Total Variation of the Control and Energy of Bilinear Quantum Systems

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***Abstract*— In the present note, we give two examples of bilinear quantum systems showing good agreement between the total variation of the control and the variation of the energy of solutions, with bounded or unbounded coupling term. The corresponding estimates in terms of the total variation of the control appear to be optimal.**

I. INTRODUCTION

A. Control of quantum systems

The state of a quantum system evolving in a Riemannian manifold Ω is described by its *wave function*, a point ψ in $L^2(\Omega, \mathbf{C})$. When the system is submitted to an electric field (e.g., a laser), the time evolution of the wave function is given, under the dipolar approximation and neglecting decoherence, by the Schrödinger bilinear equation:

$$\mathrm{i}\frac{\partial \psi}{\partial t} = (-\Delta + V(x))\psi(x,t) + u(t)W(x)\psi(x,t) \qquad (1)$$

where Δ is the Laplace-Beltrami operator on Ω, V and W are real potential accounting for the properties of the free system and the control field respectively, while the real function of the time u accounts for the intensity of the laser.

In view of applications (for instance in NMR), it is important to know whether and how it is possible to choose a suitable control $u : [0,T] \to \mathbf{R}$ in order to steer (1) from a given initial state to a given target. This question has raised considerable interest in the community in the last decade. After the negative results of [1] and [2] excluding exact controllability on the natural domain of the operator $-\Delta + V$ when W is bounded, the first, and at this day the only one, description of the attainable set for an example of bilinear quantum system was obtained by ([3], [4]). Further investigations of the approximate controllability of (1) were conducted using Lyapunov techniques ([5], [6], [7], [8], [9], [10]) and geometric techniques ([11], [12]).

B. Various notions of energies

Quantum control is a trans-disciplinary field where different communities use the same word "energy" with possibly different meaning.

Mathematically, the energy of system (1) is any norm in (a subspace of) $L^2(\Omega, \mathbf{C})$ and the energy for the control u in any norm in the space of admissible controls. A recurrent issue when studying systems of the type of (1) is to obtain a priori estimates of the energy of the system in terms of some energy of the control. Such energy estimates are crucial for many reasons, both for mathematical and engineering purposes, including for instance the proof of the well-posedness of the system and the regularity of the solutions [13], or estimates of the distance between the original infinite dimensional systems and some of its finite dimensional approximations (see Section II-C below).

Physically, the energy of the quantum system (1) with wave function ψ is $E(\psi) = \int_\Omega \left[(-\Delta + V)\overline{\psi}\right] \psi \,\mathrm{d}\mu$. The physical energy is therefore constant in time whenever the control u is zero. When the control u is nonzero, and provided suitable regularity hypotheses, the energy evolves as

$$\frac{\mathrm{d}E}{\mathrm{d}t} = 2u(t)\Im\left(\int_\Omega \left[(\Delta + V)\overline{\psi}\right] W\psi \,\mathrm{d}\mu\right). \qquad (2)$$

Note that the time derivative of the energy E at time t depends on the value $u(t)$ of the intensity of the external field *and* on the wave function $\psi(t)$.

A natural question is to relate the mathematical energy of the control with the physical energy of the system.

Standard candidates for these estimates, widely used in practice, are the L^p norms $\|u\|_{L^p(0,T)} = \left(\int_0^T |u(t)|^p \mathrm{d}t\right)^{\frac{1}{p}}$, for some suitable $p > 0$. Indeed, many previous works addressed the problem of the optimal control of the system (1) for costs involving the L^2 norm of the control (see for instance [14] or [15]). The main reason for choosing the L^2 norm is the fact that the natural Hilbert structure of L^2 allows the use of the powerful tools of Hilbert optimization. It is common belief that there is a natural relation of the L^2 norm of u and the energy of the system. The note [16] showed that, in general, the L^1-norm provides more information on the evolution of the system than other L^p-norms for $p > 1$.

A whole theory of non-autonomous linear dynamics described by unbounded linear operators has been developed in the classical work of Kato [17]. From this paper, one can deduce some energy estimates for bilinear quantum system in term of the total variation of the control. Because of their technicality, these results are not really used by the quantum engineering community.

