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. An important feature of these systems is that they can be precisely approached by finite dimensional Galerkin approximations. This property is of particular interest for the approximation of quantum system dynamics and the control of the bilinear Schrödinger equation.

The present study 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 $L^2(\Omega, \mathbf{C})$. Any physical quantity $\mathcal{O}$ (e.g. energy, position, momentum) is associated with a Hermitian operator $O : L^2(\Omega, \mathbf{C}) \rightarrow L^2(\Omega, \mathbf{C})$. The expected value of $\mathcal{O}$ for a system with wave function ψ is equal to $\int_\Omega \overline{\psi(x)} O \psi(x) \mathrm{d}\mu(x)$. For instance, a system with wave function ψ is in a subset ω of Ω with probability $\int_\omega |\psi|^2 \mathrm{d}\mu$.

The dynamics of a closed system submitted to excitations by p external fields (*e.g.* lasers) is described, under the dipolar approximation, by the bilinear Schrödinger equation

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

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

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$l \leq p$, usually called control, is a real function of the time representing the intensity of the laser l.

In recent years there has been an increasing interest in studying the controllability of the bilinear Schrödinger equation (1) mainly due to its importance for many advanced applications such as Nuclear Magnetic Resonance, laser spectroscopy, and quantum information science. The problem concerns the existence of control laws $(u_1, \ldots, u_p)$ steering the system from a given initial state to a pre-assigned final state in a given time. Considerable efforts have been made to study this problem and the main difficulty is the fact that the state space, namely $L^2(\Omega, \mathbf{C})$, has infinite dimension. Indeed in [1], a result which implies (see [2]) strong limitations on the exact controllability of the bilinear Schrödinger Equation has been proved. Hence, one has to look for weaker controllability properties as, for instance, approximate controllability or controllability between eigenstates of the Schödinger operator (which are the most relevant cases from the physical viewpoint). In dimension one, in the case $p = 1$, and for a specific class of control potentials a description of the reachable set has been provided [3], [4]. In dimension larger than one or in 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 (see for example [5], [6], [7] and references therein).

B. Finite dimensional approximations

To avoid difficulties in dealing with infinite dimensional systems, for instance in practical computations or simulations, one can project system (1) on finite dimensional subspaces of $L^2(\Omega, \mathbf{C})$. A vast literature is currently available on control of bilinear finite dimensional quantum systems (see for instance [8] and references therein) thanks, also, to general controllability methods for left-invariant control systems on compact Lie group [9]. A crucial issue is to guarantee that the finite dimensional approximations have dynamics close to the one of the original infinite dimensional system.

In [6] and [7], precise estimates of the distance between the infinite dimensional systems and some of its Galerkin approximations are used to prove that systems of type (1) are approximately controllable under physical conditions of non-degeneracy of the discrete spectrum of $-\Delta + V$. These estimates are derived for a sequence of *ad hoc* controls designed to steer the system from a given source to a given target. Besides the discretness of the spectrum of $-\Delta + V$, very few regularity assumptions are made on (1). Since the potential W is not assumed to be bounded or regular (say, not even continuous), the estimates obtained for a control u can possibly fail to hold for controls close to u, for instance, in a small neighborhood of u for some H^k norm.

Such pathological irregularities (everywhere discontinuous potentials or wave functions) are physically irrelevant. Following [10, Chapter 2.A], real potentials are at least continuous and wave functions are smooth (i.e., infinitely differentiable). As a consequence, most of the potentials and wave functions encountered in the literature are analytic. This strong regularity allows stronger estimates than those in [6] and [7].

As a matter of fact, a special class of bilinear systems of the type of (1), called weakly-coupled (see Definition 1 in Section II), exhibits very nice properties of approximations (see Theorem 4 below). Physically, for such weakly-coupled systems, the energy $\int_\Omega \overline{(-\Delta + V)\psi} \ \psi \mathrm{d}\mu$ is bounded by an explicit function of the L^1 norm of the control u (see Proposition 2), preventing propagation of the wave function to high energy levels.

The notion of weakly-coupled systems, and the fact that such systems can be precisely approached by finite dimensional bilinear systems, has many applications.

First, taking advantage of the powerful tools of the geometric control theory for finite dimensional systems [8], this definition can be used for the analysis and the open-loop control of infinite dimensional bilinear quantum systems. For instance, we used this method to prove that the rotational wave approximation (which is classical for finite dimensional systems) is still valid for infinite dimensional systems ([11]) or to exhibit an example of bilinear system approximately controllable in arbitrary small times ([12]).

Second, it provides easily computable bounds on the size of the finite dimensional systems to be considered for the numerical simulations of systems of type (1) in order to guarantee a given upper bound for the error. This has been used in [13] to implement a quantum gate in an infinite dimensional systems modelling the rotation of a 2D-molecule.

While the notion of weakly-coupled systems has been originally developed for open-loop control, the approximation results apply without modification (both for the theoretical analysis and the numerical simulation) in broader contexts. An example of Lyapunov design of open-loop control is presented in Section IV-D.

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 introduce the notion of weakly-coupled systems for bilinear quantum systems and we state some properties of their finite dimensional approximations. In particular the most important property of this class of systems is that they have a Good Galerkin Approximation (Theorem 4), that is, a finite dimensional approximation whose dynamics is arbitrarily close the the one of the infinite dimensional system. Thanks to this feature we are able to show an approximate controllability result in higher norm for such a class of systems (Proposition 5).

We then study two important examples of weakly-coupled systems, the first (Section III) covering, among others, the case where Ω is compact (Section III-B) 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 using the language of functional analysis. This reformulation allows us to treat examples slightly more general than (1), for instance, the example in Section III-A. For the convenience of the reader, we recall some basic notions of operator theory in the appendix.

