear closed quantum systems. These examples were extensively studied and may be used as a convenient and efficient test bench for new conjectures. Finally, we list some open questions, both of theoretical and practical interest.

I. INTRODUCTION

A. Control of quantum systems

The state of a quantum system (e.g. a charged particle) evolving on a Riemannian manifold Ω is described by its wave function ψ, an element of $L^2(\Omega, \mathbf{C})$. When the system is submitted to an external field (e.g. an electric field), the time evolution of the wave function is given by the Schrödinger equation

$$\mathrm{i}\frac{\partial \psi}{\partial t} = (-\Delta + V(x))\psi + uW(x)\psi(t), \quad x \in \Omega$$

where Δ is the Laplace-Beltrami operator on Ω, V is a potential describing the system in absence of control, u is the scalar (time variable) intensity of the external field and $W : \Omega \to \mathbf{R}$ is a potential accounting for the properties of the external field.

A natural question, with many practical applications, is to determine how to build (if it is possible) a control u that steers the wave function ψ from a given source to a given target.

B. Framework and notations

We set the problem in a more abstract framework. In a separable Hilbert space H, endowed with the Hermitian product $\langle , \rangle$, we consider the following control system

$$\frac{d}{dt}\psi = (A + u(t)B)\psi, \tag{1}$$

where (A, B) satisfies Assumption 1.

Assumption 1: (A, B) is a pair of (possibly unbounded) linear operators in H such that

1) A is skew-adjoint on its domain $D(A)$;
2) there exists a Hilbert basis $(\phi_k)_{k\in\mathbf{N}}$ of H made of eigenvectors of A: for every k, $A\phi_k = \mathrm{i}\lambda_k\phi_k$ with λ_k in $\mathbf{R}$ and λ_k tends to $-\infty$ as k tends to ∞ ;
3) for every j in $\mathbf{N}$, ϕ_j belongs to $D(B)$, the domain of B;
4) there exists $U \subset \mathbf{R}$ containing at least 0 and 1 such that $A+uB$ is essentially skew-adjoint (not necessarily with domain $D(A)$) for every u in U;
5) $\langle B\phi_j, \phi_k\rangle = 0$ for every j, k in $\mathbf{N}$ such that $\lambda_j = \lambda_k$ and $j \neq k$.

If (A, B) satisfies Assumption 1, for every u in U, $A+uB$ generates a unitary group of propagators $t \mapsto e^{t(A+uB)}$. By concatenation, one can define the solution of (1) for every piecewise constant functions u taking value in U, for every initial condition ψ_0 given at time t_0. We denote this solution $t \mapsto \Upsilon^u_{t,t_0}\psi_0$. To the best of our knowledge, it is not possible to define the propagator Υ^u for controls u that are not piecewise constant in the general framework of Assumption 1. With some extra regularity assumptions, it is possible to extend the definition of Υ^u to more general controls. For instance, if B is bounded, Υ admits a continuous extension to the set $L^1(\mathbf{R}, \mathbf{R})$ (see [1, Proposition 1.1]).

The framework of Assumption 1 is, in one sense, too general for the purpose of quantum mechanics. For instance, it includes the example of Section I-A with $H = L^2(\Omega, \mathbf{C})$ and V any L^∞ function. Following Cohen-Tannoudji et al., [2, Figure 7a, page 35 and Section II-A-1, page 94], one of the most physically relevant cases is precisely the one where the potentials V and W and the wave functions are smooth.

> "From a physical point of view, it is clear that the set $L^2(\Omega, \mathbf{C})$ is too wide in scope: given the meaning attributed to $|\psi(x,t)|^2$, the wave functions which are actually used possess certain properties of regularity. We can only retain the functions $\psi(x,t)$ which are everywhere defined, continuous, and infinitely differentiable"

This is the main motivation for the notion of weak-coupling (see [3]).

Definition 1: Let $k > 0$. A pair (A, B) satisfying Assumption 1 is k-weakly-coupled if

1) for every u in $\mathbf{R}$, $A+uB$ is skew-adjoint with domain $D(A)$;
2) for every $u \in \mathbf{R}$, $D(|A + uB|^{k/2}) = D(|A|^{k/2})$;

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3) there exists $d \geq 0$ and $r < k$ such that $\|B\psi\| \leq d\||A|^{r/2}\psi\|$ for every ψ in $D(|A|^{k/2})$;
4) there exists a constant C such that, for every ψ in $D(|A|^k)$, $|\Re\langle |A|^k\psi, B\psi\rangle| \leq C|\langle |A|^k\psi, \psi\rangle|$.