C. Contribution of this note

The aim of this note is to show that Kato's estimates of physical energy in terms of the total variation of the control are optimal (up to a multiplicative constant). To the best of our knowledge, this theoretical result is new. Some of the many theoretical and practical implications, both for quantum engineering and mathematical analysis of bilinear quantum system will be detailed in the last part of this paper. The difficulty of the proof consists in finding a concrete example for which the physical energy follows, up to a given multiplicative constant, Kato's estimates. For this, we use some recent explicit construction of efficient control laws (introduced in [18]) allowing explicit (yet not completely obvious) calculations.

D. Framework and notations

To take advantage of the powerful tools of the theory of linear operators, we reformulate the bilinear dynamics (1) in more abstract framework. In the separable Hilbert space H, we consider the bilinear system

$$\frac{\mathrm{d}\psi}{\mathrm{d}t}(t) = A\psi(t) + u(t)B\psi(t) \tag{3}$$

where the (time independent) linear operators A and B satisfy some regularity assumptions.

Assumption 1: The triple (A, B, Φ) is such that

1) A is skew-adjoint, possibly unbounded, on its domain $D(A)$;
2) $-\mathrm{i}A$ is positive;
3) B is bounded relatively to A: there exist a and b in $\mathbf{R}$ such that $\|B\psi\| \leq a\|A\psi\| + b\|\psi\|$;
4) $\Phi = (\phi_j)_{j\in\mathbf{N}}$ is a Hilbert basis of H made of eigenvectors of A: for every j in $\mathbf{N}$, there exists λ_j in $\mathbf{R}$ such that $A\phi_j = -\mathrm{i}\lambda_j\phi_j$;

If A and B satisfy Assumption 1.3, we denote

$$\|B\|_A = \inf\{a \in \mathbf{R} \mid \exists b \in \mathbf{R} \text{ for which } \|B\psi\| \leq a\|A\psi\| + b\|\psi\|,\ \forall \psi \in D(A)\}.$$

It is known that if (A, B, Φ) satisfies Assumption 1, then for every $u : [0, T_u] \to (-1/\|B\|_A, 1/\|B\|_A)$ with bounded variation, there exists a continuous mapping $t \mapsto \Upsilon^u_t$ taking value in the unitary group $\mathbf{U}(H)$ of H such that, for every ψ in $D(A)$, $t \mapsto \Upsilon^u_t\psi$ is differentiable almost everywhere and satsifies (3) for almost every t in $(0, T]$. For a proof of this well-posedness result, see [17] for a general theory of time dependent (non-necessarily skew-adjoint) Hamiltonians or [19] for an elementary proof adapted to the bilinear structure of (3).

Definition 1: Let (A, B, Φ) satisfy Assumption 1. The system (A, B) is *approximately controllable* if, for every ψ_0, ψ_1 in $\mathbf{S}_H$, the unit Hilbert sphere, for every $\varepsilon > 0$, there exists $u_\varepsilon : [0, T_\varepsilon] \to \mathbf{R}$ such that $\|\Upsilon^{u_\varepsilon}_{T_\varepsilon}\psi_0 - \psi_1\| < \varepsilon$.

The following sufficient criterion for approximate controllability is a reformulation of the central result of [12] where we emphasize the notion of non-degenerate (or non-resonant) transitions.

Definition 2: Let (A, B, Φ) satisfy Assumption 1. A pair (j, k) of integers is a *non-degenerate transition* of (A, B, Φ) if (i) $\langle\phi_j, B\phi_k\rangle \neq 0$ and (ii) for every (l, m) in $\mathbf{N}^2$, $|\lambda_j - \lambda_k| = |\lambda_l - \lambda_m|$ implies $(j, k) = (l, m)$ or $\langle\phi_l, B\phi_m\rangle = 0$ or $\{j, k\} \cap \{l, m\} = \emptyset$.