In a separable Hilbert space H endowed with norm $\| \cdot \|$ and Hilbert product $\langle \cdot, \cdot \rangle$, we consider the evolution problem

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = \left(A + \sum_{l=1}^{p} u_l B_l \right) \psi \qquad (2)$$

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 the domain $D(A)$ of 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 $(-\mathrm{i}\lambda_j)_{j\in\mathbf{N}}$, the sequence $(\lambda_j)_{j\in\mathbf{N}}$ is positive non-decreasing and unbounded.

In the rest of our study, we denote by $(\phi_j)_{j\in\mathbf{N}}$ a Hilbert basis of H such that $A\phi_j = -\mathrm{i}\lambda_j\phi_j$ for every j 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 state ψ_0 in H, for every piecewise constant control $u : t \in \mathbf{R} \to \sum_{n=0}^{N} u^n \chi_{[t_n, t_{n+1}]}(t) \in \mathbf{R}^p$, where $\chi_{[a,b)}(t)$ stands for the characteristic function of the interval $[a, b)$, 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

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

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

Remark 1. From Assumption 1.1 we deduce that the resolvent of A is compact, and 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 Identity (18) applied to $A + \sum_l u_l B_l$ and A, gives that the resolvent of $A + \sum_l u_l B_l$ is compact. The spectrum of $-\mathrm{i}(A + \sum_l u_l B_l)$ is discrete and accumulates only at $+\infty$ (as $-\mathrm{i}(A + \sum_l u_l B_l)$ is bounded from below).

B. Energy growth

From Assumption 1.2, the operator 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 $s \geq 0$, using (19) 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. In the case $s = 0$, we have the Hilbert space norm, thus we write $\|\psi\|$ instead of $\|\psi\|_0$.

Remark 2. The s-norm is a way to measure the regularity of the wave functions. In the case where $|A|$ is the Laplace-Beltrami operator of a smooth compact manifold and k is an integer, $D(|A|^k)$ is the set of $2k$-times differentiable functions with square integrable $(2k)^{th}$ derivative.

The notion of weakly-coupled systems is closely related to the growth of the expected value of the energy. Here $\Re$ denotes the real part of a complex number.

Definition 1. Let k be positive 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

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

Remark 3. The terminology *weak-coupling* refers to the weakness of B in the scale of A. In other words the effect of B on the spectral properties of A is small enough to have a weak coupling effect on the Galerkin approximations associated with eigenvectors of A (see Lemma 3 below) or the boundedness in the s-norm of A of the evolution (see Proposition 2 below). The weakness of this action can also be seen through the transition probabilities or energy transitions between eigenstates (see Lemma 11 below).

We have the following technical interpolation result proved in Appendix A.

Lemma 1. *Let A and A' be invertible (from their respective domains to H) 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 whose proof is in Appendix B.

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 $\sum_{l=1}^p \|u_l\|_{L^1} \leq K$, one has*

$$\|\Upsilon_T^u(\psi_0)\|_{k/2} \leq e^{c_k(A, B_1, \ldots, B_p)K}\|\psi_0\|_{k/2}. \tag{3}$$

C. Good Galerkin approximation

In this section we show that a weakly-coupled system admits a finite dimensional approximation with trajectories close, at any 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, $(A, B_1, \ldots, B_p)$ 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 $K \geq 0, n \in \mathbf{N}$, $N \in \mathbf{N}$, $(\psi_j)_{1\leq j\leq n}$ in $D(|A|^{k/2})^n$, and for every piecewise constant function $u = (u_1, \ldots, u_p)$, such that $\sum_{m=1}^p \|u_m\|_{L^1} \leq K$, one has*

$$\|B_l(\mathrm{Id} - \pi_N)\Upsilon_t^u(\psi_j)\| \leq d\lambda_{N+1}^{(r-k)/2}e^{c_k(A, B_1, \ldots, B_p)K}\|\psi_j\|_{k/2}, \tag{4}$$

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

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

$$\begin{aligned}\|(\mathrm{Id} - \pi_N)\Upsilon_t^u(\psi_j)\|_{r/2}^2 &= \sum_{n=N+1}^\infty \lambda_n^r|\langle\phi_n, \Upsilon_t^u(\psi_j)\rangle|^2 \\ &\leq \lambda_{N+1}^{r-k}\|\Upsilon_t^u(\psi_j)\|_{k/2}^2. \end{aligned} \tag{5}$$

By Proposition 2, $\|\Upsilon_t^u(\psi_j)\|_{k/2}^2 \leq e^{2c_k(A, B_1, \ldots, B_p)K}\|\psi_j\|_{k/2}^2$ for every $t > 0$ and u of L^1-norm smaller than K. Equation (4) follows as, for every $l = 1, \ldots, p$, $\|B_l\psi\| \leq d\||A|^{\frac{r}{2}}\psi\|$. $\blacksquare$

Remark 4. Since $r < k$, then $\|B_l(\mathrm{Id} - \pi_N)\Upsilon_t^u(\psi_j)\|_{r/2}$ 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

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

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 $X_{(N)}^u(t, s)$ the propagator of (Σ_N) for a p-uple of piecewise constant functions $u = (u_1, \ldots, u_p)$.

Remark 5. 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 $\mathcal{L}_N = \mathrm{span}_{1\leq j\leq N}\{\phi_j\}$. Thus, (Σ_N) can be seen as a finite dimensional bilinear dynamical system in $\mathcal{L}_N$.

The operator A written in one of its eigenvector basis is diagonal and its dynamics is decoupled on each eigenspace. Thus the projection of the dynamics coincides with the dynamics of the associated truncation.

One of the most important consequence of the weak-coupling assumption is that, even though the coupling action of the operator B can give rise to intricate dynamics, this action is weak enough to allow approximations by the dynamics of the truncations as stated in the theorem below.

