Periodic control laws for bilinear quantum systems with discrete spectrum

Nabile Boussaïd
Laboratoire de mathématiques
Université de Franche–Comté
25030 Besançon, France
Nabile.Boussaid@univ-fcomte.fr

Marco Caponigro
Dept of Mathematical Sciences and CCIB
Rutgers University
08102 Camden, NJ, USA
marco.caponigro@rutgers.edu

Thomas Chambrion
Institut Élie Cartan de Nancy and
INRIA Nancy Grand Est
54506 Vandœuvre, France
Thomas.Chambrion@inria.fr

***Abstract*— We provide bounds on the error between dynamics of an infinite dimensional bilinear Schrödinger equation and of its finite dimensional Galerkin approximations. Standard averaging methods are used on the finite dimensional approximations to obtain constructive controllability results. As an illustration, the methods are applied on a model of a 2D rotating molecule.**

I. INTRODUCTION

A. Physical context

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

When submitted to an excitation by an external field (*e.g.* a laser) the time evolution of the wave function is governed by the bilinear Schrödinger equation

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

where $V, W : \Omega \to \mathbf{R}$ are real functions describing respectively the physical properties of the uncontrolled system and the external field, and $u : \mathbf{R} \to \mathbf{R}$ is a real function of the time representing the intensity of the latter.

B. Quantum control

A natural question, with many practical implications, is whether there exists a control u steering the quantum system from a given initial position to a given target.

Considerable efforts have been made to study the controllability of (1). We refer to [14], [10], [2], [9], [1], [3] and references therein for a description of the known theoretical results on the existence of controls steering a given source to a given target. As proved in [10], [8], [11], approximate controllability is a generic property for systems of the type (1).

The main difficulty in the study of (1) is the fact that the natural state space, namely $L^2(\Omega, \mathbf{C})$, has infinite dimension. To avoid difficulties when dealing with infinite dimensional systems, for example when studying practical computations or simulations, one can project system (1) on finite dimensional subspaces of $L^2(\Omega, \mathbf{C})$. Obviously, a crucial issue is to guarantee that the finite dimensional approximations have dynamics close to the one of the original infinite dimensional system.

C. Aim and content of the paper

The contribution of this paper is twofold. First, in Section II, we provide an introduction to the class of *weakly-coupled* bilinear systems (see Definition 1). A feature of these systems is that their dynamics is precisely approached by the dynamics of their Galerkin approximations (Proposition 4). In a second part, we apply general averaging theory for the approximate control of finite dimensional bilinear conservative systems using small amplitude periodic control laws. The method is both very selective with respect to the frequency (which is a good point for quantum control) and extremely robust with respect to the shape of the control (Section III). Moreover, it provides easy and explicit estimates for the controllability time, the L^1 norm of the control and the error. Together with the results of Section II, this method provides a complete solution for the approximate control of infinite dimensional bilinear quantum systems with discrete spectrum and time estimates. As an illustration, we consider the rotation of a planar dipolar molecule in Section IV.

II. WEAKLY-COUPLED BILINEAR SYSTEMS

A. Abstract framework

We reformulate the problem (1) in a more abstract framework. This will allow us to treat examples slightly more general than (1), for instance, the example in [5, Section III.A]. In a separable Hilbert space H endowed with norm $\|\cdot\|$ and Hilbert product $\langle\cdot,\cdot\rangle$, we consider the evolution problem

$$\frac{d\psi}{dt} = (A + u(t)B)\psi \quad (2)$$

where (A, B) satisfies the following assumption.

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

1) A is skew-adjoint and has purely discrete spectrum $(-\mathrm{i}\lambda_k)_{k\in\mathbf{N}}$, the sequence $(\lambda_k)_{k\in\mathbf{N}}$ is positive non-decreasing and accumulates at $+\infty$;
2) $B : H \to H$ is skew-adjoint and bounded.

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

From Assumption 1.2 together with Kato-Rellich Theorem, we deduce that $A + uB$ is skew-adjoint on $D(A)$. Moreover, for every constant u in $\mathbf{R}$, $\mathrm{i}(A+uB)$ is bounded from below.

Hence, for every initial condition ψ_0 in H, for every u piecewise constant, $u : t \mapsto \sum_j u_j \chi_{(t_j,t_{j+1})}(t)$, with $0 = t_0 \leq t_1 \leq \ldots \leq t_{N+1}$ and $u_0, \ldots, u_N$ in $\mathbf{R}$, one can define the solution $t \mapsto \Upsilon_t^u \psi_0$ of (2) by

$$\Upsilon_t^u \psi_0 = e^{(t-t_{j-1})(A+u_{j-1}B)} \circ \\ \circ e^{(t_{j-1}-t_{j-2})(A+u_{j-2}B)} \circ \ldots \circ e^{t_0(A+u_0B)}\psi_0,$$

for $t \in [t_{j-1}, t_j)$. For a control u in $L^1(\mathbf{R})$ we define the solution using the following continuity result.

