Weakly-coupled systems in quantum control

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Abstract

Weakly-coupled systems are a class of infinite dimensional conservative bilinear control systems with discrete spectrum. A property of these systems is that they can be precisely approached by finite dimensional Galerkin approximations. This feature is of particular interest for the approximation of quantum system dynamics and the control of the bilinear Schrödinger equation.

This paper provides rigorous definitions and analysis of the dynamics of weakly-coupled systems and gives sufficient conditions for an infinite dimensional quantum control system to be weakly-coupled. As an illustration we provide examples chosen among common physical systems.

Index Terms

Quantum system, Schrödinger equation, bilinear control, approximate controllability, Galerkin approximation.

I. Introduction

A. Physical context

The state of a quantum system evolving on a finite dimensional Riemannian manifold Ω, with associated measure μ, is described by its *wave function*, that is, an element of the unit sphere of $L^2(\Omega, \mathbf{C})$. A system with wave function ψ is in a subset ω of Ω with probability $\int_\omega |\psi|^2 d\mu$.

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This work has been supported by the INRIA Nancy-Grand Est “CUPIDSE” Color program.

Second and third authors were partially supported by French Agence National de la Recherche ANR “GCM”, program “BLANC-CSD”, contract number NT09-504590. The third author was partially supported by European Research Council ERC StG 2009 “GeCoMethods”, contract number 239748.

When a system is submitted to excitations by p external fields (*e.g.* lasers) the Schrödinger equation reads

$$\mathrm{i}\frac{\partial\psi}{\partial t} = -\frac{1}{2}\Delta\psi + V(x)\psi(x,t) + \sum_{l=1}^{p} u_l(t)W_l(x)\psi(x,t), \tag{1}$$

where Δ is the Laplace-Beltrami operator on Ω, $V : \Omega \to \mathbf{R}$ is a real function, usually called potential, carrying the physical properties of the uncontrolled system, $W_l : \Omega \to \mathbf{R}$, $1 \leq l \leq p$, is a real function modeling a laser l, and u_l,$1 \leq l \leq p$, usually called control, is a real function of the time representing the intensity of the laser l.

A natural question, with many practical implications, is whether one can find a control $(u_1, \ldots, u_p)$ for which the associated dynamics generated by (1) has the desired behaviour (for instance, steering some given initial data to some given target). In the case $p = 1$, considerable efforts have been made to study the controllability. We refer to [1], [2], [3], [4], [5], [6], [7], [8], [9], [10] and references therein for a description of theoretical results concerning the existence of controls steering a given source to a given target or a neighborhood of it.

B. Finite dimensional approximations

The main difficulty in the study of (1) is the fact that the natural state space, namely $L^2(\Omega, \mathbf{C})$, has infinite dimension. To avoid difficulties when dealing with infinite dimensional systems, for example when studying practical computations or simulations, one can project system (1) on finite dimensional subspaces of $L^2(\Omega, \mathbf{C})$. A vast literature is now available on control of bilinear finite dimensional quantum system, we refer for instance to [11], [12]. A crucial issue is to guarantee that the finite dimensional approximations have dynamics close to the one of the original infinite dimensional system.

As a matter of fact, a special class of bilinear systems of the type of (1) which are said weakly-coupled (see definition in Section II) exhibits very nice properties of approximations (see Proposition 4 below). The notion of weakly-coupled system has been used in [13] implicitly, in the case $p = 1$ and W bounded.

The aim of this work is to provide an analysis of weakly-coupled systems, to present a sufficient condition for controllability for these systems, and to show that two important types of bilinear quantum systems frequently encountered in the literature are weakly-coupled.

C. Content of the paper

In Section II we define weakly-coupled systems, we state some properties of their finite dimensional approximations, and we prove a controllability result. We then study two important examples of weakly-coupled systems, the first (Section III) covering, among others, the case where Ω is compact and the second (Section IV) the case where the system (1) is tri-diagonal.

II. Weakly-coupled systems

A. Abstract framework

We reformulate (1) in a more abstract framework. This will allow us to treat examples slightly more general than (1), for instance, the example in Section III-A. In a separable Hilbert space H endowed with norm $\|\cdot\|$ and Hilbert product $\langle\cdot,\cdot\rangle$, we consider the evolution problem

$$\frac{d\psi}{dt} = (A + \sum_{l=1}^{p} u_l B_l)\psi \tag{2}$$

where $(A, B_1, \ldots, B_p)$ satisfies Assumption 1.

Assumption 1. $(A, B_1, \ldots, B_p)$ is a $(p+1)$-uple of linear operators such that

1) for every u in $\mathbf{R}^p$, $A + \sum_l u_l B_l$ is essentially skew-adjoint on $D(A)$ and $\mathrm{i}(A + \sum_l u_l B_l)$ is bounded from below;
2) A is skew-adjoint and has purely discrete spectrum $(-\mathrm{i}\lambda_k)_{k\in\mathbf{N}}$, the sequence $(\lambda_k)_{k\in\mathbf{N}}$ is positive non-decreasing and accumulates at $+\infty$.

In the rest of our study, we denote by $(\phi_k)_{k\in\mathbf{N}}$ an Hilbert basis of H such that $A\phi_k = -\mathrm{i}\lambda_k\phi_k$ for every k in $\mathbf{N}$. We denote by $D(A + \sum_l u_l B_l)$ the domain where $A + \sum_l u_l B_l$ is skew-adjoint.

Assumption 1.1 ensures that, for every constants $u_1, \ldots, u_p$ in $\mathbf{R}$, $A + \sum_l u_l B_l$ generates a group of unitary propagators. Hence, for every initial condition ψ_0 in H, for every piecewise constant control $u : t \in \mathbf{R} \to \sum_{n=0}^{N} u^n \chi_{[t_n, t_{n+1})}(t) \in \mathbf{R}^p$ with $0 = t_0 \leq t_1 \leq \ldots \leq t_{N+1}$ we can define the solution of (2) by $t \mapsto \Upsilon_t^u \psi_0$, where

$$\Upsilon_t^u = e^{(t-t_{j-1})(A+\sum u_l^{j-1} B_l)} \circ e^{(t_{j-1}-t_{j-2})(A+\sum u_l^{j-2} B_l)} \circ \ldots \circ e^{t_0(A+\sum u_l^0 B_l)},$$

for $t \in [t_{j-1}, t_j)$, $j = 1, \ldots, N$.

Remark 1. From Assumption 1.1 we deduce that for every $u \in \mathbf{R}^p$, $A + \sum_l u_l B_l$ is bounded from $D(A)$ to H as well as $\sum_l u_l B_l$. As a consequence, the resolvent of $A + \sum_l u_l B_l$ is compact. Since $\mathrm{i}(A + \sum_l u_l B_l)$ is bounded from below, the spectrum accumulates at $+\infty$.

B. Energy growth

From Assumption 1.2, the operator $\mathrm{i}A$ is self-adjoint with positive eigenvalues. For every ψ in $D(A)$, $\mathrm{i}A\psi = \sum_{j\in\mathbf{N}} \lambda_j \langle \phi_j, \psi\rangle \phi_j$. For every $s \geq 0$, we define the linear operator $|A|^s := (\mathrm{i}A)^s$ by $|A|^s\psi = \sum_{j\in\mathbf{N}} \lambda_j^s \langle \phi_j, \psi\rangle \phi_j$, for every ψ in $D(|A|^s) = \{\psi \in H \,:\, \sum_{j\in\mathbf{N}} \lambda_j^{2s} |\langle \phi_j, \psi\rangle|^2 < +\infty\}$. We define the s-norm by $\|\psi\|_s = \||A|^s\psi\|$ for every ψ in $D(|A|^s)$. The $1/2$-norm plays an important role in physics; for every ψ in $D(|A|^{1/2})$, the quantity $|\langle A\psi, \psi\rangle| = \|\psi\|_{1/2}^2$ is the expected value of the energy.

The notion of weakly-coupled systems is closely related to the growth of the expected value of the energy.

Definition 1. Let k be a positive number and let $(A, B_1, \ldots, B_p)$ satisfy Assumption 1.1. Then $(A, B_1, \ldots, B_p)$ is *k-weakly-coupled* if for every $u \in \mathbf{R}^p$, $D(|A + \sum_l u_l B_l|^{k/2}) = D(|A|^{k/2})$ and there exists a constant C such that, for every $1 \leq l \leq p$, for every ψ in $D(|A|^k)$, $|\Re\langle |A|^k\psi, B_l\psi\rangle| \leq C|\langle |A|^k\psi, \psi\rangle|$.