Definition 3: Let (A, B, Φ) satisfy Assumption 1. A subset S of $\mathbf{N}^2$ is a *non-degenerate chain of connectedness* of (A, B, Φ) if (i) for every (j, k) in S, (j, k) is a non-degenerate transition of (A, B) and (ii) for every r_a, r_b in $\mathbf{N}$, there exists a finite sequence $r_a = r_0, r_1, \ldots, r_p = r_b$ in $\mathbf{N}$ such that, for every $j \leq p - 1$, (r_j, r_{j+1}) belongs to S.

Proposition 1: Let (A, B, Φ) satisfy Assumption 1. If (A, B) admits a non-degenerate chain of connectedness, then (A, B) is approximately controllable.

E. Main result

The contribution of this note is to show the good agreement between the total variation of the control and the variation of the A-norm of the wave function. The A-norm, defined by $\|A\psi\|$ for every ψ in $D(A)$ is not equal, in general, to the energy $\||A|^{1/2}\psi\|$. However, if ϕ_j is an eigenvector of A with associated eigenvalue $-\mathrm{i}\lambda_j$, then $\|A\phi_j\| = |\lambda_j| = \||A|^{1/2}\phi_j\|^2$.

We have to distinguish between the cases where B is bounded and when it is not.

1) Bounded case: When B is bounded, the growth of the A norm of $\Upsilon^u_t\psi$ is at most linear with respect to the total variation of the control (see Section II-B.1). We present, in Section IV-A, an example for which the growth is indeed linear. More precisely, we will show the following.

Proposition 2: There exists (A, B, Φ) satisfying Assumption 1 with B bounded such that, for every M in $\mathbf{R}$, there exists $u_M : [0, T_M] \to \mathbf{R}$ with bounded variation such that $\|A\Upsilon^{u_M}_{T_M}\phi_1\| \geq M$ and $M \geq \frac{\|B\|}{4} TV_{[0,T_M]}(u_M)$.

2) Unbounded case: When B is unbounded, the growth of the A norm of $\Upsilon^u_t\psi$ is at most exponential with respect to the total variation of the control (see Section II-B.2). We present, in Section IV-B, an example for which the growth is indeed exponential. More precisely, we will show the following.

Proposition 3: There exists a triple (A, B, Φ) satisfying Assumption 1 with B unbounded such that, for every M large enough in $\mathbf{R}$, there exists $u_M : [0, T_M] \to \mathbf{R}$ with bounded variation with $\|A\Upsilon^{u_M}_{T_M}\phi_1\| \geq M$ and $M \geq \dfrac{4}{e}\exp\left(\dfrac{1}{\sqrt{6}}\|B\|_A TV_{[0,T_M]}(u_M)\right)$.

F. Content of the paper

In Section II, we review some classical estimates for the growth of $|A|^r$-norms of the wave function in terms of L^p norms (Section II-A) and total variation (Section II-B) of the control. Some examples of use of these estimates for the approximation of the infinite dimensional system (3) by its finite dimensional approximations are given in Section II-C. Section III is a quick survey of basic facts about averaging theory for finite dimensional bilinear systems.

These convergence results will be instrumental in Section IV to prove Proposition 2 (Section IV-A) and Proposition 3 (Section IV-B).

II. SOME ENERGY ESTIMATES

A. Weakness of L^p estimates

Let (A, B, Φ) satisfy Assumption 1 and admit a non-degenerate chain of connectedness. For every $r \geq 1$, for every j, k in $\mathbf{N}$ and $\varepsilon > 0$ we define $\mathcal{A}_r^{\varepsilon}(j,k)$ as the set of functions $u : [0, T_u] \to \mathbf{R}$ in $L^r([0,T_u])(\subset L^1([0,T_u]))$ such that $\|\Upsilon^u_{T_u}\phi_j - \phi_k\| < \varepsilon$. We consider the quantity

$$\mathcal{C}_r(\phi_j,\phi_k) = \sup_{\varepsilon>0}\left(\inf_{u\in\mathcal{A}_r^{\varepsilon}(j,k)} \|u\|_{L^r(0,T_u)}\right).$$

This quantity is the infimum of the L^r-norm of a control achieving approximate controllability. It clearly satisfies the triangle inequality. Next proposition states that $\mathcal{C}_r$ is a distance on the space of eigenlevels only when $r = 1$. Its proof is given in [16].