If (A, B) is k-weakly-coupled, the *coupling constant* $c_k(A, B)$ of system (A, B) of order k is the quantity

$$\sup_{\psi \in D(|A|^k)|A\psi \neq 0} \frac{|\Re\langle |A|^k\psi, B\psi\rangle|}{|\langle |A|^k\psi, \psi\rangle|}.$$

We denote by $PC(U)$ the set of piecewise constant functions u such that there exists two sequences $0 = t_1 < t_2 < \ldots < t_{p+1}$ and $u_1, u_2, \ldots, u_p$ in $U \setminus \{0\}$ with

$$u = \sum_{j=1}^{p} u_j \mathbf{1}_{[t_j, t_{j+1})}.$$

The operators A and B can be represented by infinite dimensional matrices in the basis $(\phi_k)_{k\in\mathbf{N}}$. For every j, k, we denote $b_{jk} = \langle \phi_j, B\phi_k\rangle$. For every N, the orthogonal projection $\pi_N : H \to H$ on the space spanned by the first N eigenvectors of A is defined by

$$\pi_N(x) = \sum_{k=1}^{N} \langle \phi_k, x\rangle \phi_k \qquad \text{for every } x \text{ in } H.$$

Let $\mathcal{L}_N$ be the range of π_N. The *compressions* of A and B at order N are the finite rank operators $A^{(N)} = \pi_N A_{|\mathcal{L}_N}$ and $B^{(N)} = \pi_N B_{|\mathcal{L}_N}$ respectively. The *Galerkin approximation* of (1) of order N is the system in $\mathcal{L}_N$

$$\dot{x} = (A^{(N)} + uB^{(N)})x, \tag{2}$$

whose propagator is denoted with $X^u_{(N)}$.

A pair (j, k) in $\mathbf{N}^2$ is a *non-degenerate* (also called *non-resonant*) transition of (A, B) if $b_{jk} \neq 0$ and, for every l, m, $|\lambda_j - \lambda_k| = |\lambda_l - \lambda_m|$ implies $\{j, k\} = \{l, m\}$ or $\{l, m\} \cap \{j, k\} = \emptyset$.

A subset S of $\mathbf{N}^2$ is a *chain of connectedness* of (A, B) if for every j, k in $\mathbf{N}$, there exists a finite sequence $p_1 = j, p_2, \ldots, p_r = k$ for which $(p_l, p_{l+1}) \in S$ and $\langle \phi_{p_{l+1}}, B\phi_{p_l}\rangle \neq 0$ for every $l = 1, \ldots, r-1$. A chain of connectedness S of (A, B) is *non-degenerate* if every element of S is a non-degenerate transition of (A, B).

C. Content of the paper

Sections II and III present a short review of results available in the literature about exact and approximate controllability of infinite dimensional bilinear quantum systems. Section IV collects four examples of bilinear quantum systems that were extensively studied in the last decade. Finally, we suggest five questions in Section V that we think both important and natural.

II. EXACT CONTROLLABILITY

A. Obstructions to exact controllability

The first result about bilinear control is a general negative result due to Ball, Marsden and Slemrod [4]. It was adapted to the case of bilinear quantum systems by Turinici [5] in the following form:

Proposition 1 ([5]): Let (A, B) satisfy Assumption 1 and B be bounded. Then, for every $r > 1$, for every ψ_0 in $D(A)$, the attainable set from ψ_0 with controls in L^r, $\{\Upsilon^u_{t,0}\psi_0 | u \in L^r(\mathbf{R}, \mathbf{R})\}$ is a countable union of closed sets with empty interior in $D(A)$. In particular, this attainable set has empty interior in $D(A)$.

Proposition 1 admits a natural extension in the case of weakly-coupled systems:

Proposition 2 ([3, Proposition 2]): Let (A, B) be k weakly-coupled and B be bounded. Then, for every ψ_0 in $D(|A|^{k/2})$, for every u in $L^1(\mathbf{R}, \mathbf{R})$, for every $t \geq 0$, $\Upsilon^u_{t,0}\psi_0$ belongs to $D(|A|^{k/2})$. In particular, $\{\Upsilon^u_{t,0}\psi_0 | u \in L^1(\mathbf{R}, \mathbf{R})\}$ has empty interior in $D(|A|^{r/2})$ for every $r < k$.