The *coupling constant* $c_k(A, B_1, \ldots, B_p)$ of system $(A, B_1, \ldots, B_p)$ of order k is the quantity

$$\sup_{\psi\in D(|A|^k)\setminus\{0\}} \sup_{1\leq l\leq p} \frac{|\Re\langle |A|^k\psi, B_l\psi\rangle|}{|\langle |A|^k\psi, \psi\rangle|}.$$

We have the following technical interpolation result whose proof is given in the appendix.

Lemma 1. *Let A and A' be invertible skew-adjoint operators with compact resolvent. Let k be a positive real. Assume that $D(|A|^k) = D(|A'|^k)$. Then for any real $s \in (0, k)$, $D(|A|^s) = D(|A'|^s)$.*

A first property of the propagator of a weakly-coupled system is given by the following proposition.

Proposition 2. *Let k be a positive number and let $(A, B_1, \ldots, B_p)$ satisfy Assumption 1 and be k-weakly-coupled. Then, for every $\psi_0 \in D(|A|^{k/2})$, $K > 0$, $T \geq 0$, and piecewise constant function $u = (u_1, \ldots, u_p)$ for which $\sum_{l=1}^p \|u_l\|_{L^1} < K$, one has $\|\Upsilon_T^u(\psi_0)\|_{k/2} < e^{c_k(A,B_1,\ldots,B_p)K}\|\psi_0\|_{k/2}$.*

Proof: We present here a simple proof in the special case where $D(|A|^{k+1}) = D(|A + \sum_{l\leq p} u_l B_l|^{k+1})$ for every u in $\mathbf{R}^p$. This equality holds for the most common physical examples. A general proof of Proposition 2, involving rather advanced regularization techniques to relax this extra assumption is presented in the Appendix.

First note that, for every $t \geq 0$ and for every $(u_1, \ldots, u_p)$ in $\mathbf{R}^p$, the set $D(|A|^{k+1}) = D(|A + \sum_l u_l B_l|^{k+1})$ is invariant for the unitary map $\psi \mapsto e^{t(A+\sum_l u_l B_l)}\psi$. Moreover, for every ψ in $D(|A+\sum_l u_l B_l|^{k+1})$, the map $t \mapsto |A+\sum_l u_l B_l|^k e^{t(A+\sum_l u_l B_l)}\psi = e^{t(A+\sum_l u_l B_l)}|A+\sum_l u_l B_l|^k\psi$ is C^1 from $[0, +\infty)$ to H, with derivative $t \mapsto (A + \sum_l u_l B_l)e^{t(A+\sum_l u_l B_l)}|A + \sum_l u_l B_l|^k\psi = |A + \sum_l u_l B_l|^k(A + \sum_l u_l B_l)e^{t(A+\sum_l u_l B_l)}\psi$. In other words, the map $t \mapsto e^{t(A+\sum_l u_l B_l)}\psi$ is C^1 from $[0, +\infty)$ to $D(|A + \sum_l u_l B_l|^k) = D(|A|^k)$.

Fix $u : [0, +\infty) \to \mathbf{R}^p$ piecewise constant, ψ_0 in $D(|A|^{k+1})$ and consider the real map $f : t \mapsto \langle |A|^k \Upsilon_t^u \psi_0, \Upsilon_t^u \psi_0\rangle$. Since ψ_0 belongs to $D(|A + \sum_{l=1}^p u_l(t) B_l|^{k+1})$, then f is absolutely continuous and for the argument above is piecewise C^1. For almost every t,

$$\begin{aligned}
\frac{d}{dt} f(t) &= \frac{d}{dt}\langle |A|^k \Upsilon_t^u \psi_0, \Upsilon_t^u \psi_0\rangle \\
&= \langle |A|^k \Upsilon_t^u \psi_0, (A + \sum_{l=1}^p u_l(t) B_l)\Upsilon_t^u \psi_0\rangle + \langle |A|^k (A + \sum_{l=1}^p u_l(t) B_l)\Upsilon_t^u \psi_0, \Upsilon_t^u \psi_0\rangle \\
&= 2\Re\langle |A|^k \Upsilon_t^u \psi_0, (A + \sum_{l=1}^p u_l(t) B_l)\Upsilon_t^u \psi_0\rangle \\
&= 2\sum_{l=1}^p u_l(t)\Re\langle |A|^k \Upsilon_t^u \psi_0, B_l \Upsilon_t^u \psi_0\rangle.
\end{aligned}$$

Since $(A, B_1, \ldots, B_p)$ is k-weakly-coupled, then

$$|f'(t)| \leq 2\sum_{l=1}^p |u_l(t)||\langle |A|^k \Upsilon_t^u \psi_0, B_l \Upsilon_t^u \psi_0\rangle| \leq 2c_k(A, B_1, \ldots, B_p)\sum_{l=1}^p |u_l(t)| f(t).$$

From Gronwall's lemma, we get $\langle |A|^k \psi(t), \psi(t)\rangle \leq e^{2c_k(A,B_1,\ldots,B_p)\sum_{l=1}^p \int_0^t |u_l|(\tau)d\tau}\|\psi_0\|^2_{k/2}$ for every ψ_0 in $D(|A|^{k+1})$.

Let $(\psi_0^n)_{n\in\mathbf{N}}$ be a sequence in $D(|A|^{k+1})$ converging to ψ_0 in $D(|A|^{\frac{k}{2}})$ for the $k/2$-norm. For every $\tilde{\psi}$ in $D(|A|^{\frac{k}{2}})$ and for every $t \geq 0$,

$$|\langle |A|^{\frac{k}{2}}\tilde{\psi}, \Upsilon_t^u(\psi_0^n)\rangle| \leq |\langle \tilde{\psi}, |A|^{\frac{k}{2}}\Upsilon_t^u(\psi_0^n)\rangle| \leq \|\tilde{\psi}\|\|\Upsilon_t^u(\psi_0^n)\|_{\frac{k}{2}},$$

which is bounded uniformly with respect to n from the first part of the proof. Since $\psi \mapsto \Upsilon_t^u(\psi)$ is unitary, $(\Upsilon_t^u(\psi_0^n))_{n\in\mathbf{N}}$ converges to $\Upsilon_t^u(\psi_0)$ (for the norm of H) and $|\langle |A|^{\frac{k}{2}}\tilde{\psi}, \Upsilon_t^u(\psi_0)\rangle| \leq$

$e^{2c_k(A,B_1,\dots,B_p)K}\|\tilde{\psi}\|_{\frac{k}{2}}\|\psi_0\|_{\frac{k}{2}}$. Hence, $\Upsilon^u_t(\psi_0)$ belongs to $D(|A|^{\frac{k}{2}})^* = D(|A|^{\frac{k}{2}})$ and $\|\Upsilon^u_t(\psi_0)\|_{\frac{k}{2}} \leq e^{c_k(A,B_1,\dots,B_p)K}\|\psi_0\|_{\frac{k}{2}}$, which concludes the proof in the case in which $D(|A|^{k+1}) = D(|A + \sum_{l\leq p} u_l B_l|^{k+1})$. ■

C. Good Galerkin approximation

In this section we show that a weakly-coupled system admits a finite dimensional approximation whose trajectories are close, at every time, to the solutions of the original infinite dimensional system. For every N in $\mathbf{N}$, we define the orthogonal projection

$$\pi_N : \psi \in H \mapsto \sum_{j\leq N} \langle \phi_j, \psi\rangle \phi_j \in H.$$

Lemma 3. *Let k be a positive number, $(A, B_1, \dots, B_p)$ satisfy Assumption 1, and be k-weakly-coupled. Assume that there exist $d > 0$, $0 \leq r < k$ such that $\|B_l\psi\| \leq d\|\psi\|_{r/2}$ for every ψ in $D(|A|^{r/2})$ and l in $\{1,\dots,p\}$. Then, for every $K \geq 0, n \in \mathbf{N}$, $N \in \mathbf{N}$, $(\psi_j)_{1\leq j\leq n}$ in $D(|A|^{k/2})^n$, and for every piecewise constant function $u = (u_1,\dots,u_p)$,*

$$\sum_{m=1}^{p} \|u_m\|_{L^1} \leq K \implies \|B_l(\mathrm{Id} - \pi_N)\Upsilon^u_t(\psi_j)\| < d\lambda_{N+1}^{(r-k)/2} e^{c_k(A,B_1,\dots,B_p)K}\|\psi_j\|_{k/2}, \tag{3}$$

for every $t \geq 0$, $l = 1,\dots,p$ and $j = 1,\dots,n$.