Proposition 4: $\mathcal{C}_1$ is a distance on the set $\{\phi_j, j \in \mathbf{N}\}$. For $r > 1$, $\mathcal{C}_r$ is equal to zero on the set $\{\phi_j, j \in \mathbf{N}\}$.

Proposition 4 illustrates various flaws of L^p estimates of system (3). First, and contrary to the immediate intuition, L^p norms with $p > 1$ (and in particular the L^2 norm) do not permit to distinguish among the energy levels of A. Precisely, if (A, B, Φ) admits a non-degenerate chain of connectedness, for every non empty open set $\mathcal{V}$ in $\mathbf{S}_H$, the unit sphere of H, there exists $u : [0,T] \to (-1/a, 1/a)$ in $L^p([0,T])$ with $\|u\|_{L^p([0,T])}$ arbitrarily small such that $\Upsilon^u_T\phi_1$ belongs to $\mathcal{V}$, see [20].

While the L^1 norm allows to distinguish among the energy levels of A, the distance $\mathcal{C}_1$ depends only on B and the non-degenerate chains of connectedness of (A, B, Φ) (and not on the eigenvalues of A). For instance, the computation of $\mathcal{C}_1(\phi_1, \phi_2)$ done in Section IV of [16] remains valid and the result unchanged, if one replaces A by $\pm\mathrm{i}|A|^k$ for any positive integer k.

B. Estimates based on total variation

The following estimates can be deduced from the general theory due to Kato [17]. They are valid in context much broader than Assumption 1. In particular, there is no need for H to admit a Hilbert basis made of eigenvectors of A.

In the following we will impose $u(0) = 0$. This is always the case if one replaces A by $A + u(0)B$. Moreover if (A, B, Φ) satisfies Assumption 1 then there exists Φ' and $b \in \mathbf{R}$ such that $(A + u(0)B - \mathrm{i}b, B, \Phi')$ satisfies Assumption 1 as well.

1) Bounded case:

Proposition 5: Let (A, B, Φ) satisfy Assumption 1 with B bounded. Then, for every $u : [0,T] \to \mathbf{R}$ with bounded variation and $u(0) = 0$, for every j in $\mathbf{N}$, $\big|\|A\Upsilon^u_T\phi_j\| - \|A\phi_j\|\big| \leq 2\|B\|TV_{[0,T]}(u)$.

Proof: Notice that if $u(0) = 0$ then $|u(T)| \leq TV_{[0,T]}(u)$. Hence it is enough to prove for every j in $\mathbf{N}$ that $\big|\|(A + u(T)B)\Upsilon^u_T\phi_j\| - \|A\phi_j\|\big| \leq \|B\|TV_{[0,T]}(u)$.

Any bounded variation function can be approximated pointwise by a sequence of piecewise constant functions $(u_n)_{n\in\mathbf{N}}$ such that $|u_n| \leq |u|$ and $TV_{[0,T]}(u_n) \leq TV_{[0,T]}(u)$.

Following [19], we have that $\Upsilon^{u_n}_T\phi_j \to \Upsilon^u_T\phi_j$. Thus it is sufficient to prove the statement for piecewise constant controls. The proof for piecewise constant controls follows from the estimate $\big|\|(A+uB)\exp(t(A+uB))\phi\| - \|A\phi\|\big| \leq \|B\||u|$. Indeed for a piecewise constant function the associated Υ^u_t is a product of $\exp t_i(A + u_iB)$ for different values of u_i and t_i. The details of the proof are similar to those of [19, Section 2]. ■

2) Unbounded case:

Proposition 6: Let (A, B, Φ) satisfy Assumption 1 with B unbounded. Then, for every $0 < \delta < 1$, for every $u : [0,T] \to (-(1-\delta)/a, (1-\delta)/a)$ with bounded variation and $u(0) = 0$, for every ψ in $D(A)$, $\|A\Upsilon^u_T\psi\| \leq e^{aTV_{[0,T]}(u)/\delta}\|A\psi\|$.

The proof in the unbounded case, which can be found in [19, Proposition 3], follows the lines of the bounded case.

