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Periodic control laws for bilinear quantum systems with discrete spectrum

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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 finite dimensional Riemannian manifold $\Omega$, with associated measure $\mu$, is described by its wave function, that is, a point in the unit sphere of $L^2(\Omega, C)$. A system with wave function $\psi$ is in a subset $\omega$ of $\Omega$ with the probability $\int_\omega |\psi|^2d\mu$.

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

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

where $V, W : \Omega \rightarrow \mathbb{R}$ are real functions describing respectively the physical properties of the uncontrolled system and the external field, and $u : \mathbb{R} \rightarrow \mathbb{R}$ 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 $u$ that steers 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 concerning 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 $L^2(\Omega, C)$, 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 $L^2(\Omega, C)$. 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 quantum 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 $(\cdot, \cdot)$, we consider the evolution problem

$$\frac{d\psi}{dt} = (A + u(t)B)\psi$$ \hspace{1cm} (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 $\{ -i\lambda_k \}_{k \in \mathbb{N}}$, the sequence $(\lambda_k)_{k \in \mathbb{N}}$ is positive non-decreasing and accumulates at $+\infty$;

2) $B : H \rightarrow H$ is skew-adjoint and bounded.

In the rest of our study, we denote by $(\phi_k)_{k \in \mathbb{N}}$ an Hilbert basis of $H$ such that $A\phi_k = -i\lambda_k\phi_k$ for every $k$ in $\mathbb{N}$. We denote by $D(A + uB)$ the domain where $A + uB$ is skew-adjoint.
Together with Kato-Rellich Theorem, the Assumption 1.2 ensures that for every constant \( u \in \mathbb{R} \), \( A+uB \) is essentially skew-adjoint on \( D(A) \) and \( i(A+uB) \) is bounded from below. Hence, for every initial condition \( \psi_0 \) in \( H \), for every \( u \) piecewise constant, \( t \mapsto \psi(t) = T^u_t \psi_0 \) is the solution of the following classical continuity result.

**Proposition 1:** Let \( u \) and \( \psi \) be in \( L^1(\mathbb{R}) \), \( \psi \geq 0 \) and \( \psi \) is the expected value of the energy. For every \( t \) in \( [t_{j-1}, t_j) \) for a control \( u \) in \( L^1(\mathbb{R}) \) we define the solution using the following classical continuity result.

\[
T^u_t \psi_0 = e^{(t-t_{j-1})(A+u_j-1B)} \circ e^{(t_{j-1}-t_j)(A+u_j-2B)} \circ \cdots \circ e^{0(A+u_0B)} \psi_0,
\]

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

B. Energy growth

From Assumption 1.1, the operator \( iA \) is self-adjoint with positive eigenvalues. For every \( \psi \in D(A) \), \( iA\psi = \sum_{j \in \mathbb{N}} \lambda_j \phi_j \phi_j \). For every \( \psi \) in \( D(A) \), \( \|\psi\|_2 = \|A^{1/2} \psi\|_2 \) 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 \( \psi \) in \( D(A) \), \( \|R(A)\|_2 \leq C \|A\|_2 \). The coupling constant \( C \) of system \( (A,B) \) is the quantity \( \psi \in D(A) \setminus \{0\} \) for \( \|A\|_2 \) is the expected value of the energy.

**Proposition 2:** Let \( (A,B) \) satisfy Assumption 1 and \( u \in \mathbb{R} \) be piecewise constant. Then, for every \( \psi \) in \( D(A) \), \( \sup_{t \in [0, \infty)} \|A\|_2 \leq C \|A\|_2 \), \( u \) is piecewise constant, and \( D(A^{1/2}) = D(A+uB^2) \) for every \( u \) in \( \mathbb{R} \). 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 \( D(A^{1/2}) = \{A + uB\} \) is invariant for the unitary map \( \psi \mapsto e^{i t (A+uB)} \psi \). Moreover, for every \( \psi \) in \( D(A+uB) \), the mapping \( t \mapsto e^{i t (A+uB)} \psi \) is C1 from \( [0, +\infty) \) to \( H \), with derivative \( t \mapsto (A+uB)e^{i t (A+uB)} \). In other words, the mapping \( t \mapsto e^{i t (A+uB)} \psi \) is C1 from \( [0, +\infty) \) to \( A+uB \) with \( u \) piecewise constant, \( \psi_0 \) in \( D(A^{k+1}) \) and consider the real mapping \( f : t \mapsto \langle A^k T^u_t \psi_0, T^u_t \psi_0 \rangle \). Since \( \psi_0 \) 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 \( t \),