Proof: Fix $j \in \{1,\dots,n\}$. For every $N > 1$, one has

$$\|(\mathrm{Id} - \pi_N)\Upsilon^u_t(\psi_j)\|^2_{r/2} = \sum_{n=N+1}^{\infty} \lambda_n^r |\langle \phi_n, \Upsilon^u_t(\psi_j)\rangle|^2 \leq \lambda_{N+1}^{r-k} \|\Upsilon^u_t(\psi_j)\|^2_{k/2}. \tag{4}$$

By Proposition 2, $\|\Upsilon^u_t(\psi_j)\|^2_{k/2} \leq e^{2c_k(A,B_1,\dots,B_p)K}\|\psi_j\|^2_{k/2}$ for every $t > 0$ and u of L^1-norm smaller than K. Equation (3) follows as, for every $l = 1,\dots,p$, $\|B_l\psi\| \leq d\||A|^{\frac{r}{2}}\psi\|$. ■

Remark 2. Since $r < k$, then $\|B_l(\mathrm{Id} - \pi_N)\Upsilon^u_t(\psi_j)\|_{r/2}$ tends to 0, uniformly with respect to u, as N tends to infinity.

Definition 2. Let $N \in \mathbf{N}$. The *Galerkin approximation* of (2) of order N is the system in H

$$\dot{x} = (A^{(N)} + \sum_{l=1}^{p} u_l B_l^{(N)})x \tag{Σ_N}$$

where $A^{(N)} = \pi_N A \pi_N$ and $B_l^{(N)} = \pi_N B_l \pi_N$ are the *compressions* of A and B_l (respectively).

We denote by $X^u_{(N)}(t,s)$ the propagator of (Σ_N) for a p-uple of piecewise constant functions $u = (u_1,\dots,u_p)$.

Remark 3. The operators $A^{(N)}$ and $B_l^{(N)}$ are defined on the *infinite* dimensional space H. However, they have finite rank and the dynamics of (Σ_N) leaves invariant the N-dimensional space $\mathcal{L}_N = \mathrm{span}_{1\leq l\leq N}\{\phi_l\}$. Thus, (Σ_N) can be seen as a finite dimensional bilinear dynamical system in $\mathcal{L}_N$.

Proposition 4 (Good Galerkin Approximation)**.** *Let k and s be non-negative numbers with $0 \leq s < k$. Let $(A, B_1, \ldots, B_p)$ satisfy Assumption 1 and be k-weakly-coupled. Assume that there exist $d > 0$, $0 \leq r < k$ such that $\|B_l\psi\| \leq d\|\psi\|_{r/2}$ for every ψ in $D(|A|^{r/2})$ and l in $\{1, \ldots, p\}$. Then for every $\varepsilon > 0$, $K \geq 0$, $n \in \mathbf{N}$, 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 $u = (u_1, \ldots, u_p)$*

$$\sum_{l=1}^{p} \|u_l\|_{L^1} < K \implies \|\Upsilon_t^u(\psi_j) - X_{(N)}^u(t,0)\pi_N\psi_j\|_{s/2} < \varepsilon,$$

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

Proof: Consider the case $s = 0$. Fix j in $\{1, \ldots, n\}$ and consider the map $t \mapsto \pi_N\Upsilon_t^u(\psi_j)$ that is absolutely continuous and satisfies, for almost every $t \geq 0$,

$$\frac{d}{dt}\pi_N\Upsilon_t^u(\psi_j) = (A^{(N)} + \sum_{l=1}^{p} u_l B_l^{(N)})\pi_N\Upsilon_t^u(\psi_j) + \sum_{l=1}^{p} u_l(t)\pi_N B_l(\mathrm{Id} - \pi_N)\Upsilon_t^u(\psi_j).$$

Hence, by variation of constants, for every $t \geq 0$,

$$\pi_N\Upsilon_t^u(\psi_j) = X_{(N)}^u(t,0)\pi_N\psi_j + \sum_{l=1}^{p}\int_0^t X_{(N)}^u(t,s)\pi_N B_l(\mathrm{Id} - \pi_N)\Upsilon_s^u(\psi_j)u_l(\tau)d\tau. \tag{5}$$

By Lemma 3, the norm of $t \mapsto B_l(\mathrm{Id} - \pi_N)\Upsilon_t^u(\psi_j)$ is less than $d\lambda_{N+1}^{(r-k)/2}e^{c_k(A,B_1,\ldots,B_p)K}\|\psi_j\|_{k/2}$. Since $X_{(N)}^u(t,s)$ is unitary,

$$\|\pi_N\Upsilon_t^u(\psi_j) - X_{(N)}^u(t,0)\pi_N\psi_j\| < Kd\lambda_{N+1}^{(r-k)/2}e^{c_k(A,B_1,\ldots,B_p)K}\|\psi_j\|_{k/2}. \tag{6}$$

Then

$$\begin{aligned}\|\Upsilon_t^u(\psi_j) - X_{(N)}^u(t,0)\pi_N\psi_j\| &\leq \|(\mathrm{Id} - \pi_N)\Upsilon_t^u(\psi_j)\| + \|\pi_N\Upsilon_t^u(\psi_j) - X_{(N)}^u(t,0)\pi_N\psi_j\| \\ &\leq \lambda_{N+1}^{-k/2}e^{c_k(A,B_1,\ldots,B_p)K}\|\psi_j\|_{k/2} + Kd\lambda_{N+1}^{(r-k)/2}e^{c_k(A,B_1,\ldots,B_p)K}\|\psi_j\|_{k/2}.\end{aligned} \tag{7}$$

This completes the proof for $s = 0$ since λ_N tends to infinity as N goes to infinity.

Note that, if $\mathcal{X}$ is a set and $(u_n)_{n\in\mathbf{N}}$ is a sequence of functions from $\mathcal{X}$ to H that tends uniformly to 0 (the null function) for the s-norm and is uniformly bounded for the k-norm for

$s < k$, then $(u_n)_{n\in\mathbf{N}}$ tends uniformly to 0 in the $\frac{s+k}{2}$-norm. This is a consequence of Cauchy-Schwarz inequality, indeed

$$\|u_n\|^2_{\frac{s+k}{2}} = |\langle |A|^{\frac{s+k}{2}} u_n, |A|^{\frac{s+k}{2}} u_n\rangle| = |\langle |A|^s u_n, |A|^k u_n\rangle| \leq \|u_n\|_s \|u_n\|_k.$$

We conclude the proof in the general case $s > 0$ applying this interpolation result, combined with a bootstrap argument, on the sequence $(u_N)_{N\in\mathbf{N}}$ with $u_N : (t,u) \mapsto (X^u_{(N)}(t,0)\pi_N - \Upsilon^u_t)\psi_j$, defined on $\mathcal{X} = [0,+\infty) \times \{u \in L^1 \,:\, \|u\|_{L^1} \leq K\}$. ■

Remark 4. In the case $s = 0$, there is an explicit estimate for the order of the Galerkin approximation which existence is stated in Proposition 4. For instance, by (6), $\|\pi_N \Upsilon^u_t(\psi_j) - X^u_{(N)}(t,0)\pi_N\psi_j\| < \varepsilon$ if N is such that

$$\lambda_{N+1} > \left(\frac{Kde^{c_k(A,B_1,\ldots,B_p)K}\|\psi_j\|_{k/2}}{\varepsilon}\right)^{\frac{2}{k-r}}, \tag{8}$$

for $j = 1,\ldots,n$.

D. Approximate controllability in s-norm

The *a priori* bounds on the k-norm for the solution of a system are a deep obstruction to exact controllability, but provide powerful tools for the study of the approximate controllability.

Definition 3. Let (A,B) satisfy Assumption 1. A subset S of $\mathbf{N}^2$ *couples* two levels j,k in $\mathbf{N}$, if there exists a finite sequence $\Big((s^1_1,s^1_2),\ldots,(s^q_1,s^q_2)\Big)$ in S such that

(i) $s^1_1 = j$ and $s^q_2 = k$;

(ii) $s^j_2 = s^{j+1}_1$ for every $1 \leq j \leq q-1$;

(iii) $\langle \phi_{s^j_1}, B\phi_{s^j_2}\rangle \neq 0$ for $1 \leq j \leq q$.