C. Good Galerkin Approximations

Assumption 2: The quadruple (A, B, Φ, k) is such that

1) (A, B, Φ) satisfies Assumption 1;
2) k is a positive real number;
3) for every u in $\mathbf{R}$, the domains $D(|A + uB|^k)$ of $|A + uB|^k$ and $D(|A|^k)$ of $|A|^k$ coincide;
4) there exists d, r in $\mathbf{R}$, $r < k$ such that $\|B\psi\| < d\||A|^r\psi\|$ for every ψ;
5) the supremum $c_k(A,B)$ of the subset of $\mathbf{R}$ $\{|\Re\langle|A|^k\psi, B\psi\rangle|/|\langle|A|^k\psi,\psi\rangle|, \psi \in D(|A|^k)\}$ is finite.

For every N in $\mathbf{N}$, we define the orthogonal projection

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

Definition 4: Let $N \in \mathbf{N}$. The *Galerkin approximation* of (3) of order N is the system in H

$$\dot{x} = \left(A^{(N)} + uB^{(N)}\right)x \qquad (\Sigma_N)$$

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

We denote by $X^u_{(\Phi,N)}(t,s)$ the propagator of (Σ_N).

Definition 5: The system (A, B, Φ) admits a sequence of *Good Galerkin Approximations* (GGA in short), in time $T \in (0, +\infty]$, in a subspace D (with norm $\|\cdot\|_D$) of H, in terms of a functional norm $N(\cdot)$ on a functional space $\mathbf{U}$ if, for any $K, \varepsilon > 0$, for any ψ in D, there exists N in $\mathbf{N}$ such that, for any u in $\mathbf{U}$, $N(u) \leq K$ implies $\|(X^u_{(\mathbf{\Phi},N)}(t,0) - \Upsilon^u_{t,0})\psi\|_D < \varepsilon$ for any $t < T$.

Proposition 7: Let (A, B, Φ, k) satisfy Assumption 2. Then (A, B, Φ) admits a sequence of good Galerkin approximations in infinite time, in $D(A)$ in terms of L^1 norm for locally integrable controls.

Last proposition is proved in [21] for piecewise constant controls. The generalization to L^1 controls follows from [19].

Proposition 8: Let $d > 0$, $r < 1$ and (A, B, Φ) satisfy Assumption 1 with $\|B\psi\| \leq d\||A|^r\psi\|$ for every ψ in $D(|A|^r)$. Then (A, B, Φ) admits a sequence of good Galerkin approximations in infinite time, in $D(A)$ in terms of $TV + L^1$ norm for controls with bounded variation.

This proposition is proved in [19]. Notice, that if we impose $u(0) = 0$ for the control term then the L^1 norm of the control over any finite time interval is bounded by a multiple of the total variation.

III. PERIODIC CONTROL LAWS OF BILINEAR QUANTUM SYSTEMS

A. Averaging theory

The mathematical concept of averaging of dynamical systems was introduced more than a century ago and has now developed into a well-established theory, see for instance the books of Guckenheimer & Holmes [22], Bullo & Lewis [23] or Sanders, Verhulst & Murdock [24]. It was observed that, for regular F and small ε, the trajectories of the system $\dot{x} = \varepsilon F(x, t, \varepsilon)$ remain ε close, for time of order $1/\varepsilon$, to the trajectories of the average system $\dot{x} = \widetilde{F}(x)$ where $\widetilde{F}(x) = \lim_{t\to\infty} 1/t \int_0^t F(x, t, 0)$.

In quantum physics, this concept of averaging is used intensively to transfer a system of type (3) from an eigenstate of A associated with eigenvalue $-\mathrm{i}\lambda_j$ to another associated with eigenvalue $-\mathrm{i}\lambda_k$ with a periodic control with small enough amplitude and frequency $|\lambda_j - \lambda_k|$.

The following results is proved in [18].