Theorem 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 $d > 0$ and $0 \leq r < k$ 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 $t \geq 0$,

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

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

$$\pi_N \Upsilon_t^u(\psi_j) = X_{(N)}^u(t,0)\pi_N\psi_j$$
$$+ \sum_{l=1}^{p} \int_0^t X_{(N)}^u(t,s)\pi_N B_l(\mathrm{Id} - \pi_N)\Upsilon_s^u(\psi_j)u_l(\tau)\mathrm{d}\tau. \quad (6)$$

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,

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

Then

$$\|\Upsilon_t^u(\psi_j) - X_{(N)}^u(t,0)\pi_N\psi_j\|$$
$$\leq \|(\mathrm{Id} - \pi_N)\Upsilon_t^u(\psi_j)\| + \|\pi_N \Upsilon_t^u(\psi_j) - X_{(N)}^u(t,0)\pi_N\psi_j\|$$
$$\leq \lambda_{N+1}^{-k/2}e^{c_k(A,B_1,\ldots,B_p)K}\|\psi_j\|_{k/2}$$
$$+ Kd\lambda_{N+1}^{(r-k)/2}e^{c_k(A,B_1,\ldots,B_p)K}\|\psi_j\|_{k/2}. \quad (8)$$

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 $(v_n)_{n\in\mathbf{N}}$ is a sequence of functions from $\mathcal{X}$ to H that tends uniformly to 0 (the null function) for the s_1-norm and it is uniformly bounded for the s_2-norm for $s_1 < s_2$, then $(v_n)_{n\in\mathbf{N}}$ tends uniformly to 0 in the $\frac{s_1+s_2}{2}$-norm. This is a consequence of Cauchy–Schwarz inequality, indeed

$$\|v_n\|_{\frac{s_1+s_2}{2}}^2 = |\langle |A|^{\frac{s_1+s_2}{2}}v_n, |A|^{\frac{s_1+s_2}{2}}v_n\rangle|$$
$$= |\langle |A|^{s_1}u_n, |A|^{s_2}v_n\rangle| \leq \|v_n\|_{s_1}\|v_n\|_{s_2}. \quad (9)$$

To conclude the proof in the general case $0 < s < k$, we apply iteratively this interpolation result with $v_N : (t,u) \mapsto (X_{(N)}^u(t,0)\pi_N - \Upsilon_t^u)\psi_j$, defined on $\mathcal{X} = [0,+\infty) \times \{u \in L^1 : \|u\|_{L^1} \leq K\}$. From the first part of the proof, $(v_N)_N$ tends uniformly to zero for the $s_1 = 0$ norm and it is bounded for the $s_2 = k$ norm. Hence by (9), the sequence $(v_N)_N$ tends uniformly to zero for the $k/2$ norm. Applying once again the interpolation estimate (9) with $s_1 = k/2$ and $s_2 = k$, we obtain that the sequence $(v_N)_N$ tends uniformly to zero for the $3k/4$ norm. After l interpolations, we obtain that the sequence $(v_N)_N$ tends uniformly to zero for the $k(1 - 1/2^l)$

norm. Conclusion follows by choosing an integer l such that $k(1 - 1/2^l) > s$. ∎

Remark 6. In the case $s = 0$, there is an explicit estimate for the order of the Galerkin approximation which existence is stated in Theorem 4. For instance, by (7), $\|\pi_N\Upsilon_t^u(\psi_j) - X_{(N)}^u(t,0)\pi_N\psi_j\| < \varepsilon$ if N is such that, for $j = 1, \ldots, n$,

$$\lambda_{N+1} > \left(\frac{Kde^{c_k(A,B_1,\ldots,B_p)K}\|\psi_j\|_{k/2}}{\varepsilon}\right)^{\frac{2}{k-r}}. \quad (10)$$

D. Approximate controllability in s-norm

Let $(A, B_1, \ldots, B_p)$ be a k-weakly-coupled system. For every ϕ in $D(|A|^{k/2})$, every $T \geq 0$ and every piecewise constant function $u : [0, T] \to \mathbf{R}^p$, one has $\Upsilon_T^u\phi \in D(|A|^{k/2})$, which is a deep obstruction to exact controllability. But this property also provides 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, l in $\mathbf{N}$, if there exists a finite sequence $((s_1^1, s_2^1), \ldots, (s_1^q, s_2^q))$ in S such that

(i) $s_1^1 = j$ and $s_2^q = l$;
(ii) $s_2^j = s_1^{j+1}$ for every $1 \leq j \leq q - 1$;
(iii) $\langle \phi_{s_1^j}, B\phi_{s_2^j}\rangle \neq 0$ 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-degenerate* (or sometimes *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 $\psi_1, \ldots, \psi_n \in D(|A|^s)$, $\hat{\Upsilon} \in U(H)$ such that $\hat{\Upsilon}(\psi_1), \ldots, \hat{\Upsilon}(\psi_n) \in D(|A|^s)$, and $\varepsilon > 0$, there exists a piecewise constant function $u_\varepsilon : [0, T_\varepsilon] \to \mathbf{R}$ such that

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

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

Proposition 5. *Let k be a positive number. Let (A, B) satisfy Assumption 1, be k-weakly-coupled, and admit a non-degenerate 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 $\varepsilon > 0$, $\psi_1, \ldots, \psi_n \in D(|A|^{s/2})$, and $\hat{\Upsilon} \in U(H)$ such that $\hat{\Upsilon}(\psi_1), \ldots, \hat{\Upsilon}(\psi_n) \in D(|A|^{s/2})$. Fix n_1 sufficiently large such that $\|\hat{\Upsilon}(\psi_j) - \pi_{n_1}\hat{\Upsilon}(\psi_j)\|_{s/2} < \varepsilon/3$ for every $j = 1, \ldots, n$.