Most of the bilinear quantum systems encountered in the literature are k weakly-coupled for every $k > 0$. Notice that the eigenvectors of A are in $D(|A|^k)$ for every k. As a consequence, the attainable set for such a system from any eigenvector of A is contained in $\cap_{k>0} D(|A|^k)$, the intersection of all the iterated domains of A.

B. Attainable set of the infinite square potential well

The results of Section II-A do not exclude exact controllability on a sufficiently small subset of H. In a series of paper ([6], [7]), Beauchard *et al.* determined the attainable set for the infinite square potential well.

Theorem 3: Consider the bilinear Schrödinger equation

$$\mathrm{i}\frac{\partial \psi}{\partial t} = -\Delta\psi + ux\psi(t), \quad x \in (0, 1).$$

The attainable set with L^2 controls from the first eigenstate of the Laplacian is exactly the intersection of the unit sphere of $L^2((0, 1), \mathbf{C})$ with $H^3_{(0)} = \{\psi \in H^3((0, 1), \mathbf{C}) \mid \psi(0) = \psi(1) = \psi''(0) = \psi''(1) = 0\}$.

III. APPROXIMATE CONTROLLABILITY

A. Lyapunov techniques

Because of the specific features of quantum systems and, in particular, of the effects of the measurements on its evolution, classical closed-loop control strategies cannot be directly implemented in the Schrödinger framework. Nevertheless, the strategy consisting in identifying a Lyapunov function that measures the distance from the desired final state (or the distance from a trajectory that one wants to track) and that can be forced to decrease towards zero by a suitable state-dependent choice of the control parameter can be used to obtain, via simulation, open-loop control laws that approximately steer the system towards the prescribed goal. This approach has been explored in [8] and refined in [9] for systems evolving in a finite-dimensional Hilbert space H. The proof of the convergence towards the goal adapts the classical Jurdjevic–Quinn method [10] and is based on the LaSalle invariance principle.

In the case where H is infinite-dimensional, generalizations of the previously mentioned results have been obtained by suitably adapting LaSalle invariance principle (see, in particular, [11], [1], [12], [13] for the case where the drift operator of the bilinear Schrödinger equation has discrete-spectrum).

B. Geometric techniques: general case

Definition 2: Let (A, B) satisfy Assumption 1, (j, k) be a pair of integers such that $\lambda_j \neq \lambda_k$ and $u^* : \mathbf{R} \to U$ be $T = 2\pi/|\lambda_j - \lambda_k|$-periodic and not almost everywhere zero. The number

$$\mathrm{Eff}_{(j,k)}(u^*) = \frac{\left|\int_0^T u^*(\tau) e^{\mathrm{i}(\lambda_j - \lambda_k)\tau} \mathrm{d}\tau\right|}{\int_0^T |u^*(\tau)| \mathrm{d}\tau}$$

is called the *efficiency* of u^* with respect to the transition (j, k) of (A, B).

Proposition 4 ([14, Theorem 1]): Let (A, B) satisfy Assumption 1 and U be such that $U/n \subset U$ for every $n \in \mathbf{N}$. Let $(1, 2)$ be a non-degenerate transition of (A, B). If $u^* : \mathbf{R} \to U$ is $2\pi/|\lambda_1 - \lambda_2|$-periodic with $\mathrm{Eff}_{(1,2)}(u^*) \neq 0$ and $\mathrm{Eff}_{(j,k)}(u^*) = 0$ for every j, k such that $|\lambda_j - \lambda_k| \in \mathbf{N}|\lambda_2 - \lambda_1|$ and $\{j, k\} \neq \{1, 2\}$, then there exists $T^* > 0$ such that $|\langle \phi_2, \Upsilon^{u^*/n}_{nT^*,0} \phi_1 \rangle|$ tends to 1 as n tends to infinity.

Proposition 5: Let (A, B) satisfy Assumption 1 and admit a non-degenerate chain of connectedness. Then, for every $\varepsilon > 0$, for every unitary operator $\hat{\Upsilon}$ in $\mathbf{U}(H)$, for every n in $\mathbf{N}$, there exists a piecewise constant function $u_\varepsilon : [0, T_\varepsilon] \to U$ such that $\|\Upsilon^u_{T_\varepsilon,0} \phi_j - \hat{\Upsilon} \phi_j\| < \varepsilon$ for $1 \leq j \leq n$.