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

Definition 4. Let (A,B) satisfy Assumption 1 and $s > 0$. The system (A,B) is approximately simultaneously controllable for the s-norm if for every $\hat{\Upsilon} \in U(H)$ (unitary operators acting on H) leaving $D(|A|^s)$ invariant, $\psi_1,\ldots,\psi_n \in D(|A|^s)$, and $\varepsilon > 0$, there exists a piecewise constant function $u_\varepsilon : [0,T_\varepsilon] \to \mathbf{R}$ such that

$$\|\hat{\Upsilon}\psi_j - \Upsilon^{u_\varepsilon}_{T_\varepsilon}\psi_j\|_s < \varepsilon.$$

for every $j = 1, \dots, n$.

Proposition 5. *Let k be a positive number. Let (A, B) satisfy Assumption 1, be k-weakly-coupled, and admit a non-resonant chain of connectedness. Assume that there exist $d > 0$, $0 \leq r < k$ such that $\|B\psi\| \leq d\||A|^{\frac{r}{2}}\psi\|$, for every ψ in $D(|A|^{\frac{r}{2}})$. Then (A, B) is approximately simultaneously controllable for the norm $\|\cdot\|_{s/2}$ for every $s < k$.*

Proof: Fix $\varepsilon > 0$, $\psi_1, \dots, \psi_n \in D(|A|^{s/2})$, and $\hat{\Upsilon} \in U(H)$ such that $\hat{\Upsilon}(\psi_1), \dots, \hat{\Upsilon}(\psi_n) \in D(|A|^{s/2})$. Fix n_1 sufficiently large such that $\|\hat{\Upsilon}(\psi_j) - \pi_{n_1}\hat{\Upsilon}(\psi_j)\|_{s/2} < \varepsilon/3$ for every $j = 1, \dots, n$.

There exist $l_1, \dots, l_n$ such that $t \mapsto (e^{it\lambda_{l_1}}, \dots, e^{it\lambda_{l_n}})$ is ε-dense in the torus $\mathbf{T}^n$ (see [10, Proposition 6.1]). Call $m = \max\{n_1, l_1, \dots, l_n\}$.

By [10, Remark 5.9] there exists K_1 such that for every $\eta > 0$ there exist a control u_1^η satisfying $\|u_1^\eta\|_{L^1} \leq K_1$ and $\theta_1, \theta_2, \dots, \theta_n$, such that $\|\Upsilon_{T_1}^{u_1^\eta}(\psi_j) - e^{\mathrm{i}\theta_j}\phi_{l_j}\| < \eta$, for every $j = 1, \dots, n$.

Similarly, since the hypotheses of [10, Remark 5.9] apply to the system $(-A, -B)$ (see [10, Section 6.1]), we have the existence of K_2 such that for every $\eta > 0$ there exists u_2^η satisfying $\|u_2^\eta\|_{L^1} \leq K_2$ and $\bar{\theta}_1, \dots, \bar{\theta}_n \in \mathbf{R}$ such that the solution of the system

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

at time T_2 with initial condition $\hat{\Upsilon}(\psi_j)$ and corresponding to the control u_2^η is η-close in the norm of H to $e^{\mathrm{i}\bar{\theta}_j}\phi_{l_j}$ for every $j = 1, \dots, n$.

Let τ such that $\|e^{\mathrm{i}\tau\lambda_{l_j}}e^{\mathrm{i}\theta_j} - e^{\mathrm{i}\bar{\theta}_j}\| < \eta$ for every $j = 1, \dots, n$. Let $T = T_1 + \tau + T_2$ and let $u : [0, T] \to \mathbf{R}$ be the piecewise constant control defined by

$$u^\eta(t) = \begin{cases} u_1^\eta(t) & t \in [0, T_1), \\ 0 & t \in [T_1, T_1 + \tau), \\ u_2^\eta(T_2 - (t - T_1 - \tau)) & t \in [T_1 + \tau, T], \end{cases}$$

The control u^η above steers a solution of $\dot{\psi} = (A + uB)\psi$ with initial condition ψ_j 3η-close in the norm $\|\cdot\|$ to $\hat{\Upsilon}(\psi_j)$ in a time T.

Let $K = K_1 + K_2$. By Lemma 3, we have that there exists $N = N(\varepsilon, K, s) > n$ such that

$$\|u\|_{L^1} \leq K \implies \|(\mathrm{Id} - \pi_N)\Upsilon_t^u(\psi_j)\|_{s/2} < \frac{\varepsilon}{3},$$

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

Note that, on $\mathrm{span}\{\phi_1,\dots,\phi_N\}$, we have $\|\cdot\|_{s/2}\leq\lambda_N^{s/2}\|\cdot\|$. Therefore for every $j=1,\dots,n$,

$$\begin{aligned}\|\hat\Upsilon(\psi_j)-\Upsilon_T^{u^\eta}(\psi_j)\|_{s/2}&\leq\|(\mathrm{Id}-\pi_N)(\hat\Upsilon(\psi_j)-\Upsilon_T^{u^\eta}(\psi_j))\|_{s/2}+\|\pi_N(\hat\Upsilon(\psi_j)-\Upsilon_T^{u^\eta}(\psi_j))\|_{s/2}\\&\leq\|(\mathrm{Id}-\pi_N)\hat\Upsilon(\psi_j)\|_{s/2}+\|(\mathrm{Id}-\pi_N)\Upsilon_T^{u^\eta}(\psi_j))\|_{s/2}+\lambda_N^{s/2}\|\hat\Upsilon(\psi_j)-\Upsilon_T^{u^\eta}(\psi_j)\|\\&\leq\frac{2\varepsilon}{3}+3\lambda_N^{s/2}\eta<\varepsilon,\end{aligned}$$

for η sufficiently small. ■

III. The bounded case

Proposition 6. *Let k be a positive integer. Assume that for every $u\in\mathbf{R}^p$, $D(|A|^{\frac{k}{2}})=D(|A+\sum_l u_lB_l|^{\frac{k}{2}})$ and that for every $l=1,\dots,p$ the restriction of B_l to $D(|A|^{\frac{k}{2}})$ is bounded for the $\frac{k}{2}$-norm. Then $(A,B_1,\dots,B_p)$ is k-weakly-coupled.*

Proof: For every $l=1,\dots,p$, let $\|B_l\psi\|_{k/2}\leq C_{l,k}\|\psi\|_{k/2}$ for every ψ in $D(|A|^k)$. Then $|\langle A^k\psi,B_l\psi\rangle|=|\langle|A|^{\frac{k}{2}}\psi,|A|^{\frac{k}{2}}B_l\psi\rangle|\leq\||A|^{\frac{k}{2}}\psi\|\||A|^{\frac{k}{2}}B_l\psi\|\leq C_{l,k}\||A|^{\frac{k}{2}}\psi\|^2=C_{l,k}|\langle A^k\psi,\psi\rangle|$ for every ψ in $D(|A|^k)$. ■

A. Example: single trapped ion

This example is a model of a single ion with two possible states (*excited state* and *ground state*) submitted to a superposition of external fields. It has been extensively studied (see for example [14], [15], and [16]).

The state of the system is (ψ_e,ψ_g) in $H=L^2(\mathbf{R},\mathbf{C})\times L^2(\mathbf{R},\mathbf{C})$. The dynamics is given by

$$\begin{cases}\mathrm{i}\frac{\partial\psi_e}{\partial t}&=\omega(-\Delta+x^2)\psi_e+\Omega\psi_e+\Big(u_1(t)\cos(\sqrt{2}\eta x)+u_2(t)\sin(\sqrt{2}\eta x)\Big)\psi_g\\\mathrm{i}\frac{\partial\psi_g}{\partial t}&=\omega(-\Delta+x^2)\psi_g+\Omega\psi_g+\Big(u_1(t)\cos(\sqrt{2}\eta x)+u_2(t)\sin(\sqrt{2}\eta x)\Big)\psi_e\end{cases}$$

where ω,Ω,η are positive constants related to the physical properties of the system. The two real valued controls u_1 and u_2 are usually a sum of periodic functions with positive frequencies Ω, $\Omega+\omega$ and $\Omega-\omega$. With our notations, the dynamics reads

$$\frac{d\psi}{dt}=A\psi+u_1(t)B_1\psi+u_2(t)B_2(\psi)\tag{9}$$

where A is the diagonal operator $A:(\psi_e,\psi_g)\mapsto-\mathrm{i}(\omega(-\Delta+x^2)\psi_e+\Omega\psi_e,\omega(-\Delta+x^2)\psi_g+\Omega\psi_g)$, $B_1:(\psi_e,\psi_g)\mapsto-\mathrm{i}(\cos(\sqrt{2}\eta x)\psi_g,\cos(\sqrt{2}\eta x)\psi_e)$, and $B_2:(\psi_e,\psi_g)\mapsto-\mathrm{i}(\sin(\sqrt{2}\eta x)\psi_g,\sin(\sqrt{2}\eta x)\psi_e)$.