Proposition 1: Let u and $(u_n)_{n\in\mathbf{N}}$ be in $L^1(\mathbf{R})$. If for every t in $\mathbf{R}$ $\int_0^t u_n(\tau)\mathrm{d}\tau$ converges to $\int_0^t u(\tau)\mathrm{d}\tau$ as n tends to infinity, then, for every t in $\mathbf{R}$ and every ψ_0 in H, $(\Upsilon_t^{u_n}\psi_0)_{n\in\mathbf{N}}$ converges to $\Upsilon_t^u\psi_0$ as n tends to infinity.

B. Energy growth

From Assumption 1.1, the operator $\mathrm{i}A$ is self-adjoint with positive eigenvalues. For every ψ in $D(A)$, $\mathrm{i}A\psi = \sum_{j\in\mathbf{N}} \lambda_j \langle \phi_j, \psi\rangle \phi_j$. For every $s \geq 0$, we define the linear operator $|A|^s := (\mathrm{i}A)^s$ by $|A|^s\psi = \sum_{j\in\mathbf{N}} \lambda_j^s \langle \phi_j, \psi\rangle \phi_j$, for every ψ in $D(|A|^s) = \{\psi \in H : \sum_{j\in\mathbf{N}} \lambda_j^{2s} |\langle \phi_j, \psi\rangle|^2 < +\infty\}$. We define the s-norm by $\|\psi\|_s = \||A|^s\psi\|$ for every ψ in $D(|A|^s)$. The $1/2$-norm plays an important role in physics; for every ψ in $D(|A|^{1/2})$, the quantity $|\langle A\psi, \psi\rangle| = \|\psi\|_{1/2}^2$ is the expected value of the energy.

Definition 1: Let (A, B) satisfy Assumption 1. Then (A, B) is *weakly-coupled* if there exists a constant C such that, for every ψ in $D(|A|)$, $|\Re\langle |A|\psi, B\psi\rangle| \leq C|\langle |A|\psi, \psi\rangle|$. The coupling constant $c(A, B)$ of system (A, B) is the quantity $\sup_{\psi\in D(|A|)\setminus\{0\}} |\Re\langle |A|\psi, B\psi\rangle|/|\langle |A|\psi, \psi\rangle|$.

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

Proposition 2: Let (A, B) satisfy Assumption 1 and be weakly-coupled. Then, for every $\psi_0 \in D(|A|^{1/2})$, $K > 0$, $T \geq 0$, and u in $L^1([0, \infty))$ for which $\|u\|_{L^1} < K$, one has $\|\Upsilon_T^u(\psi_0)\|_{1/2} < e^{c(A,B)K}\|\psi_0\|_{1/2}$.

Proof: We present here a simple proof in the special case where ψ_0 belongs to $D(A^2)$, u is piecewise constant, and $D(|A|^2) = D(|A + uB|^2)$ for every u in $\mathbf{R}$. This last equality holds for the most common physical examples. A general proof of Proposition 2, involving rather technical regularization techniques to relax this extra assumption is presented in [5, Appendix].

First note that, for every $t \geq 0$, the set $D(|A|^2) = D(|A + uB|^2)$ is invariant for the unitary map $\psi \mapsto e^{t(A+uB)}\psi$. Moreover, for every ψ in $D(|A + uB|^2)$, the mapping $t \mapsto |A + \sum uB|e^{t(A+uB)}\psi = e^{t(A+uB)}|A + uB|\psi$ is C^1 from $[0, +\infty)$ to H, with derivative $t \mapsto (A + uB)e^{t(A+uB)}|A + uB|\psi = |A + uB|(A + uB)e^{t(A+uB)}\psi$. In other words, the mapping $t \mapsto e^{t(A+uB)}\psi$ is C^1 from $[0, +\infty)$ to $D(|A + uB|) = D(|A|)$.