There exist $l_1, \ldots, l_n$ such that $t \mapsto (e^{it\lambda_{l_1}}, \ldots, e^{it\lambda_{l_n}})$ is ε-dense in the torus $\mathbf{T}^n$ (see [7, Proposition 6.1]). Call $m = \max\{n_1, l_1, \ldots, l_n\}$.

By [7] the existence of a non-degenerat chain of connectedness is sufficient for the approximate controllability of (A, B) in the norm of H. More precisely, by [7, Remark 5.9] there exists K_1 such that for every $\eta > 0$ there exist a control

u_1^η satisfying $\|u_1^\eta\|_{L^1} \le K_1$ and $\theta_1, \theta_2, \ldots, \theta_n$, such that $\|\Upsilon_{T_1}^{u_1^\eta}(\psi_j) - e^{i\theta_j}\phi_{l_j}\| < \eta$, for every $j = 1, \ldots, n$.

Similarly, since as shown in [7, Section 6.1] the hypotheses sufficient for controllability (and in particular the one of [7, Remark 5.9]) hold for the system $(-A, -B)$, we have existence of K_2 such that for every $\eta > 0$ there exists u_2^η satisfying $\|u_2^\eta\|_{L^1} \le K_2$ and $\bar{\theta}_1, \ldots, \bar{\theta}_n \in \mathbf{R}$ such that the solution of the system

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

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

Let τ such that $\|e^{i\tau\lambda_{l_j}}e^{i\theta_j} - e^{i\bar{\theta}_j}\| < \eta$ for every $j = 1, \ldots, n$. 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 state ψ_j, 3η-close in the norm $\|\cdot\|$ to $\hat{\Upsilon}(\psi_j)$ in a time T, namely $\|\hat{\Upsilon}(\psi_j) - \Upsilon_T^{u^\eta}(\psi_j)\| \le 3\eta$.

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

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

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

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

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

for η sufficiently small. $\blacksquare$

III. THE BOUNDED CASE

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

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

A. Example: single trapped ion

This example is a model of a two level ion trapped in a harmonic potential and under the action of an external field. This model has been extensively studied (see for example [14], [15], [16], and [17]).

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 two coupled harmonic oscillators

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

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

$$\frac{\mathrm{d}\psi}{\mathrm{d}t} = A\psi + u_1(t)B_1\psi + u_2(t)B_2\psi \qquad (11)$$

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

By [18, 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 [19, Theorem X.12]). The spectrum of A is the sequence $(-i\lambda_n)_{n\in\mathbf{N}} = -i(\omega(n+1/2)+\Omega)_{n\in\mathbf{N}}$. For every n in $\mathbf{N}$, the eigenvalue $-i\lambda_n$ 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 nth 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 $2^k C_k$ 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

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

since $(u_1B_1 + u_2B_2)\psi \in D(A^k)$ when $\psi \in D(A^k)$. Hence for every $(u_1, u_2) \in \mathbf{R}^2$, $D(|A|^k) = D(|A + u_1B_1 + u_2B_2|^k)$ and 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 $2^k C_k$.

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 [20, Theorem 7.2.6]). Note that λ_1 is not necessarily positive but this can be assumed 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 [21, 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 $C_k = 2^{2k+1} \sup_{0 \leq j \leq 2k} \|W^{(j)}\|_{L^\infty(\Omega, \mathbf{R})}$ such that $\|Wf\|_{H^{2k}} \leq C_k \|f\|_{H^{2k}}$. 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 7. As a 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 Theorem 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 $H_e^k = \{\psi \in H^{2k}(\Omega, \mathbf{C}) : \psi \text{ odd }\}$. The skew-symmetric operator $B = -\mathrm{i}\cos\theta$ is bounded on $D(|A|^{k/2})$ for every k. By Proposition 6, for every k in $\mathbf{N}$, (A, B) is k-weakly-coupled. Theorem 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 viewpoint 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 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 Schrödinger 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. Using spherical coordinates (ν, θ), the controlled Schrödinger equation is

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

Therefore, since Ω is compact, Theorem 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 ([22, Theorem 1.4.2]). It suffices to check that for every k in $\mathbf{N}$, u in $\mathbf{R}$ and $\varepsilon > 0$, there exists b_ε depending on u, k and ε such that, for every ψ in $D(A^k)$,

$$\|((A + uB)^k - A^k)\psi\| \leq \varepsilon\|A^k\psi\| + b_\varepsilon\|\psi\|. \quad (12)$$

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 $D(A^r)$,

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

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

$$
\begin{aligned}
\|Bv\|_r^2 &\leq \sum_{n=1}^{n_0} \lambda_n^{2r} |\langle v, B\phi_n \rangle|^2 + \varepsilon \sum_{n \geq n_0 - 1} \lambda_n^{2r+2} |\langle \phi_n, v \rangle|^2 \\
&\leq C_\varepsilon \|v\|^2 + \varepsilon \|v\|_{r+1}^2. \quad (13)
\end{aligned}
$$

We prove (12) by induction on k. For $k = 1$ this is a consequence of (13) with $r = 0$. The inductive step follows from the fact that

$$
\begin{aligned}
(A + uB)^{k+1} - A^{k+1} &= u((A+uB)^k B - A^k B) \\
&\quad + uA^k B + ((A+uB)^k - A^k)A
\end{aligned}
$$

for every u in $\mathbf{R}$ and from (13). ∎

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 with coupling constant*

$$
c_k(A, B) \leq \sup_n |b_{n,n+1}| \left(\frac{\lambda_{n+1}^k}{\lambda_n^k} - 1 \right).
$$

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

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

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 $n < l$ be two integers. 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,*

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

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

Proof: Let $K > 0$. We prove the result for u piecewise constant of L^1-norm smaller than K. By Propositions 9 and 10, (A, B) is k-weakly-coupled. For every $\varepsilon > 0$ by Theorem 4 there exists $N = N(K, \varepsilon) > l$ such that $\|\Upsilon_t^u(\phi_n) - X_{(N)}^u(t, 0)\phi_n\| < \varepsilon$ for every $t \geq 0$.