By [17, Theorem XIII.69 and Theorem XIII.70], the operator A is skew-adjoint with discrete spectrum and admits a family of eigenfunctions which forms an orthonormal basis of H. Since B_1 and B_2 are bounded then, for every real constants u_1 and u_2, $A+u_1B_1+u_2B_2$ is skew-adjoint with the same domain of A (see [18, Theorem X.12]). The spectrum of A is the sequence $(-\mathrm{i}\lambda_n)_{n\in\mathbf{N}} = -\mathrm{i}(\omega(n+1/2)+\Omega)_{n\in\mathbf{N}}$. For every n in $\mathbf{N}$, the eigenvalue $-\mathrm{i}\lambda_n$ has multiplicity 2 and is associated with the 2-dimensional subspace of $L^2(\mathbf{R},\mathbf{C})\times L^2(\mathbf{R},\mathbf{C})$ spanned by $\{(f_n,0),(0,f_n)\}$ where f_n is the n^{th} Hermite function. Assumption 1 is then verified. Since, for every k in $\mathbf{N}$, all derivatives up to order k of $x\mapsto\cos(\sqrt{2}\eta x)$ and $x\mapsto\sin(\sqrt{2}\eta x)$ are bounded for the L^∞-norm by $C_k = 2^{\frac{k}{2}}\eta^k$ on $\mathbf{R}$ then B_1 and B_2 are bounded by 2^kC_k on $D(|A|^{\frac{k}{2}})$ for every k. Moreover for every $(u_1,u_2)\in\mathbf{R}^2$, $D(A^k) = D((A+u_1B_1+u_2B_2)^k)$. Indeed by induction on k

$$\begin{aligned} D((A+u_1B_1+u_2B_2)^{k+1}) &= \{\psi\in D((A+u_1B_1+u_2B_2)^k)\ : \\ &\qquad (A+u_1B_1+u_2B_2)\psi\in D((A+u_1B_1+u_2B_2)^k)\} \\ &= \{\psi\in D(A^k)\ :\ (A+u_1B_1+u_2B_2)\psi\in D(A^k)\} = D(A^{k+1}), \end{aligned}$$

since $(u_1B_1+u_2B_2)\psi\in D(A^k)$ when $\psi\in D(A^k)$. Lemma 1 provides $D(|A|^s) = D(|A+u_1B_1+u_2B_2|^s)$ for any $s>0$. Hence, by Proposition 6 the system (A,B_1,B_2) is k-weakly-coupled for every k, with coupling constant smaller than 2^kC_k.

B. The case of a compact manifold

We focus here on the case where the space Ω is a compact Riemannian manifold without boundary. By Rellich-Kondrakov and Weyl theorems, if V is essentially bounded the operator $A=-\mathrm{i}(\Delta+V):H^2(\Omega)\to L^2(\Omega,\mathbf{C})$ has purely discrete spectrum $(-\mathrm{i}\lambda_n)_{n\in\mathbf{N}}$ with λ_n non-decreasing to infinity (see for instance [19, Theorem 7.2.6]). Note that λ_1 is not necessarily positive but this is the case considering $A+\mathrm{i}(\lambda_1-1)$ instead of A. This shift gives a physically irrelevant phase term, $e^{\mathrm{i}t(\lambda_1-1)}$, on the dynamics associated with A.

Lemma 7. *Let k be a positive integer, Ω be a compact Riemannian manifold, $V:\Omega\to\mathbf{R}$ be $C^{2k}(\Omega)$. Then the domain of the operator $(\Delta+V)^k$ is $H^{2k}(\Omega)$.*

Proof: Since Ω is compact it is sufficient to prove the proposition on a bounded domain of $\mathbf{R}^n$. The operator $-\mathrm{i}A=\Delta+V$ is an elliptic operator of order 2. By [20, Theorem 8.10] if $Af\in H^k(\Omega)$ then $f\in H^{k+2}(\Omega)$ and by induction we have that $D(|A|^k) = H^{2k}(\Omega)$. ■

Proposition 8. *Let k be a positive integer, Ω be a compact Riemannian manifold, $V, W : \Omega \to \mathbf{R}$ be two $C^{2k}(\Omega, \mathbf{R})$ functions on Ω. Define $A = -\mathrm{i}(\Delta + V) : D(A) \to L^2(\Omega, \mathbf{C})$ and $B = \mathrm{i}W : L^2(\Omega, \mathbf{C}) \to L^2(\Omega, \mathbf{C})$. Then (A, B) is k-weakly-coupled.*

Proof: Note that for every $f \in C^{2k}$ there exists a constant $C_k = 2^{2k+1} \sup_{0 \le j \le 2k} \|W^{(j)}\|_{L^\infty(\Omega, \mathbf{R})}$ such that $\|Wf\|_{H^{2k}} \le C_k \|f\|_{H^{2k}}$. From Lemma 7, the norm $\| \cdot \|_{H^{2k}}$ and the k-norm are equivalent. Therefore, by Proposition 6, the system is k-weakly-coupled. ■

Remark 5. As consequence of Lemma 7 and Proposition 8 we have that, in the case of a compact manifold, if the potentials are in $C^m(\Omega)$ then Proposition 4 applies with $k = m/2 - 1$ and $r = 0$.

C. Example: orientation of a rotating molecule in the plane

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 $H^k_e = \{\psi \in H^{2k}(\Omega, \mathbf{C}) : \psi \text{ odd } \}$. The skew-symmetric operator $B = -\mathrm{i}\cos\theta$ is bounded on $D(|A|^{k/2})$ for every k. By Proposition 6, for every k in $\mathbf{N}$, (A, B) is k-weakly-coupled. Proposition 4 applies for every k with $r = 0$ and $d = 1$. In Section IV-C we also give an estimate on the coupling constant $c_k(A, B)$ for this system.

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-resonant connectedness chain for (A, B). Therefore, by Proposition 5 the system provides an example of approximately simultaneously controllable system in norm $H^k(\Omega)$ for every k. Note that, since the eigenstates belong to $H^k(\Omega)$ for every k then the reachable set from any eigenstate is contained in $H^k(\Omega)$ for every k.

D. Example: orientation of a rotating molecule in the space

We present the physical example of a rotating rigid bipolar molecule. Unlike last example the motion of the molecule is not confined to a plane. The model then can be represented by the Schödinger equation on the sphere. In this case, $\Omega = \mathbf{S}^2$ is the unit sphere, the family $(Y_\ell^m)_{\ell\geq 0, |m|\leq \ell}$ of the spherical harmonics is an Hilbert basis of $H = L^2(\Omega, \mathbf{C})$, and the control is represented by three piecewise constant functions u_1, u_2, u_3. The controlled Schrödinger equation is

$$\mathrm{i}\frac{\partial \psi(\nu,\theta,t)}{\partial t} = (-\Delta + u_1(t)\cos\theta\sin\nu + u_2(t)\sin\theta\sin\nu + u_3(t)\cos\nu)\psi(\nu,\theta,t), \quad (\nu,\theta)\in\mathbf{S}^2.$$

Therefore, since Ω is compact, Proposition 4 applies for every integer k with $d = 1$ and $r = 0$.

IV. Tri-diagonal systems

We deal with the case where $p = 1$ and B couples only adjacent levels of A.

A. Tri-diagonal systems

Definition 5. A system (A, B) satisfying Assumption 1 is *tri-diagonal* if for every j, k in $\mathbf{N}$, $|j - k| > 1$ implies $\langle \phi_j, B\phi_k\rangle = 0$.

In the following, we denote $b_{j,k} = \langle \phi_j, B\phi_k\rangle$.