Proof: The original proof given in [15] is a particular case of Proposition 4 (see [15, Proof of Lemma 4.3] for an explicit construction of u^*). This proof is valid if U accumulates at zero. Thanks to [16, Proposition 3], one can replace the sequence u^*/n by a sequence of controls taking value in $\{0, 1\}$. ■

Proposition 6: Let (A, B) satisfy Assumption 1 and admit a non-degenerate chain of connectedness S. Then, for every $\varepsilon > 0$, for every (j, k) in S, there exists a piecewise constant function $u_\varepsilon : [0, T_\varepsilon] \to U$ such that $\|\Upsilon^u_{T_\varepsilon,0} \phi_j - \phi_k\| < \varepsilon$ and

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

Proof: In the case where U accumulates at zero, this is [15, Proposition 2.8]. The general case $U = \{0, 1\}$ follows from [16, Proposition 3]. ■

A lower bound of the L^1 norm of the control needed to induce a transfer from a wave function ψ_a in the unit sphere of H is given by [17, Proposition 4.6]:

$$\sup_{n \in \mathbf{N}} \frac{\big||\langle \phi_n, \psi_a \rangle| - |\langle \phi_n, \Upsilon^u_{t,0} \psi_a \rangle|\big|}{\|B\phi_n\|} \leq \int_0^t |u(\tau)| \mathrm{d}\tau$$

for every (A, B) satisfying Assumption 1, every $t \geq 0$, and every piecewise constant u taking value in U.

C. Geometric techniques: weakly-coupled systems

Proposition 7 ([3, Proposition 2]): Let (A, B) satisfy Assumption 1 and be k-weakly-coupled. Then, for every $\psi_0 \in D(|A|^{k/2})$, $K > 0$, $T \geq 0$, and u piecewise constant such that $\|u\|_{L^1} < K$, one has $\left\| |A|^{\frac{k}{2}} \Upsilon^u_T(\psi_0) \right\| \leq e^{c_k(A,B)K} \||A|^{\frac{k}{2}} \psi_0\|$.

Proposition 8 ([3, Proposition 4]): Let k in $\mathbf{N}$ and (A, B) satisfy Assumption 1 and be k-weakly-coupled. Then for every $\varepsilon > 0$, $s < k$, $K > 0$, $n \in \mathbf{N}$, and $(\psi_j)_{1 \leq j \leq n}$ in $D(|A|^{k/2})^n$ there exists $N \in \mathbf{N}$ such that for every piecewise constant function u

$$\|u\|_{L^1} < K \Rightarrow \||A|^{\frac{s}{2}} (\Upsilon^u_t(\psi_j) - X^u_{(N)}(t, 0) \pi_N \psi_j)\| < \varepsilon,$$

for every $t \geq 0$ and $j = 1, \ldots, n$.

Remark 1: Notice that, in Propositions 7 and 8, the upper bound of the $|A|^{k/2}$ norm of the solution of (1) or the bound on the error between the infinite dimensional system and its finite dimensional approximation only depend on the L^1 norm of the control, not on the time.

The a priori bound for the $|A|^{k/2}$ norm combined with an interpolation argument allows to deduce approximate controllability in $|A|^{r/2}$ norm from the approximate controllability in A^0 norm (i.e., the norm of H):

Proposition 9: Let (A, B) satisfy Assumption 1, be k-weakly-coupled and admit a non-degenerate chain of connectedness. Then, for every $\varepsilon > 0$, for every n in $\mathbf{N}$, for every unitary operator $\hat{\Upsilon}$ in $\mathbf{U}(H)$, for every $r < k/2$, there exists $u_\varepsilon : [0, T_\varepsilon] \to \{0, 1\}$ such that $\||A|^r (\hat{\Upsilon} \phi_j - \Upsilon^{u_\varepsilon}_{T_\varepsilon,0} \phi_j)\| < \varepsilon$ for $j \leq n$.

Proof: This would be [3, Proposition 5] if the controls u_ε took value in $(0, 1)$. The case $U = \{0, 1\}$ follows from [16, Proposition 3]. ■

D. Other results

Let us mention in this section some other results concerning quantum control problems on infinite-dimensional spaces which do not satisfy Assumption 1.