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

$$\begin{aligned} \frac{d}{dt}f(t) &= \frac{d}{dt}\langle |A|\Upsilon_t^u\psi_0, \Upsilon_t^u\psi_0\rangle \\ &= 2\Re\langle |A|\Upsilon_t^u\psi_0, (A + u(t)B)\Upsilon_t^u\psi_0\rangle \\ &= 2u(t)\Re\langle |A|\Upsilon_t^u\psi_0, B\Upsilon_t^u\psi_0\rangle. \end{aligned}$$

Since (A, B) is weakly-coupled, one has

$$\begin{aligned} |f'(t)| &\leq 2|u(t)||\langle |A|\Upsilon_t^u\psi_0, B\Upsilon_t^u\psi_0\rangle| \\ &\leq 2c(A, B)|u(t)|f(t). \end{aligned}$$

From Gronwall's lemma, we get

$$\langle |A|\psi(t), \psi(t)\rangle \leq e^{2c(A,B)\int_0^t |u|(\tau)\mathrm{d}\tau}\|\psi_0\|_{1/2}^2$$

for every ψ_0 in $D(|A|^2)$. ∎

C. Good Galerkin approximation

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

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

Proposition 3: Let (A, B) satisfy Assumption 1, and be weakly-coupled. Then, for every $n \in \mathbf{N}$, $N \in \mathbf{N}$, $(\psi_j)_{1\leq j\leq n}$ in $D(|A|^{1/2})^n$, and for every L^1 function u,

$$\|(\mathrm{Id} - \pi_N)\Upsilon_t^u(\psi_j)\| < \frac{e^{c(A,B)\|u\|_{L^1}}\|\psi_j\|_{1/2}}{\sqrt{\lambda_{N+1}}}. \qquad (3)$$

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

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

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

By Proposition 2, for every $t > 0$, $\|\Upsilon_t^u(\psi_j)\|_{1/2}^2 \leq e^{2c(A,B)\|u\|_{L^1}}\|\psi_j\|_{1/2}^2$. The conclusion then follows by Proposition 1. ∎

Remark 1: Since B is bounded, then $\|B(\mathrm{Id} - \pi_N)\Upsilon_t^u(\psi_j)\|$ tends to 0 as N tends to infinity uniformly with respect to u of L^1-norm smaller than a given constant.

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

$$\dot{x} = (A^{(N)} + u(t)B^{(N)})x \qquad (\Sigma_N)$$

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

We denote by $X_{(N)}^u(t, s)$ the propagator of (Σ_N) associated with a L^1 function u.

Remark 2: The operators $A^{(N)}$ and $B^{(N)}$ are defined on the *infinite* dimensional space H. However, they have finite rank and the dynamics of (Σ_N) leaves invariant the N-dimensional space $\mathcal{L}_N = \mathrm{span}_{1\leq l\leq N}\{\phi_l\}$. Thus, (Σ_N) can be seen as a finite dimensional bilinear system in $\mathcal{L}_N$.

Proposition 4 (Good Galerkin Approximation): Let (A, B) satisfy Assumption 1 and be weakly-coupled. Then for every $\varepsilon > 0$, $K \geq 0$, $n \in \mathbf{N}$, and $(\psi_j)_{1\leq j\leq n}$ in $D(|A|^{1/2})^n$ there exists $N \in \mathbf{N}$ such that for every L^1 function u

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

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

Proof: Fix j in $\{1, \ldots, n\}$ and consider the map $t \mapsto \pi_N\Upsilon^u_t(\psi_j)$ that is absolutely continuous and satisfies, for almost every $t \geq 0$,

$$\frac{d}{dt}\pi_N\Upsilon^u_t(\psi_j) = (A^{(N)} + u(t)B^{(N)})\pi_N\Upsilon^u_t(\psi_j) + u(t)\pi_N B(\mathrm{Id} - \pi_N)\Upsilon^u_t(\psi_j). \quad (4)$$

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

$$\pi_N\Upsilon^u_t(\psi_j) = X^u_{(N)}(t,0)\pi_N\psi_j + \int_0^t X^u_{(N)}(t,s)\pi_N B(\mathrm{Id} - \pi_N)\Upsilon^u_s(\psi_j)u(\tau)\mathrm{d}\tau. \quad (5)$$

By Proposition 3, the norm of $t \mapsto B(\mathrm{Id} - \pi_N)\Upsilon^u_t(\psi_j)$ is less than $\|B\|\lambda_{N+1}^{-1/2}e^{c(A,B)K}\|\psi_j\|_{1/2}$. Since $X^u_{(N)}(t,s)$ is unitary, $\|\pi_N\Upsilon^u_t(\psi_j) - X^u_{(N)}(t,0)\pi_N\psi_j\| < \|u\|_{L^1}\|B\|\lambda_{N+1}^{-1/2}e^{c(A,B)K}\|\psi_j\|_{k/2}$. Then

$$\begin{aligned}\|\Upsilon^u_t(\psi_j) - X^u_{(N)}(t,0)\pi_N\psi_j\| &\leq \|(\mathrm{Id} - \pi_N)\Upsilon^u_t(\psi_j)\| \\ &\quad + \|\pi_N\Upsilon^u_t(\psi_j) - X^u_{(N)}(t,0)\pi_N\psi_j\| \\ &\leq \lambda_{N+1}^{-1/2}(1 + K\|B\|)e^{c(A,B)K}\|\psi_j\|_{1/2}.\end{aligned}$$

This completes the proof since λ_N tends to infinity as N goes to infinity. ∎

III. Control of finite dimensional conservative bilinear systems

A. Averaging results

In this Section, we focus on the control system (Σ_N) of Definition 2. The matrix $A^{(N)}$ is diagonal with eigenvalues $(-\mathrm{i}\lambda_j)_{1\leq j\leq N}$ with $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_N$. We denote with $(b_{jk})_{1\leq j,k\leq N}$ the entries of $B^{(N)}$.