Proposition 9: Let (A, B, Φ) satisfy Assumption 1. Assume that (j, k) is a non-degenerate transition of (A, B, Φ). Define $T = 2\pi/|\lambda_j - \lambda_k|$ and let $u^* : \mathbf{R} \to (-1/\|B\|_A, 1/\|B\|_A)$ be T-periodic and with bounded variation on $[0, T]$. If $\int_0^T u^*(\tau)e^{\mathrm{i}(\lambda_j-\lambda_k)\tau}\mathrm{d}\tau \neq 0$ and $\int_0^T u^*(\tau)e^{\mathrm{i}(\lambda_l-\lambda_m)\tau}\mathrm{d}\tau = 0$ for every (l, m) such that (i) $\{j, k\} \neq \{l, m\}$, and (ii) $\{j, k\} \cap \{l, m\} \neq \emptyset$, and (iii) $|\lambda_l - \lambda_m| \in (\mathbf{N} \setminus \{1\})|\lambda_j - \lambda_k|$ and (iv) $b_{lm} \neq 0$, then, for every n in $\mathbf{N}$, there exists T_n^* in $(nT^* - T, nT^* + T)$ such that $|\langle \phi_k, X^u_{(\Phi,N)}(T_n^*, 0)\phi_j\rangle|$ tends to 1 as n tends to infinity, with

$$T^* = \frac{\pi T}{2|b_{j,k}| \left|\int_0^T u^*(\tau)e^{\mathrm{i}(\lambda_j-\lambda_k)\tau}\mathrm{d}\tau\right|}, \quad I = \int_0^T |u^*(\tau)|\mathrm{d}\tau,$$

$$K = \frac{IT^*}{T} \text{ and } C = \sup_{(j,k)\in\Lambda} \left| \frac{\int_0^T u^*(\tau)e^{\mathrm{i}(\lambda_l-\lambda_m)\tau}\mathrm{d}\tau}{\sin\left(\pi \frac{|\lambda_l-\lambda_m|}{|\lambda_j-\lambda_k|}\right)} \right|,$$

where Λ is the set of all pairs (l, m) in $\{1, \ldots, N\}^2$ such that $b_{lm} \neq 0$ and $\{l, m\} \cap \{j, k\} \neq \emptyset$ and $|\lambda_l - \lambda_m| \notin \mathbf{Z}|\lambda_2 - \lambda_1|$.

Notice that Proposition 9 does not claim that $\|A(X^u_{(\Phi,N)}(T_n^*, 0)\phi_j - \phi_k)\|$ tends to zero as n tends to infinity. However,

$$\liminf_{n\to\infty} \|AX^u_{(\Phi,N)}(T_n^*, 0)\phi_j\| \geq \liminf_{n\to\infty} \lambda_k |\langle \phi_k, X^u_{(\Phi,N)}(T_n^*, 0)\phi_j\rangle| = \lambda_k.$$

Using Propostion 7 or Proposition 8 these can be extended to inifinite dimensional system (3) with (A, B, Φ, k) satisfing Assumption 2 or Assumption 1 with $\|B\psi\| \leq d\||A|^r\psi\|$ for every ψ in $D(|A|^r)$ for some $d > 0$ and $r < 1$.

B. Averaging using the sine function

Let (A, B, Φ) satisfy Assumption 1 and (j, k) be a non-degenerate transition of (A, B, Φ). We define $\omega = |\lambda_j - \lambda_k|$. We apply Proposition 9 with $u^* : t \mapsto \sin(\omega t)$. For n large enough, $\|u^*(t)/n\|_{L^\infty} \leq 1/\|B\|_A$. Straightforward computations give

$$T = \frac{2\pi}{\omega}, \quad T^* = \frac{\pi}{|b_{jk}|}, \quad I = \frac{4}{\omega},$$

and we compute

$$TV_{[0,T_n^*)}\left(\frac{u^*}{n}\right) = \frac{1}{n}\int_0^{T_n^*} \omega|\cos(\omega t)|\mathrm{d}t = \frac{\omega}{n}\left(\int_0^{\left\lfloor \frac{nT_n^*}{T}\right\rfloor T} |\cos(\omega t)|\mathrm{d}t + \int_{\left\lfloor \frac{nT_n^*}{T}\right\rfloor T}^{T_n^*} |\cos(\omega t)|\mathrm{d}t\right).$$