First of all, some papers deal with the case where the drift Hamiltonian has some continuous spectrum and consider the problem of approximately controlling between the eigenstates corresponding to the discrete part of the spectrum. In particular, in [18] Mirrahimi considers the case of a drift operator of the form $-\Delta + V$ on $\mathbf{R}^d$, where V is a potential decaying at infinity. The controllability is proved using a Lyapunov technique and estimating the interaction with continuum spectrum thanks to Strichartz estimates.

Another important class of systems exhibiting continuous spectrum is obtained by considering the ensemble control of Bloch equations. The corresponding system consists in a continuum of finite-dimensional systems coupled by the control parameter only. Each system of the ensemble is parameterized by a characteristic frequency. Controllability results in this setting have been obtained in [19], [20], [21].

Other interesting class of problems is given by models for a quantum oscillator coupled with a spin (see [22], [23]). The spectrum in this case is discrete, but it *intrinsically* presents degenerate transitions. The controllability results are obtained exploiting the presence of more than one control.

Let us finally mention the widely used adiabatic methods. They require the use of several controls (not only one, as in Equation (1)) and rely on adiabatic theory and the interesections of eigenvalues. Approximate controllability is obtained through slow variations of the different controls (see [24]).

IV. FOUR EXAMPLES

A. Infinite square potential well

The first example we consider describes a particle confined in a 1D box $(0, \pi)$. This model has been extensively studied by several authors in the last few years and it has been the first quantum system for which a positive controllability result has been obtained. Beauchard proved exact controllability in some dense subsets of L^2 first using Coron's return method ([6]), then standard linear test ([7]). Nersesyan obtained approximate controllability results using Lyapunov techniques ([11], [13]), which allowed to obtain the global result (i.e., Theorem 3 recalled in Section II-B).

The Schrödinger equation writes

$$\mathrm{i}\frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \psi}{\partial x^2} - u(t)x\psi(x,t) \tag{3}$$

with boundary conditions $\psi(0,t) = \psi(\pi,t) = 0$ for every $t \in \mathbf{R}$.

With our notations, $H = L^2\left((0,\pi), \mathbf{C}\right)$ endowed with the Hermitian product $\langle \psi_1, \psi_2 \rangle = \int_0^\pi \overline{\psi_1(x)}\psi_2(x)dx$. The operators A and B are defined by $A\psi = \mathrm{i}\frac{1}{2}\frac{\partial^2 \psi}{\partial x^2}$ for every ψ in $D(A) = (H_2 \cap H_0^1)\left((0,\pi), \mathbb{C}\right)$, and $B\psi : x \mapsto \mathrm{i}x\psi(x)$. A Hilbert basis of H is $(\phi_k)_{k\in\mathbf{N}}$ with $\phi_k : x \mapsto \sin(kx)/\sqrt{2}$. For every k, $A\phi_k = -\mathrm{i}(k^2/2)\phi_k$.

For every j, k in $\mathbf{N}$,

$$b_{jk} = \langle \phi_j, B\phi_k \rangle = \begin{cases} (-1)^{j+k}\frac{2jk}{(j^2-k^2)^2} & \text{if } j-k \text{ odd} \\ 0 & \text{otherwise.} \end{cases}$$

Despite numerous degenerate transitions, the system is approximately controllable (see [15, Section 7]).

One can directly check that (A, B) is 2-weakly-coupled. By Proposition 2, the system cannot be k-weakly-coupled for $k > 3$ (since the attainable set from any eigenvector of A contains the intersection of the unit L^2 sphere with $H^3_{(0)} = D(|A|^{3/2})$).

For example of control designs and numerical simulations, we refer to [25, Section IV].

B. Harmonic oscillator

The quantum harmonic oscillator is among the most important examples of quantum system (see, for instance, [26, Complement G_V]). Its controlled version has been extensively studied (see, for instance, [27], [28]). In this example $H = L^2(\mathbf{R}, \mathbf{C})$ and equation (1) reads

$$\mathrm{i}\frac{\partial \psi}{\partial t}(x,t) = \frac{1}{2}(-\Delta + x^2)\psi(x,t) + u(t)x\psi(x,t). \tag{4}$$