Proposition 9. *Assume that (A, B) is tri-diagonal, that the sequence $\left(\frac{\lambda_{n+1}}{\lambda_n}\right)_{n\in\mathbf{N}}$ is bounded, and that the sequences $\left(\frac{b_{n,n-1}}{\lambda_n}\right)_{n\in\mathbf{N}}, \left(\frac{b_{n,n}}{\lambda_n}\right)_{n\in\mathbf{N}}$ tend to zero. Then, for every k in $\mathbf{N}$ and u in $\mathbf{R}$, $D((A + uB)^k) = D(A^k)$. Moreover, $D(A^k)$ is invariant for $e^{t(A+uB)}$ for any u in $\mathbf{R}$ and t in $\mathbf{R}$.*

Proof: The equality of $D((A+uB)^k)$ and $D(A^k)$ will follow from the Kato-Rellich theorem ([21, Theorem 1.4.2]). It suffices to check that for every k in $\mathbf{N}$, u in $\mathbf{R}$, $\varepsilon > 0$, and every ψ in $D(A^k)$, there exists $\varepsilon < 1$ and b_ε such that

$$\|((A + uB)^k - A^k)\psi\| \leq \varepsilon\|A^k\psi\| + b_\varepsilon\|\psi\|. \tag{10}$$

Let us prove that B is bounded from $D(A^{r+1})$ to $D(A^r)$ for every integer $r \geq 0$. For every v in $D(A^r)$,

$$\begin{aligned}
\|Bv\|_r^2 &= \sum_{n=1}^{\infty} \lambda_n^{2r} |\langle Bv, \phi_n \rangle|^2 \\
&= \sum_{n=1}^{\infty} \lambda_n^{2r} |\langle v, B\phi_n \rangle|^2 \\
&\leq \sum_{n=1}^{\infty} \lambda_n^{2r} (b_{n,n-1}^2 |\langle \phi_{n-1}, v \rangle|^2 + b_{n,n}^2 |\langle \phi_n, v \rangle|^2 + b_{n,n+1}^2 |\langle \phi_{n+1}, v \rangle|^2) \\
&= \sum_{n=1}^{\infty} \lambda_{n-1}^{2r+2} \left(\frac{\lambda_n}{\lambda_{n-1}} \right)^{2r} \frac{b_{n,n-1}^2}{\lambda_{n-1}^2} |\langle \phi_{n-1}, v \rangle|^2 + \lambda_n^{2r+2} \frac{b_{n,n}^2}{\lambda_n^2} |\langle \phi_n, v \rangle|^2 + \\
&\quad + \lambda_{n+1}^{2r+2} \left(\frac{\lambda_n}{\lambda_{n+1}} \right)^{2r} \frac{b_{n,n+1}^2}{\lambda_{n+1}^2} |\langle \phi_{n+1}, v \rangle|^2.
\end{aligned}$$

Now for every $\varepsilon > 0$, let n_0 such that $\sup_{n \geq n_0} \frac{b_{n,n-1}^2}{\lambda_{n-1}^2} < \frac{\varepsilon}{3C^{2r}}$, $\sup_{n \geq n_0} \frac{b_{n,n}^2}{\lambda_n^2} < \varepsilon/3$, and $\sup_{n \geq n_0} \frac{b_{n,n+1}^2}{\lambda_{n+1}^2} < \frac{\varepsilon}{3}$. Note that the sequence $(\lambda_n)_{n \in \mathbf{N}}$ is non-decreasing. Then there exists C_ε such that

$$\|Bv\|_r^2 \leq \sum_{n=1}^{n_0} \lambda_n^{2r} |\langle v, B\phi_n \rangle|^2 + \varepsilon \sum_{n \geq n_0 - 1} \lambda_n^{2r+2} |\langle \phi_n, v \rangle|^2 \leq C_\varepsilon \|v\|^2 + \varepsilon \|v\|_{r+1}^2. \tag{11}$$

We prove (10) by induction on k. For $k = 1$ this is a consequence of (11) with $r = 0$. The inductive step follows from the fact that

$$(A + uB)^{k+1} - A^{k+1} = u((A + uB)^k B - A^k B) + uA^k B + ((A + uB)^k - A^k)A$$

for every u in $\mathbf{R}$ and from inequality (11). ■

Proposition 10. *Let (A, B) be a tri-diagonal system and let k be a positive integer. Assume that the sequence $\left(\frac{\lambda_{n+1}}{\lambda_n}\right)_{n \in \mathbf{N}}$ is bounded, that the sequences $\left(\frac{b_{n,n-1}}{\lambda_n}\right)_{n \in \mathbf{N}}, \left(\frac{b_{n,n}}{\lambda_n}\right)_{n \in \mathbf{N}}$ tend to zero, and that the sequence $\left(|b_{n,n+1}| \left(\frac{\lambda_{n+1}^k}{\lambda_n^k} - 1 \right) \right)_{n \in \mathbf{N}}$ is bounded. Then (A, B) is k-weakly-coupled.*

Proof: For every ψ in $D(A)$, write $\psi = \sum_{j=1}^{\infty} x_j \phi_j$ where $x_j = \langle \phi_j, \psi \rangle$. Since $\Re(b_{j,j}) = 0$

then

$$\begin{aligned}\Re\left(\langle |A|^k\psi, B\psi\rangle\right) &= \Re\left(\sum_{j=1}^{\infty}\lambda_j^k\bar{x}_j b_{j+1,j}x_{j+1}+\lambda_{j+1}^k\bar{x}_{j+1}b_{j,j+1}x_j\right)\\ &= \Re\left(\sum_{j=1}^{\infty}\lambda_j^k(\bar{x}_j b_{j+1,j}x_{j+1}-x_j\bar{b}_{j+1,j}\bar{x}_{j+1})+(\lambda_{j+1}^k-\lambda_j^k)\bar{x}_{j+1}b_{j,j+1}x_j\right)\\ &= \Re\left(\sum_{j=1}^{\infty}(\lambda_{j+1}^k-\lambda_j^k\bar{x}_{j+1}b_{j,j+1}x_j\right)\\ &\leq \sum_{j=1}^{\infty}(\lambda_{j+1}^k-\lambda_j^k)|b_{j,j+1}|\frac{|x_j|^2+|x_{j+1}|^2}{2}.\end{aligned}$$

By hypothesis, there exists C such that $|b_{j,j+1}|(\lambda_{j+1}^k-\lambda_j^k)\leq C\lambda_j^k$ for every j. Hence, $|\Re\langle|A|^k\psi,B\psi\rangle|\leq C\sum_{j=1}^{\infty}\lambda_j^k|x_j|^2\leq C\langle|A|^k\psi,\psi\rangle$. The equality of the domains follows by Proposition 9. ■

B. Estimates for tri-diagonal systems

Lemma 11. *Let (A,B) be a tri-diagonal system and l be an integer. Assume that the sequence $\left(\frac{\lambda_{n+1}}{\lambda_n}\right)_{n\in\mathbf{N}}$ is bounded, that the sequences $\left(\frac{b_{n,n-1}}{\lambda_n}\right)_{n\in\mathbf{N}}, \left(\frac{b_{n,n}}{\lambda_n}\right)_{n\in\mathbf{N}}$ tend to zero, and that there exists a positive integer k and $0\leq r<k/2$ such that the sequences $\left(|b_{n,n+1}|\left(\frac{\lambda_{n+1}^k}{\lambda_n^k}-1\right)\right)_{n\in\mathbf{N}}$, $\left(\frac{b_{n,n}}{|\lambda_n|^r}\right)_{n\in\mathbf{N}}$ and $\left(\frac{b_{n,n-1}}{|\lambda_n|^r}\right)_{n\in\mathbf{N}}$ are bounded. Then for every $t\geq 0$, for every piecewise constant control u,*

$$|\langle\phi_{l+1},\Upsilon_t^u\phi_1\rangle|\leq\frac{3^l}{l!}\prod_{j=l+1}^{2l+1}L(j)\left(\int_0^t|u(\tau)|d\tau\right)^l,$$

where for $j\in\mathbf{N}$, $L(j)=\sup_{n,m\leq j}|b_{n,m}|$.

Proof: Let $K>0$. We prove the result for u piecewise constant of L^1-norm smaller than K. For every $\varepsilon>0$ by Proposition 4 there exists $N=N(K,\varepsilon)>l$ such that $\|\Upsilon_t^u(\phi_1)-X_{(N)}^u(t,0)\phi_1\|<\varepsilon$ for every $t\geq 0$.