\[
\frac{d}{dt} f(t) = \frac{d}{dt} \langle |A|^k T^u_t \psi_0, T^u_t \psi_0 \rangle = 2 Re |\langle A|^k T^u_t \psi_0, (A+u(t)B)T^u_t \psi_0 \rangle = 2u(t) Re \langle |A|^k T^u_t \psi_0, BT^u_t \psi_0 \rangle.
\]

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

\[
|f'(t)| \leq 2|u(t)| \langle |A|^k T^u_t \psi_0, BT^u_t \psi_0 \rangle \leq 2c(2A,B) \langle |A|^k \psi_0, BT^u_t \psi_0 \rangle \langle |A|^k \psi_0, BT^u_t \psi_0 \rangle.
\]

From Gronwall’s lemma, we get

\[
\langle |A|^k \psi_0, \psi_0 \rangle \leq e^{2c(2A,B) \langle |A|^k \psi_0, BT^u_t \psi_0 \rangle \langle |A|^k \psi_0, BT^u_t \psi_0 \rangle}
\]

for every \( \psi_0 \) in \( D(|A|^2) \).

C. Good Galerkin approximation

For every \( N \in \mathbb{N} \), we define the orthogonal projection

\[
\pi_N : \psi \in H \mapsto \sum_{j \leq N} (\phi_j \psi) \phi_j \in H.
\]

**Proposition 3:** Let \( (A,B) \) satisfy Assumption 1, and \( u \) be weakly-coupled. Then, for every \( u \in \mathbb{N} \), \( N \in \mathbb{N} \), \( \psi \in \mathbb{N} \), \( |\psi_j| \leq \lambda_{N+1}^2 \)

\[
\langle (\pi_N - \pi_N) T^u_t \psi_0, \psi_0 \rangle \langle (\pi_N - \pi_N) T^u_t \psi_0, \psi_0 \rangle \leq \frac{e^{c(2A,B) \|\psi_0\|_2}}{\sqrt{\lambda_{N+1}^2}}
\]

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

**Proof:** Fix \( j \in \{1, \ldots, n\} \). For every \( N \geq 1 \), one has

\[
\langle (\pi_N - \pi_N) T^u_t \psi_0, \psi_0 \rangle \langle (\pi_N - \pi_N) T^u_t \psi_0, \psi_0 \rangle \leq \frac{e^{c(2A,B) \|\psi_0\|_2}}{\sqrt{\lambda_{N+1}^2}}
\]

By Proposition 2, for every \( t \geq 0 \), \( \|T^u_t \psi_0\|_2 \leq \frac{e^{c(2A,B) \|\psi_0\|_2}}{\sqrt{\lambda_{N+1}^2}} \). The conclusion then follows by Proposition 2.

**Remark 1:** Since \( B \) is bounded, then \( B(\pi_N - \pi_N) T^u_t \psi_0 \) 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 \( N \in \mathbb{N} \). The Galerkin approximation of (2) of order \( N \) is the system in \( H \)

\[
\dot{x} = (A^{(N)} + u(t)B^{(N)})x \quad (\Sigma_N)
\]

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 \( X^u_{(N)}(t,s) \) the propagator of \( (\Sigma_N) \) for 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 \( (\Sigma_N) \) leaves invariant the \( N \)-dimensional space \( L_N = \text{span}_{1 \leq j \leq N} \{\phi_j\} \). Thus, \( (\Sigma_N) \) can be seen as a finite dimensional bilinear system in \( L_N \).