A Hilbert basis of H made of eigenvectors of A is given by the sequence of the Hermite functions $(\phi_n)_{n\in\mathbf{N}}$, associated with the sequence $(-\mathrm{i}\lambda_n)_{n\in\mathbf{N}}$ of eigenvalues where $\lambda_n = n - 1/2$ for every n in $\mathbf{N}$. In the basis $(\phi_n)_{n\in\mathbf{N}}$, B admits a tri-diagonal structure

$$\langle \phi_j, B\phi_k \rangle = \begin{cases} -\mathrm{i}\sqrt{\frac{k}{2}} & \text{if } j = k-1, \\ -\mathrm{i}\sqrt{\frac{k+1}{2}} & \text{if } j = k+1, \\ 0 & \text{otherwise.} \end{cases}$$

For every k in $\mathbf{N}$, the system (A, B) is k-weakly-coupled (see [3]) and

$$c_k(A,B) \quad \leq \quad 3^k - 1.$$

The quantum harmonic oscillator is not controllable (in any reasonable sense) as proved in [27]. However, the Galerkin approximations of (4) of every order are exactly controllable (see [29]), and Proposition 8 ensures that any trajectory of the infinite dimensional system is a uniform limit of trajectories of its Galerkin approximations. This is not a contradiction, since Proposition 8 does not say that every trajectory of every Galerkin approximation is close to the trajectory of the infinite-dimensional system having the same initial condition and corresponding to the same control. What happens for the quantum oscillator is that if one wants to steer the Galerkin approximation of order N of (4) from a given state (say, the first eigenstate) to an ε-neighbourhood of another given target (say, the second eigenstate), the L^1 norm of the control blows up as N tends to infinity. It is compatible with Proposition 8 that the sequence of these trajectories does not converge to a trajectory of (4).

To obtain an estimate of the order N of the Galerkin approximation whose dynamics remains ε close to the one of the infinite dimensional system when using control with L^1-norm K, one can use [3, Remark 8] and we find that $\|X_u^{(N)}(t,0)\phi_1 - \pi_N \Upsilon_t^u \phi_1\| \leq \varepsilon$ provided $\|u\|_{L^1} \leq K$ and

$$\frac{2^{N-1}\sqrt{N+2}}{(N-1)!}\sqrt{\frac{(2N)!}{(N+1)!}}K^N < \varepsilon.$$

For instance, if $K = 3$ and $\varepsilon = 10^{-4}$, this is true for $N = 413$.

C. Planar rotation of a linear molecule

The next example involves a bilinear Schrödinger equation on a manifold with non-trivial topology.

We consider a rigid bipolar molecule rotating in a plane. Its only degree of freedom is the rotation around its centre of mass. The molecule is submitted to an electric field of constant direction with variable intensity u. The orientation of the molecule is an angle in $\Omega = SO(2) \simeq \mathbf{R}/2\pi\mathbf{Z}$. The dynamics is governed by the Schrödinger equation

$$\mathrm{i}\frac{\partial \psi(\theta,t)}{\partial t} = \left(-\frac{\partial^2}{\partial \theta^2} + u(t)\cos\theta\right)\psi(\theta,t), \quad \theta \in \Omega.$$

Note that the parity (if any) of the wave function is preserved by the above equation. We consider then the Hilbert space $H = \{\psi \in L^2(\Omega, \mathbf{C}) : \psi \text{ odd}\}$, endowed with the Hilbert product $\langle f, g \rangle = \int_\Omega \bar{f}g$. The eigenvalue of the skew-adjoint operator $A = \mathrm{i}\frac{\partial^2}{\partial \theta^2}$ associated with the eigenfunction $\phi_k : \theta \mapsto \sin(k\theta)/\sqrt{\pi}$ is $-\mathrm{i}\lambda_k = -\mathrm{i}k^2$, $k \in \mathbf{N}$. The domain of $|A|^k$ is the Hilbert space $H_e^k = \{\psi \in H^{2k}(\Omega, \mathbf{C}) : \psi \text{ odd}\}$. The skew-symmetric operator $B = -\mathrm{i}\cos\theta$ is bounded on $D(|A|^{k/2})$ for every k. For every k in $\mathbf{N}$, (A, B) is k-weakly-coupled ([3, proposition 8]). For every k in $\mathbf{N}$, $c_k(A,B) \leq \frac{2^{2k}-1}{2}$.