Theorem 5: Let $u^* : [0, +\infty) \to \mathbf{R}$ be a locally integrable function. Assume that $\lambda_1 \neq \lambda_2$ and that, for every $l, m \leq N$, $|\lambda_l - \lambda_m| = |\lambda_2 - \lambda_1|$ implies $\{l, m\} = \{1, 2\}$ or $b_{lm} = 0$ or $\{l, m\} \cap \{1, 2\} = \emptyset$.

Assume that u^* is periodic with period $T = \frac{2\pi}{|\lambda_2 - \lambda_1|}$ and that $\int_0^T u^*(\tau)e^{\mathrm{i}(\lambda_l - \lambda_m)\tau}\mathrm{d}\tau = 0$ for every $\{l, m\}$ such that $\{l, m\} \cap \{1, 2\} \neq \emptyset$ and $\lambda_l - \lambda_m \in (\mathbf{Z} \setminus \{\pm 1\})(\lambda_1 - \lambda_2)$ and $b_{lm} \neq 0$.

If $\int_0^T u^*(\tau)e^{\mathrm{i}(\lambda_2 - \lambda_1)\tau}\mathrm{d}\tau \neq 0$, then, for every n in $\mathbf{N}$, there exists T^*_n in $(nT^* - T, nT^* + T)$ such that

$$\frac{1 - |\langle\phi_2, X^{\frac{u}{n}}_{(N)}(T^*_n, 0)\phi_1\rangle|}{(1 + 2K\|B^{(N)}\|)I} \leq \frac{(1 + C)\|B^{(N)}\|}{n}, \quad (6)$$

with

$$T^* = \frac{\pi T}{2|b_{1,2}|\left|\int_0^T u^*(\tau)e^{\mathrm{i}(\lambda_1 - \lambda_2)\tau}\mathrm{d}\tau\right|}, \quad I = \int_0^T |u^*(\tau)|\mathrm{d}\tau,$$

$$K = \frac{IT^*}{T}, C = \sup_{(j,k)\in\Lambda}\left|\frac{\int_0^T u^*(\tau)e^{\mathrm{i}(\lambda_j - \lambda_k)\tau}\mathrm{d}\tau}{\sin\left(\pi\frac{|\lambda_j - \lambda_k|}{|\lambda_2 - \lambda_1|}\right)}\right|,$$

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

Theorem 5 above states that $|\langle\phi_k, X^{\frac{u^*}{n}}(nT^*, 0)\phi_j\rangle|$ tends to one as n tends to infinity. This convergence result may be obtained using classical averaging theory (see for instance [13]). Another proof based on the particular algebraic structure of the system is given in [6]. The estimates given here are given in [6, Proposition 2].

B. Efficiency of the transfer

Using the notations of the last paragraph, for every periodic function u^* with period $T = \frac{2\pi}{|\lambda_j - \lambda_k|}$, we define the efficiency of u^* with respect to the transition (j, k) as the real quantity:

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

For every u, $0 \leq E^{(j,k)}(u) \leq 1$. For every $\{j, k\}$, $\sup_u E^{(j,k)}(u) = 1$ (consider a sequence of controls that tends to a periodic sum of Dirac functions). An example of u^* with zero efficiency is presented in Section IV.

An intuitive explanation of the efficiency could be the following: asymptotically, the L^1-norm of the control needed to induce the transition between levels j and k using periodic controls of the form u_n is equal to $\pi/(2|b_{jk}|E^{(j,k)}(u^*))$.

C. Design of control laws

The system (2) being given, the design of an effective control law fulfilling the hypotheses of Theorem 5 is an important practical issue. To generate a transfer from level j to level k, one should choose a control u such that $E^{(j,k)}(u)$ is as large as possible and $E^{(l,m)}(u)$ is zero (or arbitrarily close to zero) for every l, m such that $\lambda_l - \lambda_m \in (\lambda_j - \lambda_k)(\mathbf{Z} \setminus \{1\})$.