Consider the solution $\psi : t \mapsto X_{(N)}^u(t, 0)\phi_n$ of (Σ_N) with initial state ϕ_n. Then $\psi(t) = e^{tA^{(N)}}\phi_n +$

$\int_0^t e^{(t-s)A^{(N)}} u(s) B^{(N)} \psi(s) \mathrm{d}s$. After $l-n$ iterations we get

$$\psi(t) = e^{tA^{(N)}}\Big(\phi_n +$$
$$+ \sum_{j=1}^{l-n-1} \int_{0 \le s_j \le \cdots \le s_1 \le t} e^{(t-s_1)A^{(N)}} B^{(N)} \cdots e^{(s_{j-1}-s_j)A^{(N)}} B^{(N)} \times$$
$$\times e^{s_j A^{(N)}} \phi_n \prod_{m=1}^{j} u(s_m) \mathrm{d}s_1 \ldots \mathrm{d}s_j +$$
$$+ \int_{0 \le s_{l-n} \le \cdots \le s_1 \le t} e^{(t-s_1)A^{(N)}} B^{(N)} e^{(s_1-s_2)A^{(N)}} B^{(N)} \times \cdots$$
$$\times e^{(s_{l-n-1}-s_{l-n})A^{(N)}} B^{(N)} \psi(s_{l-n}) \prod_{m=1}^{l-n} u(s_m) \mathrm{d}s_1 \ldots \mathrm{d}s_{l-n}\Big).$$

For the tri-diagonal structure of the system we have

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

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

$$\langle \phi_l, \psi(t) \rangle = e^{tA^{(N)}} \times$$
$$\int_{0 \le s_{l-n} \le \cdots \le s_1 \le t} \langle \phi_l, e^{(t-s_1)A^{(N)}} B^{(N)} e^{(s_1-s_2)A^{(N)}} B^{(N)} \times$$
$$\cdots \times e^{(s_{l-n-1}-s_{l-n})A^{(N)}} B^{(N)} \psi(s_{l-n}) \rangle \prod_{m=1}^{l-n} u(s_m)$$
$$\mathrm{d}s_1 \ldots \mathrm{d}s_{l-n}$$

Now,

$$\sup_{s_1,\ldots,s_{l-n} \in [0,t]} \| B^{(N)} e^{(s_{l-n}-s_{l-n-1})A^{(N)}} B^{(N)} \times \cdots$$
$$\times e^{(s_2-s_1)A^{(N)}} B^{(N)} e^{(s_1-t)A^{(N)}} \phi_l \| \le 3^{l-n} \prod_{j=l+1}^{2l-n} L(j) \quad (14)$$

Then

$$|\langle \phi_l, \psi(t) \rangle|$$
$$\le 3^{l-n} \prod_{j=l+1}^{2l-n} L(j) \int_{0 \le s_1 \le \cdots \le s_{l-n} \le t} |u(s_1)| \ldots |u(s_{l-n})| \mathrm{d}s_1 \ldots \mathrm{d}s_{l-n}$$
$$= 3^{l-n} \frac{\left(\int_0^t |u(s)| \mathrm{d}s\right)^{l-n}}{(l-n)!} \prod_{j=l+1}^{2l-n} L(j),$$

hence $|\langle \phi_l, \Upsilon_t^u(\phi_n) \rangle| \le 3^{l-n} \frac{K^{l-n}}{(l-n)!} \prod_{j=l+1}^{2l-n} L(j) + \varepsilon$, 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 [19, Section X.12, Example 1]).

Remark 8. In the case in which the diagonal of B is zero then equation (14) reads

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

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

Proposition 12. *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 $0 \le r < k/2$ 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 N in $\mathbf{N}$, for every $t \ge 0$, $n \le N \in \mathbf{N}$, for every piecewise constant control u,*

$$\|\pi_N \Upsilon_t^u(\phi_n) - X_{(N)}^u(t,0)\phi_n\| \le$$
$$\frac{3^{N-n}}{(N-n)!} L(N+1) \prod_{j=N+1}^{2N-n} L(j) \left(\int_0^t |u(\tau)| \mathrm{d}\tau\right)^{N-n+1}$$

where for $j \in \mathbf{N}$, $L(j) = \sup_{p,q \le j} |b_{p,q}|$.

Proof: Because of the tri-diagonal structure, (6) gives

$$\|\pi_N \Upsilon_t^u(\phi_n) - X_{(N)}^u(t,0)\phi_n\|$$
$$\le |b_{N,N+1}| \left(\int_0^t |u(\tau)| \mathrm{d}\tau\right) \sup_{\tau \in [0,t]} |\langle \phi_N, \Upsilon_\tau^u \phi_n \rangle|.$$

Conclusion follows from Lemma 11. ∎

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,l in $\mathbf{N}$, $\lambda_l = l^2$, $\langle \phi_j, B\phi_l \rangle \ne 0$ if and only if $|j-l| = 1$ 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 $\mathbf{N}$,

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

In particular $c_1(A,B) \le 3/2$ and, by (10), we obtain that $\|\pi_N \Upsilon_t^u(\phi_1) - X_{(N)}^u(t,0)\pi_N \phi_1\| < \varepsilon$ 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 8 and Proposition 12, we get

$$\|X_{(N)}^u(t,0)\phi - \pi_N \Upsilon_t^u(\phi)\| \le \frac{K^{N-1}}{(N-2)!}$$

for any u such that $\|u\|_{L^1} \le K$ and any ϕ in $\mathrm{span}(\phi_1, \phi_2)$ with norm 1.