From the point of view of the controllability problem, notice that the operator B couples only adjacent eigenstates, that is, $\langle \phi_l, B\phi_j \rangle = 0$ if and only if $|l-j| > 1$. Since $\lambda_{l+1} - \lambda_l = 2l+1$ then $\{(j,l) \in \mathbf{N}^2 : |l-j| = 1\}$ is a non-degenerate connectedness chain for (A,B). Therefore, by [3, Proposition 5] the system provides an example of approximately controllable system in norm $H^k(\Omega, \mathbf{C})$ for every k. Note that, since the eigenstates are in $H^k(\Omega, \mathbf{C})$ for every k then the reachable set from any eigenstate is contained in $H^k(\Omega, \mathbf{C})$ for every k.

D. Everywhere dense attainable set and no Good Galerkin Approximation

To the best of our knowledge, the following academic example does not appear in the physics literature. For α in $\mathbf{N}$, consider the following bilinear Schrödinger equation

$$\mathrm{i}\frac{\partial \psi}{\partial t} = \left[\left(-\frac{1}{2}\Delta + x^2 \right)^{\alpha} + \left(-\frac{1}{2}\Delta + x^2 \right)^{-1} \right] \psi + u(t) x^4 \psi(x,t), \qquad x \in \mathbf{R}. \tag{5}$$

This strongly perturbed harmonic oscillator checks the controllability conditions of [15, Proposition 2.8], with H equal to the set of even L^2 functions on $\mathbf{R}$, $A = -\mathrm{i}[(-\Delta/2 + x^2)^{\alpha} + (-\Delta/2 + x^2)^{-1}]$ and $B = -\mathrm{i}x^4$. The bilinear Schrdinger equation is well-posed for piecewise constant nonnegative controls u (see [30, Theorems XIII.69 and XIII.70]). A basis of H made of eigenvectors of A is given by $(\phi_{2n})_n$ where ϕ_k is the kth Hermite function. A non-degenerate chain of connectedness of (A,B) is $\{(j, j+1), j \in \mathbf{N}\}$. Since $|\langle \phi_j, B\phi_{j+1} \rangle| \sim j^{-2}$, $(|\langle \phi_j, B\phi_{j+1} \rangle|^{-1})_j \in \ell^1$. As a consequence, it is possible to join (approximately) any energy level from the first one with a control of L^1 norm less than $(5\pi/4) \sum_{j \in \mathbf{N}} |\langle \phi_j, B\phi_{j+1} \rangle|^{-1} < +\infty$. Hence the system does not admit Good Galerkin Approximations in the spirit of Proposition 8, since it is possible to reach arbitrary high energy levels using controls with a given finite L^1 norm.

V. FIVE OPEN QUESTIONS

A. Attainable set of weakly-coupled systems

Most of the bilinear quantum systems we encountered in the physics literature are k-weakly-coupled for every $k > 0$. We have already seen that if (A,B) is k-weakly-coupled for every $k > 0$, then the attainable set from any eigenvector of A is contained in $\cap_{k>0} D(|A|^k)$, the intersection of the domains of all the iterations of A. This prevents a direct application of the linear test used in [7] because of the difficulty to endow $\cap_{k>0} D(|A|^k)$ (or a subspace of it) with a Banach structure. But it does not forbid (a priori) the eigenstates of A to be in the attainable set of the first eigenstate. The complete description of the attainable set from the first eigenstate is likely out of reach without new powerful methods. One may consider the less challenging

Question 1: Let (A,B) be k-weakly-coupled for every $k > 0$. Give (explicitly) a state ψ_b not colinear to ϕ_1 such that there exist a control u in $L^1(\mathbf{R}, \mathbf{R})$ and a time $T > 0$ for which $\Upsilon^u_{T,0}\phi_1 = \psi_b$.

B. Minimal time

Let (A,B) satisfy Assumption 1 and admit a non-degenerate chain of connectedness. From Proposition 5, we know that $\cup_{t \geq 0} \{\Upsilon^u_{t,0}\phi_1 | u \in PC\}$ is dense in H. We define $\rho = \inf \left\{ T \geq 0 \text{ such that } \overline{\cup_{0 \leq t \leq T} \{\Upsilon^u_{t,0}\phi_1 | u \in PC\}} = H \right\}$. It is classical that $\rho > 0$ if A is bounded, which is the case for instance if H is finite dimensional. The computation of ρ is difficult in practice. At present time, ρ is unknown for all the examples of Section IV. An example ($H = L^2(\mathbf{R}/2\pi\mathbf{Z}, \mathbf{C})$, $A = \mathrm{i}(-\Delta)^{\alpha}$ with $\alpha > 5/2$, $B : \psi \mapsto \mathrm{i}\cos(\theta)\psi$) has been recently exhibited for which $\rho = 0$, see [31].