A natural choice for the control law can be $t \mapsto \cos(|\lambda_j - \lambda_k|t)$. The efficiency with respect to transition (j, k) is equal to $\pi/4 \approx 0.79$. All other efficiencies are zeros.

This cosine control law may however not match every desirable property of the control law. For instance, if for some reason the control law has to be positive, one could choose $t \mapsto 1 + \cos(|\lambda_j - \lambda_k|t)$. The efficiency with respect to transition (j, k) is equal to $1/2$. All other efficiencies are zeros.

If there are no resonances, that is if $\lambda_j - \lambda_k \notin (\lambda_l - \lambda_m)\mathbf{Z}$ for every $\{l, m\} \neq \{j, k\}$, one could consider the choice of a periodic Dirac comb $t \mapsto \sum_{n\in\mathbf{Z}}\delta_{n2\pi|\lambda_j - \lambda_k|}(t)$, whose efficiency with respect to transition (j, k) is equal to one. If one desires to avoid the use of distributional control

laws (Equation (2) has then to be understood in the measure sense), one may consider standard L^1 function close enough to Dirac combs. Examples are presented in Section IV.

Finally, let us mention the algorithm described in [3] that allows to build u^* positive and piecewise constant. If $\lambda_j - \lambda_k = 1$ and the only resonances to be considered are such that $|\lambda_l - \lambda_m| \in \{a_1, a_2, \dots, a_p\}$, then the efficiency of u^* with respect to transition (j,k) is

$$\prod_{n=1}^{p} \cos\left(\frac{\pi}{2a_n}\right).$$

In the worst case, this algorithm guarantees $E^{(j,k)}(u) \geq \prod_{n\geq 2} \cos(\pi/2n) > 0.43$, a very low efficiency if compared to the cosine law. However, this algorithm is especially useful to handle the case of high order resonances. Indeed, if $a_1, a_2, \dots, a_p$ are all greater than N, then the efficiency with respect to transition (j,k) is greater than

$$\exp\left(-\frac{\pi^2}{4N} - \frac{\pi^4}{48N^3}\right),$$

which tends to one as N tends to infinity.

IV. Rotation of a planar molecule

In this Section, we apply our results to the well studied example of the rotation of a planar molecule (see, for instance, [12], [4], [3]).

A. Presentation of the model

We consider a linear molecule with fixed length and center of mass. We assume that the molecule is constrained to stay in a fixed plane and that its only degree of freedom is the rotation, in the plane, around its center of mass. The state of the system at time t is described by a point $\theta \mapsto \psi(t,\theta)$ of $L^2(\Omega, \mathbf{C})$ where $\Omega = \mathbf{R}/2\pi\mathbf{Z}$ is the one dimensional torus. The Schrödinger equation writes

$$\mathrm{i}\frac{\partial \psi}{\partial t}(t,\theta) = -\Delta\psi(t,\theta) + u(t)\cos(\theta)\psi(t,\theta), \qquad (7)$$

where Δ is the Laplace-Beltrami operator on Ω. The self-adjoint operator $-\Delta$ has purely discrete spectrum $\{k^2, k \in \mathbf{N}\}$. All its eigenvalues are double but zero which is simple. The eigenvalue zero is associated with the constant functions. The eigenvalue k^2 for $k > 0$ is associated with the two eigenfunctions $\theta \mapsto \frac{1}{\sqrt{\pi}}\cos(k\theta)$ and $\theta \mapsto \frac{1}{\sqrt{\pi}}\sin(k\theta)$. The Hilbert space $H = L^2(\Omega, \mathbf{C})$ splits in two subspaces H_e and H_o, the spaces of even and odd functions of H respectively. The spaces H_e and H_o are stable under the dynamics of (7), hence no global controllability is to be expected in H.

B. Non-resonant case

We first focus on the space H_o. The restriction A of $\mathrm{i}\Delta$ to H_o is skew adjoint, with simple eigenvalues $(-\mathrm{i}k^2)_{k\in\mathbf{N}}$ associated to the eigenvectors

$$\left(\phi_k : \theta \mapsto \frac{1}{\sqrt{\pi}}\sin(k\theta)\right)_{k\in\mathbf{N}}.$$

The restriction B of $\psi \mapsto -\mathrm{i}\cos(\theta)\psi$ to H_o is skew-adjoint and bounded. The pair (A,B) satisfies Assumption 1 and is weakly-coupled (see [5, Section III.C]).