The second estimates is significantly better than the first one. For instance, if one has $\|u\|_{L^1} = 4$ 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, $\|u\|_{L^1}^{N-1} < \varepsilon(N-2)!$, is true for $N = 20$.

D. Example: Lyapunov design of open-loop control of the rotation of a planar molecule

A classical method to design controls steering the system (2) from a given source to a given target is to use Lyapunov techniques (see [23]). In practice, a suitable function $V : H \to H$ is used to measure the distance between the current point ψ and the target (that could be a precise wave function or a subset of the Hilbert sphere of H). Under suitable regularity assumptions, the mapping $t \mapsto V(\psi(t))$ is differentiable and

$$\frac{\mathrm{d}}{\mathrm{d}t}V(\psi(t)) = \mathrm{D}_{\psi(t)}V((A + u(t)B)\psi(t))$$

is an affine function in $u(t)$. A suitable choice of $u(t)$ depending of $\psi(t)$ ensures that the function $t \mapsto V(\psi(t))$ is decreasing. The proof that ψ actually converges to the target is non-trivial and usually relies on LaSalle invariance principles.

When the system (A, B) is weakly-coupled, the Good Galerkin Approximations may be used to obtain precise estimates on the quality of the controls obtained with Lyapunov techniques. For instance, consider the system of Section III-C with the source equal to $\phi = \cos(\eta)\phi_1 + \sin(\eta)\phi_2$, and the target equal to $\{e^{i\theta}\phi_2 | \theta \in \mathbf{R}\}$ where ϕ_1 and ϕ_2 are the first eigenstates of the Laplacian and $\eta = 10^{-3}$. On the Galerkin approximation of size $N = 20$ of the system (2), we use the Lyapunov function $V : \psi \mapsto 1 - |\langle \phi_2, \psi \rangle|^2$ which satisfies

$$\frac{\mathrm{d}}{\mathrm{d}t}V(\psi(t)) = -2u(t)\Re(\langle \phi_2, B\psi \rangle \overline{\langle \phi_2, \psi \rangle})$$

To ensure that V decreases along the trajectories of (2), we chose, for every t, $\tilde{u}(t) := \Re(\langle \phi_2, X^u_{(20)}(t, 0)(\phi) \rangle \langle \phi_2, BX^u_{(20)}(t, 0)(\phi) \rangle)$. We find numerically $|\langle \phi_2, X^{\tilde{u}}_{(20)}(120, 0)(\cos(\eta)\phi_1 + \sin(\eta)\phi_2) \rangle| > 1 - 3.10^{-8}$ and $\int_0^{120} |u(t)| \mathrm{d}t < 4$, see [24] for the source of the **Scilab** program. From Proposition 12, we obtain $|\langle \phi_2, \Upsilon^{\tilde{u}}_{120,0}(\cos(\eta)\phi_1 + \sin(\eta)\phi_2) \rangle| > 1 - 10^{-4}$.

E. Example: quantum harmonic oscillator

The quantum harmonic oscillator is among the most important examples of quantum system (see, for instance, [10, Complement G_V]). Its controlled version has been extensively studied (see, for instance, [25], [26]). In this example $H = L^2(\mathbf{R}, \mathbf{C})$ and equation (2) reads

$$\mathrm{i}\frac{\partial \psi}{\partial t}(x, t) = \frac{1}{2}(-\Delta + x^2)\psi(x, t) + u(t)x\psi(x, t). \quad (15)$$

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

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

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

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

The quantum harmonic oscillator is not controllable (in any reasonable sense) as proved in [25]. However, the Galerkin approximations of (15) of every order are exactly controllable (see [27]), and Theorem 4 ensures that any trajecory of the infinite dimensional system is a uniform limit of trajectories of its Galerkin approximations. This is not a contradiction, since the infinite dimensional system cannot track, in general, every trajectory of its Galerkin approximations. In particular, there is no reason for which the infinite dimensional system could track a sequence of trajectories of its Galerkin approximations associated with controls with L^1 norm tending to infinity. As a matter of fact, if one wants to steer a solution of the Galerkin approximation of order N of (15) from a given state (say, the first eigenstae) to an ε-neighbourhood of a given target (say, the second eigenstate), the L^1 norm of the control blows up as N tends to infinity.

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 Theorem 4 with $k = 2$, $r = 1$, $d = 1$, and $\|\phi_1\|_1 = 1/2$. The resulting bound, as given by (10),

$$N > \frac{K^2 e^{16K}}{4\varepsilon^2} - \frac{1}{2} \quad (16)$$

is however rather weak. As in the example of Section IV-C, the tri-diagonal structure of B allows better estimates. Using Remark 8, we find that $\|X^{(N)}_u(t, 0)\phi_1 - \pi_N\Upsilon^u_t\phi_1\| \leq \varepsilon$ 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 $N = 413$, while (16) is false for $N < 10^{29}$.

V. CONCLUSION

In our study we focused on the notion of weak-coupling. We established some interesting consequence in control theory and in numerical simulations which applies to common physical models. We prove a result, Theorem 4, providing a uniform bound on the difference from dynamics of a finite dimensional Galerkin approximation and dynamics of the infinite dimensional system. Moreover, an estimate on size of the Galerkin approximation has been explicitly provided for some relevant class of systems, allowing, in particular, *a priori* estimates on the error in numerical simulations on finite dimensional

approximations. In some case, the result permits to adapt finite dimensional control techniques to study the challenging problem of the control of the bilinear Schrödinger equation. For this reason we believe that the notion of weak-coupling will be a main tool in the study of controllability with relaxed controls, such as Dirac impulses, which represent, in some case, a better modelization of the physical experiences. Finally, we believe that the strong properties of convergence of the finite dimensional approximations of weakly-coupled systems will allow to address the study of a general controllabilty result for the bilinear Schrödinger equation with mixed spectrum.