Question 2: Does it exist (A,B) k-weakly-coupled for every $k > 0$ such that A is unbounded, B has no eigenvector and $\rho > 0$?

A related question has been investigated by Beauchard and Morancey in [32], where they give a set of sufficient conditions for the attainable set of a 3-weakly-coupled system in small time with small controls to have empty or non-empty interior in $D(|A|^{3/2})$.

C. Transfer time and size of controls

As previously said, large controls may, for some examples, allow approximate controllability in arbitrarily small time. For weakly-coupled systems, it can be easily proved (see [31]) that an a priori bound on the L^1 norm of the control is not compatible with approximate controllability in arbitrarily small time. In practice (in particular when using adiabatic methods), one often applies very small controls, what results in large transfer time.

Question 3: An upper bound on the L^1 norm of the control being given, what is the smallest possible time needed to transfer a given system (A,B) from the first eigenstate of A to the second one?

D. Minimal number of switches

In the case where B is bounded, the following computation

$$\begin{aligned} \|Ae^{t(A+uB)}\psi\| &= \|(A + uB - uB)e^{t(A+uB)}\psi\| \\ &\leq \|(A+uB)e^{t(A+uB)}\psi\| + |u|\|B\| \\ &\leq \|e^{t(A+uB)}(A+uB)\psi\| + |u|\|B\| \\ &\leq \|A\psi\| + 2|u|\|B\|, \end{aligned}$$

valid for every u in U, $t \geq 0$ and ψ in the intersection of the unit sphere of H and $D(A)$, gives an upper bound of variation of the energy of the system in term of the total variation of the control u. This provides a lower bound of the number of discontinuities of a piecewise constant control taking value in $\{0,1\}$ to reach a given target.

Let (A,B) satisfy Assumption 1. If (A,B) admits a non-degenerate chain of connectedness, then for every ψ_b in the unit sphere of H, for every $\varepsilon > 0$, there exists $u_\varepsilon : [0, T_\varepsilon] \to \{0,1\}$ such that $\|\Upsilon^u_{T_u,0}\phi_1 - \psi_b\| < \varepsilon$. Using [16, Proposition 3], it is possible to build u_ε with a number of discontinuities of the order of $1/\varepsilon$.

Question 4: Is it possible to build u_ε with a number of discontinuities of order $o_{\varepsilon \to 0}\left(\frac{1}{\varepsilon}\right)$?

E. Good Galerkin Approximations for general systems

The existence of Good Galerkin Approximations is of crucial interest for the theoretical analysis and the numerical simulation of bilinear quantum systems. For systems that are not weakly-coupled (e.g., example of Section IV-D), there is no equivalent of Proposition 8 in general. However, if (A, B) has the particular form $A = -\mathrm{i}(\Delta + V)$, $B = \mathrm{i}W$, with Δ the Laplace-Beltrami operator on a compact manifold Ω and $V : \Omega \to \mathbf{R}$ a smooth function, then for any measurable bounded $W : \Omega \to \mathbf{R}$, (A, B) admits a Good Galerkin Approximation. This can be proved by considering $W_\eta : \Omega \to \mathbf{R}$ a smooth function η-close in L^1 norm to W. $(A, \mathrm{i}W_\eta)$ is k-weakly-coupled for every k, thus Proposition 8 applies, and the trajectory of $(A, \mathrm{i}W_\eta)$ with control u is $\|u\|_{L^1}\eta$ close to the trajectory of $(A, \mathrm{i}W)$ with control u. Conclusion follows by letting η tend to zero.

Question 5: Does it exist a system (A, B) with unbounded B that satisfies Assumption 1, is not k-weakly-coupled for any $k > 0$ and that can be approached, uniformly with respect of the L^1 norm of the control, by its Galerkin approximations?

Notice that the example of Section IV-D with $\alpha \geq 3$ is a counter-example to the natural idea "If B is A-bounded, then (A, B) admits Good Galerkin Approximations".

VI. CONCLUSIONS

The variety of approaches and methods developed by different authors in the last years to tackle the difficult problem of the controllability of infinite dimensional bilinear quantum systems is essentially the sign of the rich structure and subtle nature of control issues in this context. It is likely that new methods will be necessary to answer the many open problems in the fields.

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