As n tends to infinity, $\frac{\omega}{n}\int_{\left\lfloor \frac{nT_n^*}{T}\right\rfloor T}^{T_n^*} |\cos(\omega t)|\mathrm{d}t$ tends to zero, hence

$$\lim_{n\to\infty} TV_{[0,T_n^*)}\left(\frac{u^*}{n}\right) = \lim_{n\to\infty} \frac{\omega}{n}\left\lfloor \frac{nT_n^*}{T}\right\rfloor \int_0^T |\cos(\omega t)|\mathrm{d}t = \lim_{n\to\infty} 4\frac{\omega T_n^*}{n} = \frac{2\omega}{|b_{jk}|}.$$

IV. EXAMPLES

A. The bounded case: 2D rotation of a linear molecule

Consider a linear molecule whose only degree of freedom is the planar rotation, in a fixed plan, about its fixed center of mass. This system has been thoroughly studied (see the references given in [25] or [21] for instance).

In this model, the Schrödinger equation reads

$$\mathrm{i}\frac{\partial\psi}{\partial t} = -\Delta\psi + \cos\theta\psi, \quad \theta \in \Omega, \tag{4}$$

$\Omega = \mathbf{R}/2\pi\mathbf{Z}$ is the unit circle endowed with the Riemannian structure inherited from $\mathbf{R}$, H is the space of odd functions of $L^2(\Omega, \mathbf{C})$, $A = \mathrm{i}\Delta$ (Δ is the restriction to H of the Laplace-Beltrami operator of Ω) and $B : \psi \mapsto (\theta \mapsto \cos(\theta)\psi(\theta))$ is the multiplication by cosine.

In the Hilbert basis $\Phi = (\theta \mapsto \sin(k\theta))_{k\in\mathbf{N}}$ of H, A is diagonal with diagonal $-\mathrm{i}k^2, k = 1 \ldots \infty$ and B is tri-diagonal with $b_{k,k} = 0, b_{k,k+1} = -\mathrm{i}/2$, $b_{j,k} = 0$ for every k, j in $\mathbf{N}$ such that $|j - k| > 1$.

The triple (A, B, Φ) satisfies Assumption 1, B is bounded and $\|B\psi\| \leq 0\|A\psi\| + \sqrt{2}\|\psi\|$ for every ψ in H. The set $\{(k, k + 1), k \in \mathbf{N}\}$ is a non-degenerate chain of connectedness for (A, B, Φ).

For every j and n_j in $\mathbf{N}$, we define the control $u^{*,j,n_j} : t \in [0, 2n_j\pi] \mapsto \sin((2j + 1)t)/n_j$, and for every N in $\mathbf{N}$, we define $u^{*,(n_1,n_2,\ldots,n_{N-1})}$ by the concatenation of $u^{*,1,n_1}$, $u^{*,2,n_2}$, …, $u^{*,N-1,n_{N-1}}$.

By Proposition 9,

$$\liminf_{n_1,\ldots,n_{N-1}\to\infty} \|A\Upsilon^{u^{*,(n_1,n_2,\ldots,n_{N-1})}}\phi_1\| \geq \lambda_N = N^2.$$

From Section III-B, we compute

$$\liminf_{n_1,n_2,\ldots,n_{N-1}\to\infty} TV_{[0,2\pi(n_1+n_2+\ldots+n_{N-1}]}(u^{*,(n_1,n_2,\ldots,n_{N-1})}) = \sum_{j=1}^{N-1} 4(2j+1) = 4N^2,$$

which proves Proposition 2.

B. The unbounded case: perturbation of the harmonic oscillator

The second model we consider is a perturbation of the quantum harmonic oscillator, with dynamics given by

$$\mathrm{i}\frac{\partial \psi}{\partial t} = \left[(-\Delta + x^2) + (-\Delta + x^2)^{-1}\right]\psi + u(t)x^2\psi. \quad (5)$$