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

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

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

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

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

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

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

By Proposition 3, the norm of $t \mapsto B(Id - \pi_N)Y^u_t(\psi_j)$ is less than $\|B\|\frac{\lambda^{1/2}}{\lambda^{1/2} + K}\|\psi_j\|_{L^1}$. Since $X^u_{(N)}(t,s)$ is unitary, $\|\pi_N Y^u_t(\psi_j) - X^u_{(N)}(t,0)\pi_N \psi_j\| < \|u\|_{L^1}\|B\|\frac{\lambda^{1/2}}{\lambda^{1/2} + K}\|\psi_j\|_{L^1}$.

Then,

$$\|Y^u_t(\psi_j) - X^u_{(N)}(t,0)\pi_N \psi_j\| \leq \|Id - \pi_N\|\|Y^u_t(\psi_j)\| + \|\pi_N Y^u_t(\psi_j) - X^u_{(N)}(t,0)\pi_N \psi_j\| \leq \lambda^{1/2}\|Id - \pi_N\|\|Y^u_t(\psi_j)\| + \|\pi_N Y^u_t(\psi_j) - X^u_{(N)}(t,0)\pi_N \psi_j\|.$$

This completes the proof since $\lambda_N$ 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 $(\Sigma_N)$ of Definition 2. The matrix $A(N)$ is diagonal with eigenvalues $(-\alpha_j)_{1 \leq j \leq N}$ with $\alpha_1 \leq \alpha_2 \leq \cdots \leq \alpha_N$. We denote with $(b_{jk})_{1 \leq j \leq k \leq N}$ the entries of $B(N)$.

**Theorem 5:** Let $j, k$ be two integers such that $1 \leq j < k \leq N$. Assume that $b_{jk} \neq 0$ and that for every $l, m \leq N$, $|\alpha_l - \alpha_m| \in \mathbb{N}[|\alpha_j - \alpha_k|]$ implies $(j, k) \in \{(l, m)\}$ or $b_{lm} = 0$.

Define $T = \frac{\pi\sqrt{k-j-1}}{\alpha_j - \alpha_k}$. Then, for every $u^* \in L^1(\mathbb{R})$ satisfying

$$\int_0^T u^*(\tau)e^{i(\lambda_k - \lambda_j)\tau}d\tau \neq 0 \text{ and } \int_0^T u^*(\tau)e^{i(\lambda_l - \lambda_m)\tau}d\tau = 0,$$

for every $l, m$ such that $|\alpha_l - \alpha_m| \in \mathbb{N}[|\alpha_j - \alpha_k|]$ and $b_{lm} \neq 0$, one has

$$1 - \|\phi_k, X^{nT^*0}(nT^*0,0)\phi_j]\| \leq C \frac{\pi}{n2|b_{jk}|} \left(\int_0^T |u^*(\tau)|d\tau\right)^2 \text{ with } \frac{C}{\inf_{|\alpha_l - \alpha_m| \in \mathbb{N}[|\alpha_j - \alpha_k|]} \sin \left(2\pi\frac{\alpha_j - \alpha_m}{\alpha_j - \alpha_k}\right)}.$$
with respect to transition weakly-coupled (see [5, Section III.C]).

**B. Non-resonant case**

The spaces hence no global controllability is to be expected in the worst case, this algorithm guarantees that \( \epsilon \sim \frac{1}{N^2 \sqrt{2}} \), what may seem poor with respect to the cosine law. However, this algorithm is especially useful to handle the case of high order resonances. Indeed, if \( a_1, a_2, \ldots, a_p \) 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 \( L^2(\Omega,C) \) where \( \Omega = \mathbb{R}/2\pi \mathbb{Z} \) is the one dimensional torus. The Schrödinger equation writes

\[
\frac{\partial \psi}{\partial t}(t,\theta) = -\Delta \psi(t,\theta) + u(t) \cos(\theta) \psi(t,\theta),
\]

where \( \Delta \) is the Laplace-Beltrami operator on \( \Omega \). The self-adjoint operator \( -\Delta \) has purely discrete spectrum \( \{ k^2, k \in \mathbb{N} \} \). 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 \( H = L^2(\Omega,C) \) splits in two subspaces \( H_0 \) and \( H_\infty \), the spaces of even and odd functions of \( H \) respectively. The spaces \( H_0 \) and \( H_\infty \) are stable under the dynamics of (6), hence no global controllability is to be expected in \( H \).