Consider the solution $\psi: t\mapsto X_{(N)}^u(t,0)\phi_1$ of (Σ_N) with initial condition ϕ_1. Then $\psi(t)=e^{tA^{(N)}}\phi_1+\int_0^t e^{(t-s)A^{(N)}}u(s)B^{(N)}\psi(s)ds$. Iterating $l-1$ times we get

$$\begin{aligned}\psi(t)=e^{tA^{(N)}}\Big(&\phi_1+\\ &+\sum_{j=1}^{l-1}\int_{0\leq s_j\leq\cdots\leq s_1\leq t}e^{(t-s_1)A^{(N)}}B^{(N)}\cdots e^{(s_{j-1}-s_j)A^{(N)}}B^{(N)}e^{s_jA^{(N)}}\phi_1\prod_{m=1}^{j}u(s_m)ds_1\ldots ds_j+\\ &+\int_{0\leq s_l\leq\cdots\leq s_1\leq t}e^{(t-s_1)A^{(N)}}B^{(N)}e^{(s_1-s_2)A^{(N)}}B^{(N)}\cdots e^{(s_{l-1}-s_l)A^{(N)}}B^{(N)}\psi(s_l)\prod_{m=1}^{l}u(s_m)ds_1\ldots ds_l\Big).\end{aligned}$$

For the tri-diagonal structure of the system we have

$$\langle \phi_{l+1}, e^{(t-s_1)A^{(N)}} B^{(N)} \cdots e^{(s_{j-1}-s_j)A^{(N)}} B^{(N)} e^{s_j A^{(N)}} \phi_1 \rangle = 0$$

for every $0 \leq s_j \leq \cdots \leq s_1 \leq t$ and $j \leq l-1$. Then

$$\langle \phi_{l+1}, \psi(t) \rangle = e^{tA^{(N)}} \int_{0 \leq s_l \leq \cdots \leq s_1 \leq t} \langle \phi_{l+1}, e^{(t-s_1)A^{(N)}} B^{(N)} e^{(s_1-s_2)A^{(N)}} B^{(N)} \cdots e^{(s_{l-1}-s_l)A^{(N)}} B^{(N)} \psi(s_l) \rangle \prod_{m=1}^{l} u(s_m) ds_1 \ldots ds_l$$

Now,

$$\sup_{s_1,\ldots,s_l \in [0,t]} \| B^{(N)} e^{(s_l - s_{l-1})A^{(N)}} B^{(N)} \cdots e^{(s_2-s_1)A^{(N)}} B^{(N)} e^{(s_1-t)A^{(N)}} \phi_{l+1} \| \leq 3^l \prod_{j=l+1}^{2l+1} L(j). \quad (12)$$

Then

$$|\langle \phi_{l+1}, \psi(t) \rangle| \leq 3^l \prod_{j=l+1}^{2l+1} L(j) \int_{0 \leq s_1 \leq \cdots \leq s_l \leq t} \prod_{m=1}^{l} |u(s_m)| ds_1 \ldots ds_l = 3^l \frac{\left(\int_0^t |u(s)| ds \right)^l}{l!} \prod_{j=l+1}^{2l+1} L(j),$$

as a consequence

$$|\langle \phi_{l+1}, \Upsilon_t^u(\phi_1) \rangle| \leq 3^l \frac{K^l}{l!} \prod_{j=l+1}^{2l+1} L(j) + \varepsilon,$$

and the result follows as ε tends to zero. ■

From a physical point of view, Lemma 11 provides an estimation of the probability of energy transitions (in the spirit, for instance, of [18, Section X.12, Example 1]).

Remark 6. In the case in which the diagonal of B is zero then equation (12) reads

$$\sup_{s_1,\ldots,s_l \in [0,t]} \| B^{(N)} e^{(s_l - s_{l-1})A^{(N)}} B^{(N)} \cdots e^{(s_2-s_1)A^{(N)}} B^{(N)} e^{(s_1-t)A^{(N)}} \phi_{l+1} \| \leq 2^l \prod_{j=l+1}^{2l+1} L(j).$$

This gives the better estimate in this case $|\langle \phi_{l+1}, \Upsilon_t^u \phi_1 \rangle| \leq 2^l \prod_{j=l+1}^{2l+1} L(j) \left(\int_0^t |u(\tau)| d\tau \right)^l / l!$.

C. Example: orientation of a rotating molecule in the plane II

The system of Section III-C provides also an example of tri-diagonal system. Recall that for this system, for every j, k in $\mathbf{N}$, $\lambda_k = k^2$, $\langle \phi_j, B\phi_k \rangle \neq 0$ if and only if $|j-k| = 1$ and $\langle \phi_j, B\phi_{j+1} \rangle = -\mathrm{i}/2$. We deduce a bound for the coupling constants from Proposition 10. For every k in $\mathbf{N}$,

$$c_k(A,B) \leq \sup_{n \in \mathbf{N}} |\langle \phi_n, B\phi_{n+1} \rangle| \left(\frac{\lambda_{n+1}^k}{\lambda_n^k} - 1 \right) = \sup_{n \in \mathbf{N}} \frac{1}{2} \left(\left(1 + \frac{1}{n} \right)^{2k} - 1 \right) = \frac{2^{2k} - 1}{2}.$$

In particular $c_1(A,B) \leq 3/2$ and, by (8), we obtain that $\|\pi_N \Upsilon^u_t(\phi_1) - X^u_{(N)}(t,0)\pi_N\phi_1\| < \varepsilon$ if $\lambda_{N+1} = (N+1)^2 > \left(\frac{\|u\|_{L^1} e^{3/2\|u\|_{L^1}}}{\varepsilon}\right)^2$.

The tri-diagonal structure allows to obtain better estimates on N. From Remark 6, we get

$$|\langle \phi_{N+1}, \Upsilon^u_t(\phi_1)\rangle| \leq \frac{(2K)^N}{N!} \prod_{j=N+1}^{2N+1} L(j) = \frac{K^N}{N!}.$$

Therefore, by (5), for every $\varepsilon > 0$, if N is such that $\|u\|_{L^1}^{N+1} < 2\varepsilon N!$ then $\|\pi_N \Upsilon^u_t(\phi_1) - X^u_{(N)}(t,0)\phi_1\| < \varepsilon$.

The second estimates is significantly better than the first one. For instance, if one has $\|u\|_{L^1} = 3$ and one desires $\varepsilon < 10^{-4}$, the condition $\varepsilon(N+1) > \|u\|_{L^1} e^{3/2\|u\|_{L^1}}$ is false for every $N < 2.7\ 10^6$ while the second condition, $\|u\|_{L^1}^{N+1} < 2\varepsilon N!$, is true for $N = 14$.

D. Example: quantum harmonic oscillator

The quantum harmonic oscillator is among the most important examples of quantum system (see, for instance, [22, Complement G_V]). Its controlled version has been extensively studied (see, for instance, [23], [24]). In this example $H = L^2(\mathbf{R}, \mathbf{C})$ and equation (2) becomes

$$\mathrm{i}\frac{\partial \psi}{\partial t}(x,t) = \frac{1}{2}(-\Delta + x^2)\psi(x,t) + u(t)x\psi(x,t). \tag{13}$$

An 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:

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

Proposition 9 and Proposition 10 apply so that, for every k in $\mathbf{N}$, the system (A,B) is k-weakly-coupled and

$$\begin{aligned} c_k(A,B) &\leq \sup_n \sqrt{n}\left(\frac{(n+1/2)^k}{(n-1/2)^k} - 1\right) \\ &\leq \sup_n \sqrt{n}\left(1 + \frac{1}{n-\frac{1}{2}} - 1\right)\sum_{j=0}^{k-1}\left(1 + \frac{1}{n-\frac{1}{2}}\right)^j \\ &\leq \frac{3^{k+1}-1}{2}\sup_n \frac{\sqrt{n}}{n-\frac{1}{2}} \\ &\leq 3^{k+1} - 1. \end{aligned}$$

The quantum harmonic oscillator is not controllable (in any reasonable sense), however, the Galerkin approximations of (13) of every order are controllable (see [23]). This is not a contradiction, indeed Proposition 4 states that there exists a size of the Galerkin approximation for which the trajectories of the infinite dimensional system can be approximately tracked by the Galerkin approximation, provided that there exists a uniform bound on the L^1-norm of the control. As a matter of fact, there is no such bound for system (13).

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 could use Proposition 4 with $k = 2$, $r = 1$, $d = 1$, and $\|\phi_1\|_1 = 1/2$. The resulting bound, as given by (8),

$$N > \frac{K^2 e^{16K}}{4\varepsilon^2} - \frac{1}{2} \tag{14}$$

is however very weak. Like in the example of Section IV-C, the tri-diagonal structure of B allows better estimates. Using Remark 6, 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

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

For instance, if $K = 3$ and $\varepsilon = 10^{-4}$, this is true for $N = 420$, while (14) is false for $N < 10^{29}$.

V. Conclusion

In our study we focused on the notion of weak coupling. We have established some interesting consequences in control theory and numerical simulation which applies to common and interesting physical models.