The Galerkin approximations of A and B at order N are

$$A^{(N)} = -\begin{pmatrix} \mathrm{i} & 0 & \cdots & 0 \\ 0 & 4\mathrm{i} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & N^2\mathrm{i} \end{pmatrix} \quad \text{and}$$

$$B^{(N)} = -\mathrm{i}\begin{pmatrix} 0 & 1/2 & 0 & \cdots & 0 \\ 1/2 & 0 & 1/2 & \ddots & \vdots \\ 0 & \ddots & 0 & \ddots & 0 \\ \vdots & \ddots & 1/2 & 0 & 1/2 \\ 0 & \cdots & 0 & 1/2 & 0 \end{pmatrix}.$$

Our aim is to transfer the wave function from the first eigenspace to the second one. The numerical simulation will be done on some finite dimensional space $\mathbf{C}^N$. We will use controls with L^1 norm less than $13/3$. By Proposition 2 and since $c(A,B) \leq 3/2$ (see [5, Section IV-C]), the $|A|^{\frac{1}{2}}$ norm of $\Upsilon^u_t(\phi_1)$ will remain less than $\exp(13/2) \approx 665$ for all time. From [5, Remark 4], the error done when replacing the original system by its Galerkin approximation is smaller than $\varepsilon = 10^{-2}$ provided that the Galerkin approximation has order at least $\sqrt{13e^{13/2}/3/10^{-2}} \approx 537$. This estimate is indeed very conservative and it can be improved using the regularity of the operator B.

From [5, Section IV.C], for every integer k, for every t in $[0,+\infty)$, for every locally integrable control u,

$$|\langle \phi_{k+1}, \Upsilon^u_t \phi_1\rangle| \leq \frac{1}{k!}\left(\int_0^t |u(\tau)|\mathrm{d}\tau\right)^k.$$

As a consequence, if $\|u\|_{L^1} \leq 13/3$, then $\|\pi_{22}B(\mathrm{Id} - \pi_{22})\Upsilon^u_t(\phi_1)\| \leq 5.10^{-7}$ for every t in $[0,+\infty)$. Using this inequality, one gets that the error made when replacing the original system by its Galerkin approximation of order 22 is smaller than $\varepsilon = 3.10^{-6}$ whenever $\|u\|_{L_1} \leq 13/3$.

The transition between the levels 1 and 2 is degenerate, indeed, $5^2 - 4^2 = 9 = 3(2^2 - 1^2)$. Nevertheless, for every $\{l_1, l_2\} \neq \{1,2\}$ such that $\lambda_{l_1} - \lambda_{l_2} \in 3\mathbf{Z}$ and $\langle \phi_{l_1}, B\phi_{l_2}\rangle \neq 0$, one has $l_1 > 2$ and $l_2 > 2$. Hence, for every $\frac{2\pi}{3}$-periodic function u, the limit of the propagator $X^{u/n}_{(N)}(t,0)$ leaves invariant the subspace generated by ϕ_1 and ϕ_2 and the result of Theorem 5 applies (with no need to check that all efficiencies of u for the transition (l_1,l_2) with $l_1 - l_2 \in 3(\mathbf{Z}\setminus\{1\})$ are zero).

We illustrate the notion of efficiency on some examples of control, namely $u^* : t \mapsto \cos^l(3t)$ for $l \in \{1,2,3,4,5\}$.

The efficiency is zero when l is even. In numerical simulations, the quantity $|\langle \phi_2, X^{u^*}_{(22)}(t,0)\phi_1\rangle|$ is less than 2.10^{-5} for every $t < 500$ (see Figure 1 for $l = 2$).

When l is odd, the efficiency is not zero. To estimate numerically the efficiency, one considers, for $n \in \{1, 10, 30\}$,

TABLE I

NUMERICAL EFFICIENCIES OF SOME PERIODIC SHAPES

Control u^* (Efficiency)	n	Time $t^\dagger$	Precision $1-p^\dagger$	Numerical Efficiency
$t \mapsto \cos(3t)$ $\pi/4 \approx 79\%$	$n=1$	6.8	2.10^{-2}	73%
	$n=10$	63	4.10^{-4}	78%
	$n=30$	189	3.10^{-5}	78%
$t \mapsto \cos(3t)^3$ $9\pi/32 \approx 88\%$	$n=1$	8.9	2.10^{-2}	83%
	$n=10$	84	2.10^{-4}	88%
	$n=30$	252	2.10^{-5}	88%
$t \mapsto \cos(3t)^5$ $75\pi/256 \approx 92\%$	$n=1$	10	7.10^{-3}	93%
	$n=10$	101	2.10^{-4}	92%
	$n=30$	302	2.10^{-5}	92%

the first maximum $p^\dagger$ of $t \mapsto |\langle \phi_2, X_{(N)}^{u^*/n}(t,0)\phi_1\rangle|$, reached at time $t^\dagger$, and computes

$$\frac{(1-p^\dagger)n\pi}{2|\langle \phi_1, B\phi_2\rangle| \int_0^{t^\dagger} |u^*(\tau)| \mathrm{d}\tau}.$$

The **Scilab** source codes used for the simulation are available on the web page [7]. We sum up the results in Table 1.