With the notations of Section I-D, H is the Hilbert space of the odd functions of $L^2(\mathbf{R},\mathbf{C})$, $A = -\mathrm{i}\left[(-\Delta + x^2) + (-\Delta + x^2)^{-1}\right]$ where Δ is the restriction of the Laplacian to the space of odd functions and B is the multiplication, in H by $-\mathrm{i}x^2$. Denoting by H_n the n^{th} Hermite function, we check that $AH_{2n-1} = -\mathrm{i}((4n-1) + (4n-1)^{-1})H_{2n-1}$, hence $\Phi = (H_{2n-1})_{n\in\mathbf{N}}$ is a Hilbert basis of H made of eigenvectors of A. Moreover, $BH_1 = -\mathrm{i}(1/2H_1 + \sqrt{3/2}H_3)$ and, for every n in $\mathbf{N}$, $n \geq 2$,

$$BH_{2n-1} = -\mathrm{i}\left[\sqrt{n\left(n-\frac{1}{2}\right)}H_{2n-3} + \left(n-\frac{1}{2}\right)H_{2n-1} + \sqrt{n\left(n+\frac{1}{2}\right)}H_{2n+1}\right].$$

In the basis Φ, A is diagonal with diagonal entries $(-\mathrm{i}((4n-1)+(4n-1)^{-1}))_{n\in\mathbf{N}}$ and B is tri-diagonal. The system (A,B,Φ) is tri-diagonal in the sense of [19] and satisfies Assumption 1 with $\|B\|_A \leq \frac{\sqrt{6}}{4}$ (Proposition 12 of [19] applied with $r = 1$ and $C = 1/4$).

For every j and n_j in $\mathbf{N}$, we define the control

$$u^{*,j,n_j} : t \in [0, 2n_j\pi] \mapsto \frac{1}{n_j}\sin\left(4\frac{16j^2+8j-7}{(4j+3)(4j-1)}t\right),$$

and for every N in $\mathbf{N}$, we define $u^{*,(n_1,n_2,\ldots,n_{N-1})}$ by the concatenation of $u^{*,1,n_1}$, $u^{*,2,n_2}$, $\ldots$, $u^{*,N-1,n_{N-1}}$.

By Proposition 9,

$$\liminf_{n_1,\ldots,n_{N-1}\to\infty} \|A\Upsilon^{u^{*,(n_1,n_2,\ldots,n_{N-1})}}\phi_1\| \geq \lambda_N \geq 4N-1.$$

From Section III-B, we compute, similarly to what we have done in Section II-B.1,

$$\begin{aligned}\liminf_{n_1,n_2,\ldots,n_{N-1}\to\infty} TV_{[0,2\pi(n_1+n_2+\ldots+n_{N-1}]}(u^{*,(n_1,n_2,\ldots,n_{N-1})}) &\leq \sum_{j=1}^{N-1}\frac{4}{j} \\ &\leq 4(1+\log(N-1)),\end{aligned}$$

which proves Proposition 3.

V. CONCLUSIONS

A. Contribution

We exhibited two examples showing that the Kato estimates for the A-norm of the solutions of a bilinear quantum system, with bounded or unbounded coupling term, are optimal up to a multiplicative constant. These estimates are given in terms of the total variation of the control.

B. Physical significance

The classical Kato's estimates in terms of total variation are a major improvement with respect to the more usual energy estimates in terms of the L^p norm of the control, for several reasons. First, they apply to much more general systems, involving in particular unbounded control terms and provide more precise results. Second, the total variation of a constant control is zero. Hence a constant control applied for a long time will result, using Kato's estimates, in a constant upper bound for the energy (this is obviously not the case for the L^p estimates).

In the present analysis, we have stressed the crucial role of the control oscillations. We knew from the estimates by Kato that low oscillations prevent high variations of the physical energy of the system, see [19]. The result we present here shows that if the control oscillates at the right frequency then the energy of the system can be modified up to the limits imposed by the estimates by Kato. Incidentally, it is striking fact that rough models, like the semi-classical bilinear ones considered in the examples, exhibit some of the fundamental oscillatory aspects of quantum systems.

C. Perspectives

An interesting, and probably difficult, question is the optimal control of bilinear quantum systems when the cost is the total variation of the control. Approximation procedures (as the Good Galerkin Approximations presented in this note) allow to consider only a finite dimensional problem. The main difficulty will come from the non-smoothness of the cost (total variation) which will lead to the use of tools of non-smooth analysis.

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