APPENDIX

A. 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 bases 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 $D(|A|^k) \subset D(|A'|^k)$, 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

$$\sum_n \lambda'^{2k}_n \sum_l \lambda_l^{-k}\overline{\langle\widetilde{\psi},\phi_l\rangle\langle\phi_l,\phi'_n\rangle} \sum_j \lambda_j^{-k}\langle\widetilde{\psi},\phi_j\rangle\langle\phi_j,\phi'_n\rangle$$
$$\le C_k\|\widetilde{\psi}\|^2. \tag{17}$$

and the equality holds for $k = 0$ and $C_0 = 1$. Consider $\psi \in H$ and $f_{\widetilde{\psi}} : z = s + iy \mapsto \sum_n \lambda'^{2(s+iy)}_n\langle|A|^{-s+iy}\widetilde{\psi},\phi'_n\rangle\langle\phi'_n,|A|^{-s-iy}\widetilde{\psi}\rangle$ 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 (17) for $s = 0$ and $s = k$ we have $\left|f_{\widetilde{\psi}}(s+iy)\right| \le C_s\||A|^{-s+iy}\widetilde{\psi}\|_s\||A|^{-s-iy}\widetilde{\psi}\|_s \le C_s\|\widetilde{\psi}\|^2$.

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 [19, 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. ∎

B. 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 state 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, see (20) or [28, 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 $t \in (t_{j-1}, t_j)$,

$$\frac{\mathrm{d}}{\mathrm{d}t}f_\varepsilon^j(t)$$
$$= \frac{\mathrm{d}}{\mathrm{d}t}\langle|A|^k\Big(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1\Big)^{-1}\psi(t),$$
$$\Big(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1\Big)^{-1}\psi(t)\rangle$$
$$= \langle|A|^k\Big((A + \sum_l u_l^{j-1}B_l)\varepsilon + 1\Big)^{-1}\psi(t),$$
$$(A + \sum_l u_l(t)B_l)(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t)\rangle$$
$$+ \langle|A|^k\Big(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1\Big)^{-1}$$
$$\Big(A + \sum_l u_l(t)B_l\Big)\psi(t), \Big(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1\Big)^{-1}\psi(t)\rangle$$
$$= 2\Re\langle|A|^k\Big(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1\Big)^{-1}\psi(t),$$
$$\Big(A + \sum_l u_l(t)B_l\Big)\Big(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1\Big)^{-1}\psi(t)\rangle$$
$$= 2\sum_l u_l(t)\Re\langle|A|^k\Big(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1\Big)^{-1}\psi(t),$$
$$B_l\Big(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1\Big)^{-1}\psi(t)\rangle,$$

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

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}f_\varepsilon^j(t)\right|$$
$$\le 2c_k(A, B_1, \ldots, B_p) \times$$
$$\times \sum_l |u_l(t)||\langle|A|^k(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t),$$
$$(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t)\rangle|$$
$$\le 2c_k(A, B_1, \ldots, B_p)\sum_l |u_l(t)|f_\varepsilon^j(t).$$

Gronwall's lemma implies that $f_\varepsilon^j(t) = \langle|A|^k(\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t), (\varepsilon(A + \sum_l u_l^{j-1}B_l) + 1)^{-1}\psi(t)\rangle \le$

$e^{2c_k(A,B_1,...,B_p)\sum_l \int_{t_{j-1}}^t |u_l|(\tau)\mathrm{d}\tau} f_\varepsilon^j(t_{j-1})$. Passing to the limit ε to 0 and using (20), this gives $f(t) = \langle |A|^k\psi(t), \psi(t)\rangle \leq e^{2c_k(A,B_1,...,B_p)\sum_l \int_{t_{j-1}}^t |u_l|(\tau)\mathrm{d}\tau} f(t_{j-1})$. An immediate iteration in j concludes the proof. ∎

C. Linear operator in Hilbert spaces

For the reader's sake, this section recalls some basic facts of the theory of linear operators in a Hilbert space. We refer to [29], [28] for more details.

1) Closed operator and adjoints: Consider a separable Hilbert space H endowed with norm $\|\cdot\|$ and Hilbert product $\langle \cdot, \cdot \rangle$.

A linear operator is the coupled data $(A, D(A))$ where $D(A)$ is a subspace of H and A a linear operator from $D(A)$ to H. To simplify the notation we often write A instead and refer to $D(A)$ as the domain of A. An operator A' is an extension of A if $D(A) \subset D(A')$ and $A' = A$ on $D(A)$. Below we will write $A \subset A'$.

An operator is densely defined if its domain is dense.

An operator A is closed if its graph $\{(\psi, A\psi), \quad \psi \in D(A)\}$ is a closed subspace of $H \times H$ (endowed with its natural product topology). Notice that from the closed graph theorem, closed operator A with $D(A) = H$ are exactly bounded operators on H.

An operator A is closable if it has a closed extension. In this case, there exists a smallest (in the sense of the extension) closed extension which is called the closure and denoted $\overline{A}$. Notice that in this case the closure of the graph of A is the graph of the closure of A.

If A is a densely defined operator, we define its adjoint A^* by

$$D(A^*) = \{\phi \in H, \text{s.t.} \exists \eta \in H, \forall \psi \in D(A), \langle \phi, A\psi \rangle = \langle \eta, \psi \rangle\}$$

and for any $\phi \in D(A^*)$, $A^*\phi = \eta$, uniqueness of η follows from the density of the domain.