#### B. Non-resonant case

We first focus on the space \( H_0 \). The restriction \( A \) of \( i\Delta \) to \( H_0 \) is skew-adjoint, with simple eigenvalues \( (-ik^2)_{k \in \mathbb{N}} \) associated to the eigenvectors

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

The restriction \( B \) of \( \psi \mapsto -i \cos(\theta) \psi \) to \( H_0 \) 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

\[
A^{(N)} = \begin{pmatrix}
0 & 0 & \cdots & 0 \\
4i & \ddots & \cdots & \vdots \\
\vdots & \ddots & \ddots & \vdots \\
0 & \cdots & 0 & 0
\end{pmatrix}
\]

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

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 \( C^N \). The controls we will use in the following have \( L^1 \) norm less than 13/3 and, from Proposition 2, the \( |A|^\frac{1}{2} \) norm of \( T_\tau^{(N)}(\phi_1) \) will remain less than \( \exp(13/2) \approx 665 \) for all time. From [5, Remark 4], the error made when replacing the original system by its Galerkin approximation of order \( \sqrt{13e^{13/2}/310^{-2}} \approx 288228 \) is smaller than \( \epsilon = 10^{-2} \). 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 \( l \), for every \( t \) in \([0, +\infty)\), for every locally integrable control \( u \) (not necessarily periodic),

\[
|\langle \phi_{k+1}, T_\tau^{(N)}(\phi_1) \rangle| \leq \frac{1}{k!} \left( \int_{[0,t]} |u(\tau)| d\tau \right)^k.
\]

As a consequence, if \( \|u\|_{L^1} \leq 13/3 \), then \( \|\pi_{22} B (\Id - \pi_{22}) T_\tau^{(N)}(\phi_1)\| \leq 5.10^{-7} \) 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 \( \epsilon = 3.10^{-6} \) when \( \|u\|_{L^1} \leq 13/3 \).

The transition between the levels 1 and 2 is resonant, indeed, \( 5^2 - 4^2 = 9 = 3(2^2 - 1) \). Nevertheless, for every \( \{l_1, l_2\} \neq \{1, 2\} \) such that \( \lambda_{l_1} - \lambda_{l_2} \in 3\mathbb{Z} \) and \( \langle \phi_1, B\phi_2 \rangle \neq 0 \), one has \( l_1 > 2 \) and \( l_2 > 2 \). Hence, for every \( \frac{2\pi}{\lambda_k} \)-periodic function \( u \), the limit of the propagator \( X^{(N)}(t,0) \) leaves invariant the subspace generated by \( \phi_1 \) and \( \phi_2 \) and the result of Theorem 5 applies (without having to check that all efficiencies of \( u \) for the transition \( (l_1, l_2) \) with \( l_1 - l_2 \in 3\mathbb{Z} \setminus \{1\} \) 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 \( |\langle \phi_2, X^{(N)}(t,0)\phi_1 \rangle| \) 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 \( n \in \{1, 10, 30\} \), the first maximum \( p^l \) of \( t \mapsto |\langle \phi_2, X^{(N)}(t,0)\phi_1 \rangle| \), reached at time \( t^l \), and computes

\[
\frac{(1 - p^l)n\pi}{2|\langle \phi_1, B\phi_2 \rangle| \int_{[0,t^l]} |u(\tau)| d\tau}.
\]
The Scilab source codes used for the simulation are available on the web page [7]. We sum up the results in Table 1.