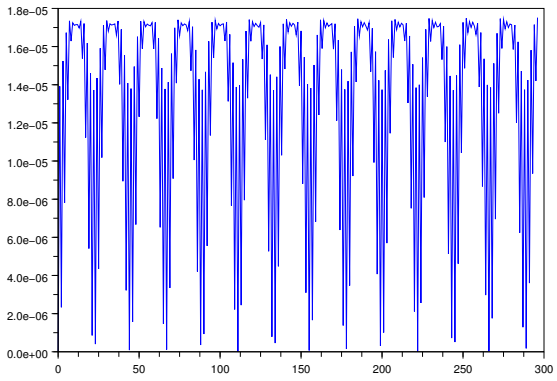

Fig. 1. Evolution of the square of the modulus of the second coordinate when applying the control : $t \mapsto \cos^2(3t)/30$ on the planar molecule (odd subspace) with initial condition ϕ_1. The simulation has been done on a Galerkin approximation of size $N = 22$.

C. Resonant case

We focus on the space H_e. The restriction A of $\mathrm{i}\Delta$ to H_e is skew adjoint, with simple eigenvalues $(-\mathrm{i}k^2)_{k\in\mathbf{N}\cup\{0\}}$ associated with the eigenvectors $(\phi_k)_{k\in\mathbf{N}\cup\{0\}}$, with $\phi_k : \theta \mapsto \frac{1}{\sqrt{\pi}}\cos(k\theta)$ for k in $\mathbf{N}$ and $\phi_0 : \theta \mapsto \frac{1}{\sqrt{2\pi}}$. The restriction B of $\psi \mapsto -\mathrm{i}\cos(\theta)\psi$ to H_e is skew-symmetric. The pair $(A+\mathrm{i}, B)$ satisfies Assumption 1. The translation from A to $A+\mathrm{i}$ induces just a phase shift and will be neglected in the following.

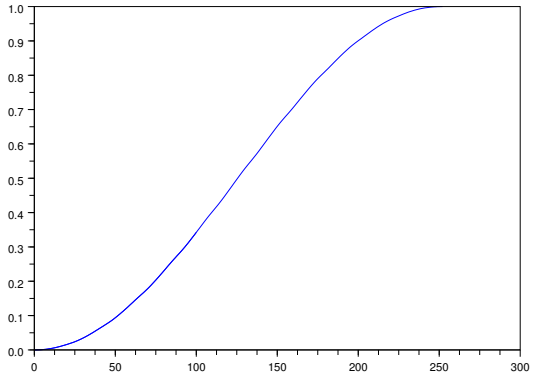

Fig. 2. Evolution of the square of the modulus of the second coordinate when applying the control $t \mapsto \cos^3(3t)/30$ on the planar molecule (odd subspace) with initial condition ϕ_1. The simulation has been done on a Galerkin approximation of size $N = 22$.

The Galerkin approximation of A and B at order N are

$$A^{(N)} = -\begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & \mathrm{i} & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & (N-1)^2\mathrm{i} \end{pmatrix} \text{ and}$$

$$B^{(N)} = -\mathrm{i}\begin{pmatrix} 0 & 1/\sqrt{2} & 0 & \cdots & 0 \\ 1/\sqrt{2} & 0 & 1/2 & \ddots & \vdots \\ 0 & \ddots & 0 & \ddots & 0 \\ \vdots & \ddots & 1/2 & 0 & 1/2 \\ 0 & \cdots & 0 & 1/2 & 0 \end{pmatrix}.$$

Our aim is to transfer the population from the first eigenspace, associated with eigenvalue 0, to the second one, associated with eigenvalue i. The transition $(1,2)$ is degenerate (indeed $2^2 - 1^2 = 3 = 3(1^2 - 0^2)$), and unlike what happens in H_o, the propagator $X_{(N)}^{u^*/n}(t,0)$ does not necessarily (approximately) stabilize the space spanned by ϕ_1 and ϕ_2 for every 2π-periodic function u^*. Note however that B only couples level 2 to levels 1 and 3. In other words, it is enough to find a 2π-periodic function u^* such that $E^{(2,3)}(u^*)$ is zero and $E^{(1,2)}(u^*)$ is not zero (and as large as possible) to induce the desired transfer. This is achieved, for instance, with the sequence of piecewise constant controls build in [3], for which the efficiency with respect to transition $(1,2)$ tends to $\cos(\pi/6)$ and the efficiency with respect to transition $(2,3)$ is zero. Another example is presented on Figure 3.