However, our assumptions are not optimal and in forthcoming works we expect generalization to rough control such as Dirac impulses. We hope that we will include systems with continuous spectrum in the scope of such technology.

Appendix

Proof of Lemma 1

Proof of Lemma 1: Without loss of generality we can assume that the operators $|A|$ and $|A'|$ are positive and invertible. Let $(\phi_n)_{n\in\mathbf{N}}$ and $(\phi'_n)_{n\in\mathbf{N}}$ be unitary basis of H made

of eigenvectors of A and A' respectively. Then $\lambda_n\phi_n = |A|\phi_n$ for $n \in \mathbf{N}$ and $D(|A|^s) = \{\psi \in H : \sum_{j\in\mathbf{N}} \lambda_j^{2s}|\langle\phi_j,\psi\rangle|^2 < +\infty\}$. Similarly, we can define λ'_n and $D(|A'|^s)$.

Since $D(|A|^k) \subset D(|A'|^k)$ and by the closed graph theorem, we deduce the existence of $C_k > 0$ such that for every $\psi \in D(|A|^k)$

$$\sum_n \lambda'^{2k}_n |\langle\psi,\phi'_n\rangle|^2 \le C_k \sum_n |\lambda_n|^{2k}|\langle\psi,\phi_n\rangle|^2$$

so that

$$\sum_n \lambda'^{2k}_n \left|\sum_j \langle\psi,\phi_j\rangle\langle\phi_j,\phi'_n\rangle\right|^2 \le C_k \sum_n |\lambda_n|^{2k}|\langle\psi,\phi_n\rangle|^2.$$

For all $\psi \in D(|A|^k)$ let $\widetilde{\psi}$ in H such that $\psi = |A|^{-k}\widetilde{\psi} = \sum \lambda_j^{-k}\langle\widetilde{\psi},\phi_j\rangle\phi_j$. Then, for all $\widetilde{\psi} \in H$, we have

$$\sum_n \lambda'^{2k}_n \sum_l \lambda_l^{-k}\overline{\langle\widetilde{\psi},\phi_l\rangle\langle\phi_l,\phi'_n\rangle} \sum_j \lambda_j^{-k}\langle\widetilde{\psi},\phi_j\rangle\langle\phi_j,\phi'_n\rangle \le C_k\|\widetilde{\psi}\|^2. \tag{15}$$

and the equality holds for $k = 0$ and $C_0 = 1$. Consider $\widetilde{\psi} \in H$ and

$$f_{\widetilde{\psi}} : z = s + \mathrm{i}y \mapsto \sum_n \lambda'^{2s+i2y}_n \langle|A|^{-s+\mathrm{i}y}\widetilde{\psi},\phi'_n\rangle\langle\phi'_n,|A|^{-s-\mathrm{i}y}\widetilde{\psi}\rangle$$

where, for every z in $\mathbf{C}$, $|A|^z\widetilde{\psi} = \sum_j \lambda_j^z\langle\widetilde{\psi},\phi_j\rangle\phi_j$. Then, by (15) for $s = 0$ and $s = k$ we have

$$\left|f_{\widetilde{\psi}}(s+iy)\right| \le C_s\||A|^{-s+\mathrm{i}y}\widetilde{\psi}\|_s\||A|^{-s-\mathrm{i}y}\widetilde{\psi}\|_s \le C_s\|\widetilde{\psi}\|^2.$$

If $\widetilde{\psi}$ is finite linear combination of the vectors $\{\phi_j\}_{j\in\mathbf{N}}$ then the function $f_{\widetilde{\psi}}$ analytic on the strip $\{z \in \mathbf{C} : 0 < \Re z < k\}$ and continuous on its closure as uniform limits of a partial sum on n. Since it is bounded on the boundary, by Hadamard three-lines theorem [18, Appendix IX.4], it is bounded on the strip, and, moreover, $\log(\sup_{\Re z=s}|f_{\widetilde{\psi}}(z)|)$, is a convex function of $s \in [0,k]$. So that for $s \in (0,k)$, we obtain

$$\sum_n \lambda'^{2s}_n |\langle\psi,\phi'_n\rangle|^{2s} \le C_k^{\frac{s}{k}} \sum_n |\lambda_n|^{2s}|\langle\psi,\phi_n\rangle|^2,$$

and by density $D(|A|^s) \subset D(|A'|^s)$. The hypothesis and the proof being symmetric in A and A' we have actually the equality. ■

APPENDIX
PROOF OF PROPOSITION 2

In this Appendix, we use regularization techniques to provide a proof of Proposition 2.

Proof of Proposition 2: Note that for every $u \in \mathbf{R}^p$, $D(|A+\sum_l u_l B_l|^{k/2}) = D(|A|^{k/2})$, the function $|A|^{k/2}e^{t(A+\sum u_l B_l)}\psi_0$ is in $C(\mathbf{R}, H)$ and for every $\varepsilon > 0$ the function $|A|^{k/2}(\varepsilon(A + \sum_l u_l B_l) + 1)^{-1}e^{t(A+\sum u_l B_l)}\psi_0$ is in $C^1(\mathbf{R}, H)$ whenever $\psi_0 \in D(|A|^{k/2})$.

If $t \mapsto \psi(t)$ is the solution of (2) with initial condition ψ_0 in $D(|A|^{k/2})$, the real mapping $f : t \mapsto \langle |A|^k\psi(t), \psi(t)\rangle$ is absolutely continuous from $\mathbf{R}$ to $\mathbf{R}$. We make a regularization to obtain extra regularity, we introduce $f_\varepsilon^j : t \mapsto \langle |A|^k(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t), (\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t)\rangle$. From the functional calculus [25, Theorem VIII.5] the sequence f_ε^j is pointwise convergent to f as ε tends to 0.

The function f_ε^j is absolutely continuous from $\mathbf{R}$ to $\mathbf{R}$ and it is differentiable on the interval (t_{j-1}, t_j), for every $t \in (t_{j-1}, t_j)$,

$$\begin{aligned}
\frac{d}{dt}f_\varepsilon^j(t) &= \frac{d}{dt}\langle |A|^k(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t), (\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t)\rangle \\
&= \langle |A|^k((A + \sum_l u_l^{j-1}B_l)\varepsilon + 1)^{-1}\psi(t), (A + \sum_{l=1}^p u_l(t)B_l)(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t)\rangle \\
&\quad + \langle |A|^k(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}(A + \sum_{l=1}^p u_l(t)B_l)\psi(t), (\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t)\rangle \\
&= 2\Re\langle |A|^k(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t), (A + \sum_{l=1}^p u_l(t)B_l)(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t)\rangle \\
&= 2\sum_{l=1}^p u_l(t)\Re\langle |A|^k(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t), B_l\psi(t)(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\rangle,
\end{aligned}$$

and since $(A, B_1, \ldots, B_p)$ is k-weakly-coupled,

$$\begin{aligned}
|\frac{d}{dt}f_\varepsilon^j(t)| &\leq 2c_k(A, B_1, \ldots, B_p)\times \\
&\qquad \times \sum_{l=1}^p |u_l(t)||\langle |A|^k(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t), (\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t)\rangle| \\
&\leq 2c_k(A, B_1, \ldots, B_p)\sum_{l=1}^p |u_l(t)|f_\varepsilon^j(t).
\end{aligned}$$

Gronwall's lemma implies that $f_\varepsilon^j(t) = \langle |A|^k(\varepsilon(A+\sum_l u_l^{j-1}B_l)+1)^{-1}\psi(t), (\varepsilon(A+\sum_l u_l^{j-1}B_l)+1)^{-1}\psi(t)\rangle \leq e^{2c_k(A,B_1,\ldots,B_p)\sum_{l=1}^p \int_{t_{j-1}}^t |u_l|(\tau)d\tau} f_\varepsilon^j(t_{j-1})$. Passing to the limit ε to 0, this gives $f(t) =$

$\langle |A|^k \psi(t), \psi(t) \rangle \leq e^{2c_k(A,B_1,\ldots,B_p)\sum_{l=1}^{p}\int_{t_{j-1}}^{t}|u_l|(\tau)d\tau} f(t_{j-1})$. An immediate iteration concludes the proof. ■

ACKNOWLEDGMENT

It is a pleasure for the authors to thank Ugo Boscain, Chitra Rangan, Pierre Rouchon, Mario Sigalotti, and Dominique Sugny for valuable inputs and advices.

The second and third authors are grateful to the Institut Henri Poincaré (Paris, France) for providing research facilities and a stimulating environment during the "Control of Partial and Differential Equations and Applications" program in the Fall 2010.

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