<table>
<thead>
<tr>
<th>Control $u^*$</th>
<th>$n$</th>
<th>Time $t^\dagger$</th>
<th>Precision $1 - p^\dagger$</th>
<th>Numerical Efficiency</th>
</tr>
</thead>
<tbody>
<tr>
<td>$t \mapsto \cos(3\pi t)$</td>
<td>$n = 1$</td>
<td>6.8</td>
<td>$2 \cdot 10^{-2}$</td>
<td>73%</td>
</tr>
<tr>
<td>$\pi/4 \approx 79%$</td>
<td>$n = 10$</td>
<td>63</td>
<td>$4 \cdot 10^{-4}$</td>
<td>78%</td>
</tr>
<tr>
<td>$\pi/4 \approx 79%$</td>
<td>$n = 30$</td>
<td>189</td>
<td>$3 \cdot 10^{-5}$</td>
<td>78%</td>
</tr>
<tr>
<td>$t \mapsto \cos(3\pi t)^3$</td>
<td>$n = 1$</td>
<td>8.9</td>
<td>$2 \cdot 10^{-2}$</td>
<td>83%</td>
</tr>
<tr>
<td>$9\pi/32 \approx 88%$</td>
<td>$n = 10$</td>
<td>84</td>
<td>$2 \cdot 10^{-4}$</td>
<td>88%</td>
</tr>
<tr>
<td>$9\pi/32 \approx 88%$</td>
<td>$n = 30$</td>
<td>252</td>
<td>$2 \cdot 10^{-5}$</td>
<td>88%</td>
</tr>
<tr>
<td>$t \mapsto \cos(3\pi t)^5$</td>
<td>$n = 1$</td>
<td>10</td>
<td>$7 \cdot 10^{-3}$</td>
<td>93%</td>
</tr>
<tr>
<td>$75\pi/256 \approx 92%$</td>
<td>$n = 10$</td>
<td>101</td>
<td>$2 \cdot 10^{-4}$</td>
<td>92%</td>
</tr>
<tr>
<td>$75\pi/256 \approx 92%$</td>
<td>$n = 30$</td>
<td>302</td>
<td>$2 \cdot 10^{-5}$</td>
<td>92%</td>
</tr>
</tbody>
</table>

C. Resonant case

We focus on the space $H_e$. The restriction $A$ of $i\Delta$ to $H_e$ is skew adjoint. We have simple eigenvalues $(-i k^2)_{k \in \mathbb{N} \cup \{0\}}$ associated to the eigenvectors $\langle \phi_k \rangle_{k \in \mathbb{N} \cup \{0\}}$, with $\phi_k : \theta \mapsto \frac{\sqrt{3}}{k} \cos(k \theta)$ for $k$ in $\mathbb{N}$ and $\phi_0 : \theta \mapsto \frac{\sqrt{2}}{\sqrt{3}}$. The restriction $B$ of $\psi \mapsto -i \cos(\theta) \psi$ to $H_e$ is skew-symmetric. The pair $(A + i, B)$ satisfies Assumption 1. The translation from $A$ to $A + i$ induces just a phase shift and will be neglected in the following.

The Galerkin approximation of $A$ and $B$ at order $N$ are

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

and

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

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 resonant (indeed $2^2 - 1^2 = 3 = 3(1^2 - 0^2)$), and unlike what happens on the space of odd eigenfunctions, the limit matrix $M^\dagger$ does not necessarily stabilize the space spanned by $\phi_1$ and $\phi_2$ for every $2\pi$-periodic function $u^*$. Note however that $B$ only connects level 2 to levels 1 and 3. In other words, it is enough to find a $2\pi$-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 have shown how simple regularity hypotheses can be used to approach with arbitrary precision an infinite dimensional system with 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.
Fig. 3. Evolution of the square of the modulus of the second coordinate when applying the control $\frac{1}{10} \cos(t) + \frac{1}{100}$ on the planar molecule (even subspace) with initial condition $\phi_1$. The simulation has been done on a Galerkin approximation of size $N = 22$. Precision $1 - p^1$ 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).

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.

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