V. CONCLUSIONS AND FUTURE WORKS

A. Conclusions

The contribution of this paper is twofold. First, we showed how simple regularity hypotheses can be used to approach with arbitrary precision an infinite dimensional system with

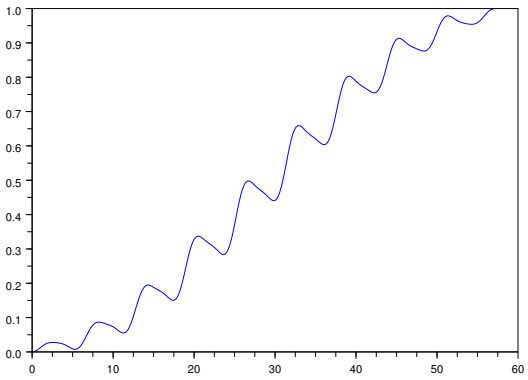

Fig. 3. Evolution of the square of the modulus of the second coordinate when applying the control $\frac{3}{40}\cos(t) + \frac{1}{10}$ on the planar molecule (even subspace) with initial condition ϕ_1. The simulation has been done on a Galerkin approximation of size $N = 22$. Precision $1 - p^\dagger$ is equal to 2.10^{-3}. Numerical efficiencies are 38% (theoretical: $3/8$) for the transition $(1, 2)$ and less than 5.10^{-4} for the transition $(2, 3)$ (theoretical: 0).

its finite dimensional Galerkin approximations. Using this finite dimensional reduction, we then used classical averaging techniques to obtain a proof of a well known experimental result about periodic control laws for the bilinear Schrödinger equation. As byproduct, we introduced the notion of efficiency, which characterizes the quality of the shape of a given control law.

B. Future Works

Most of the points in this paper are merely a starting point to further investigations. Among other, we plan to study the generalization of the notion of weakly-coupled systems for systems with continuous or mixed spectrum.

VI. ACKNOWLEDGMENTS

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

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

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

REFERENCES

[1] Karine Beauchard and Camille Laurent. Local controllability of 1D linear and nonlinear Schrödinger equations with bilinear control. *J. Math. Pures Appl.*, 94(5):520–554, 2010.

[2] Karine Beauchard and Mazyar Mirrahimi. Practical stabilization of a quantum particle in a one-dimensional infinite square potential well. *SIAM J. Control Optim.*, 48(2):1179–1205, 2009.

[3] Ugo Boscain, Marco Caponigro, Thomas Chambrion, and Mario Sigalotti. A weak spectral condition for the controllability of the bilinear Schrödinger equation with application to the control of a rotating planar molecule. arXiv:1101.4313v1, 2011.

[4] Ugo Boscain, Thomas Chambrion, Paolo Mason, Mario Sigalotti, and Dominique Sugny. Controllability of the rotation of a quantum planar molecule. In *Proceedings of the 48th IEEE Conference on Decision and Control*, pages 369–374, 2009.

[5] Nabile Boussaïd, Marco Caponigro, and Thomas Chambrion. Weakly-coupled systems in quantum control. arXiv:1109.1900v1.

[6] Thomas Chambrion. Periodic excitations of bilinear quantum systems. *ArXiv 1103.1130*, 2011.

[7] Thomas Chambrion. Supplementary material to preprint "Periodic excitations of bilinear quantum systems", 2011. `http://www.iecn.u-nancy.fr/~chambrio/PreprintUK.html`.

[8] Paolo Mason and Mario Sigalotti. Generic controllability properties for the bilinear Schrödinger equation. *Communications in Partial Differential Equations*, 35:685–706, 2010.

[9] Mazyar Mirrahimi. Lyapunov control of a quantum particle in a decaying potential. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 26(5):1743–1765, 2009.

[10] Vahagn Nersesyan. Global approximate controllability for Schrödinger equation in higher Sobolev norms and applications. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 27(3):901–915, 2010.

[11] Yannick Privat and Mario Sigalotti. The squares of the Laplacian–Dirichlet eigenfunctions are generically linearly independent. *ESAIM: COCV*, 16:794–807, 2010.

[12] Julien Salomon and Gabriel Turinici. Control of molecular orientation and alignment by monotonic schemes. In *Proceedings of the 24-th IASTED International Conference on modelling, identification and control*, pages 64–68, February 16-18, 2005.

[13] Jan A. Sanders and Ferdinand Verhulst. *Averaging methods in nonlinear dynamical systems*. Applied mathematical sciences. Springer-Verlag, 1985.

[14] Gabriel Turinici. On the controllability of bilinear quantum systems. In M. Defranceschi and C. Le Bris, editors, *Mathematical models and methods for ab initio Quantum Chemistry*, volume 74 of *Lecture Notes in Chemistry*. Springer, 2000.