Using transformation $(\psi, \eta) \mapsto (-\eta, \psi)$ in $H \times H$, Riesz lemma and Closed Graph theorem we deduce that A^* is closed and A is closable if and only if $D(A^*)$ is dense, [28, Theorem VIII.1].

Notice that if $A \subset A'$ then $(A')^* \subset A^*$.

2) Spectrum and resolvent: Let A be a closed densely defined operator. A complex number λ is in the resolvent set $\rho(A)$ of A if $A - \lambda I_H$ is invertible (with bounded inverse) from $D(A)$ to H. The complementary set of $\rho(A)$ is the spectrum $\sigma(A)$ of A.

For any $\lambda \in \rho(A)$, the operator $R_A(\lambda) := (A - \lambda I_H)^{-1}$ is a bounded operator. Moreover for $\lambda, \lambda' \in \rho(A)$, $R_A(\lambda)$ commutes to $R_A(\lambda')$ and we have the following resolvent identity

$$R_A(\lambda) - R_A(\lambda') = (\lambda - \lambda')R_A(\lambda)R_A(\lambda'). \quad (18)$$

Thus for $\lambda' \neq \lambda$ in the resolvent set of A, we have

$$I_H = (\lambda' - \lambda)(I_H - (\lambda - \lambda')R_A(\lambda'))\left((\lambda' - \lambda)^{-1}I_H - R_A(\lambda)\right)$$

from which we deduce that the spectrum of $R_A(\lambda)$ is the closure of the image of the spectrum of A by $\lambda' \mapsto (\lambda' - \lambda)^{-1}$.

Riesz-Schauder theorem [28, Theorem VI.15] gives that if one of the resolvents of A is compact then the spectrum of A is made of isolated eigenvalues of finite algebraic multiplicity (the corresponding algebraic kernel is finite dimensional) possibly accumulating at infinity.

Notice that if one of the resolvents is compact then all of them are.

3) Symmetric operators: A densely defined operator A is symmetric if $A \subset A^*$. A symmetric operator is thus always closable. A symmetric operator is self-adjoint if $A = A^*$. A self-adjoint operator is thus always closed. A symmetric operator is essentialy self-adjoint if its closure is self-adjoint.

A densely defined operator A is skew-symmetric if iA is symmetric. A skew-symmetric operator is skew-adjoint if $A = -A^*$, that is iA is self-adjoint. A skew-symmetric operator is essentialy skew-adjoint if its closure is skew-adjoint.

Given a skew-adjoint operator A for every ψ in $D(A)$,

$$\|(A - zI_H)\psi\|^2 = \|(A + \Im zI_H)\psi\|^2 + |\Re z|^2\|\psi\|^2$$

from which we deduce that any non-purely imaginary complex number is in the resolvent set of A, or the spectrum of A is purely imaginary, and for every ψ in H, $\|R_A(z)\psi\| \leq \frac{1}{|\Re z|}\|\psi\|$ which, from the Hille-Yosida theorem [19, Theorem X.47a], provides the existence of a continuous family of unitary operators $t \in \mathbf{R} \mapsto e^{tA}$ such that for any $\psi_0 \in H$, $\psi : t \in \mathbf{R} \mapsto e^{tA}\psi_0$ is the unique strong solution of the Cauchy problem $\partial_t \psi = A\psi \quad \psi(0) = \psi_0$ if $\psi_0 \in D(A)$ and defines a mild solution in the other cases.

A symmetric operator A is said to be positive if the associated quadratic form $\langle A\psi, \psi \rangle$ defined on $D(A)$ is positive and it is said bounded from below if there exists a real c such that $A - c$ is positive.

If A is skew-adjoint and one of the resolvent of A is compact then the spectrum of A is made of purely imaginary eigenvalues of finite multiplicity possibly accumulating at infinity in modulus. Moreover there exists a Hilbert basis made of eigenvectors. If iA is bounded from below the only accumulation point is $+i\infty$.

Reciprocally if A is skew-adjoint with a spectrum made of isolated eigenvalues of finite multiplicity accumulating only at infinity then A has a compact resolvent. In this framework, the operator A can be redefined the following way (see [28, Theorem VI.17]). Denote by $(\lambda_n)_{n \in \mathbf{N}}$ the spectrum of A and $(\phi_n)_{n \in \mathbf{N}}$ a Hilbert basis of eigenvectors of A such that $A\phi_n = \lambda_n\phi_n$ then $D(A) = \left\{\psi \in H, \quad \sum_n |\lambda_n|^2|\langle\psi, \phi_n\rangle|^2 < +\infty\right\}$ and $A\psi = \sum_n \lambda_n\langle\psi, \phi_n\rangle\phi_n$.

For $\psi \in D(|A|^s)$, we define

$$|A|^s\psi = \sum_n |\lambda_n|^s\langle\psi, \phi_n\rangle\phi_n, \quad (19)$$

where $D(|A|^s) = \left\{\psi \in H, \quad \sum_n |\lambda_n|^{2s}|\langle\psi, \phi_n\rangle|^2 < +\infty\right\}$.

One can also notice that for any $\psi \in H$, $e^{tA}\psi = \sum_n e^{t\lambda_n}\langle\psi, \phi_n\rangle\phi_n$ and on $D(|A|^s)$, $|A|^s$ and

e^{itA} commutes. Thus

$$(\varepsilon A + 1)^{-1}\psi = \sum_n (\varepsilon\lambda_n + 1)^{-1}\langle\psi, \phi_n\rangle\phi_n \qquad (20)$$

which, by the Dominated Convergence Theorem, tends to ψ in $D(|A|^s)$, for any $s \in \mathbf{R}$, as ε goes to 0.

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