Implementation of logical gates on infinite dimensional quantum oscillators

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*— In this paper we study the error in the approximate simultaneous controllability of the bilinear Schrödinger equation. We provide estimates based on a tracking algorithm for general bilinear quantum systems and on the study of the finite dimensional Galerkin approximations for a particular class of quantum systems, weakly-coupled systems. We then present two physical examples: the perturbed quantum harmonic oscillator and the infinite potential well.**

I. Introduction

A. Logical gates

Quantum computation relies on the idea to store an information in the state of quantum system. This state is described by the *wave function*, that is, a point ψ in the Hilbert sphere of $L^2(\Omega, \mathbf{C})$, where Ω is a Riemannian manifold.

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

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

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.

When the manifold Ω is compact, the linear operator $i(\Delta/2 - V)$ admits a set of eigenstates $(\phi_n)_{n\in\mathbf{N}}$. A *logical gate*, or *quantum gate*, is a unitary transformation in $L^2(\Omega, \mathbf{C})$ for which some finite dimensional space of the form $\operatorname{span}\{\phi_1, \phi_2, \ldots, \phi_n\}$ is invariant. To build a given logical gate $\widehat{\Upsilon}$ from the system (1), one has to find a control law u such that the propagator Υ^u_T at a certain time T of (1) satisfies $\Upsilon^u_T(\phi_j) = \widehat{\Upsilon}\phi_j$ for every $j = 1, \ldots, n$.

The main difficulty with this problem is that the space $L^2(\Omega, \mathbf{C})$ has infinite dimension. For the sake of simplicity, one often considers the case where Ω is a finite union of points (or, equivalently, $L^2(\Omega, \mathbf{C})$ is finite dimensional). Nevertheless, most of the usual quantum systems evolve on non-trivial manifolds Ω. This papers deals with the effective implementation of some simple logical gates on models of quantum oscillators on 1-dimensional manifolds.

B. Quantum control

The problem of driving the solutions of (1) to a given target has been intensively studied in the past decades, both in the finite and infinite dimensional case. Many advances have been made in the infinite dimensional case, when there is only one source and one target. The interested reader may refer, for instance and among many other references, to [5], [7] for the theoretical viewpoint and to [8] for numerical aspects. In particular, it was proved in [3] that *exact* controllability is impossible in general. This does not prevent to study *approximate* controllability of (1), that is to replace the condition $\Upsilon^u_T(\phi_j) = \widehat{\Upsilon}\phi_j$ by $\|\Upsilon^u_T(\phi_j) - \widehat{\Upsilon}\phi_j\| \leq \varepsilon$ for every $j = 1, \ldots, n$. To the best of our knowledge, there are only very few results of *simultaneous* controllability in the infinite dimensional case and the only available effective control techniques have been described in [9] and [11].

Recently, we noticed in [10] that a certain class of bilinear systems are precisely approached by their Galerkin approximations. Two important examples of these so-called *weakly-coupled* systems are the quantum harmonic oscillator and the infinite potential well. The structure of weakly-coupled systems permits precise numerical simulations for the construction of quantum gates.

C. Content of the paper

The theoretical background is recalled in Section II. After a quick survey on simultaneous control techniques for Equation (1), we give precise definitions and approximation results for weakly-coupled systems. In Section III we apply these results to induce a permutation among the first three eigenstates of a perturbation of the quantum harmonic oscillator and we provide numerical simulations and estimates for the error. Similarly, in Section IV we induce a permutation among the first three eigenstates of the infinite potential well.

II. General theoretical results

A. Framework and notations

We reformulate the problem (1) in a more abstract framework. In a separable Hilbert space H endowed with norm $\|\cdot\|$ and Hilbert product $\langle\cdot,\cdot\rangle$, we consider the evolution problem

$$\frac{d\psi}{dt} = (A + uB)\psi \quad (2)$$

where (A, B) satisfies Assumption 1.

Assumption 1: (A, B) is a pair of linear operators with domains $D(A)$ and $D(B)$ such that

1) for every u in $\mathbf{R}$, $A + uB$ is essentially skew-adjoint on $D(A) \cap D(B)$;
2) A is skew-adjoint and has purely discrete spectrum $(-i\lambda_k)_{k\in\mathbf{N}}$. associated with the Hilbert basis $(\phi_k)_{k\in\mathbf{N}}$ of eigenvectors of A.

From Assumption 1.2, one deduces that there exists a Hilbert basis $(\phi_k)_{k\in\mathbf{N}}$ of eigenvectors of A with $A\phi_k = -\mathrm{i}\lambda_k\phi_k$.

From Assumption 1.1, one deduces that, for every piecewise constant u, $u : t \mapsto \sum_j u_j\chi_{(t_j,t_{j+1})}(t)$, with $0 = t_0 \leq t_1 \leq \ldots \leq t_{N+1}$ and $u_0, \ldots, u_N$ in $\mathbf{R}$, the solution $t \mapsto \Upsilon^u_t\psi_0$ of (2) has the form

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

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

Remark 1: Under extra regularity hypotheses, it is possible to define the propagator of (2) for a larger class of controls. For instance, when B is bounded, for every t, $\Upsilon_t : u \mapsto \Upsilon^u_t$ admits a unique continuous extension to $L^1_{\mathrm{loc}}(\mathbf{R}, \mathbf{R})$.

B. Control results

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

(i) $s^1_1 = j$ and $s^q_2 = k$;
(ii) $s^j_2 = s^{j+1}_1$ for every $1 \leq j \leq q-1$;
(iii) $\langle \phi_{s^j_1}, B\phi_{s^j_2}\rangle \neq 0$ for $1 \leq j \leq q$.

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

Definition 2: Let (A, B) satisfy Assumption 1. The system (A, B) is approximately simultaneously controllable if for every $\widehat{\Upsilon} \in U(H)$ (unitary operators acting on H), $\psi_1, \ldots, \psi_n \in H$, and $\varepsilon > 0$, there exists a piecewise constant function $u_\varepsilon : [0, T_\varepsilon] \to \mathbf{R}$ such that

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

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

The following sufficient condition for approximate simultaneous controllability has been given in [9].

Proposition 1: Let (A, B) satisfy Assumption 1 and admit a non-resonant chain of connectedness. Then (A, B) is approximately simultaneously controllable.

C. Weakly-coupled systems

Definition 3: Let k be a positive number and let (A, B) satisfy Assumption 1.1. Then (A, B) is k *weakly-coupled* if for every $u \in \mathbf{R}$, $D(|A + uB|^{k/2}) = D(|A|^{k/2})$ and there exists a constant C such that, for every ψ in $D(|A|^k)$, $|\Re\langle|A|^k\psi, B\psi\rangle| \leq C|\langle|A|^k\psi, \psi\rangle|$.

Definition 4: Let $N \in \mathbf{N}$. The *Galerkin approximation* of (2) of order N is the system in H

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

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 $X^u_{(N)}(t, s)$ the propagator of (Σ_N) associated with a piecewise constant functions u. The following proposition is a special case of [10, Proposition 4].

Proposition 2: Let k and s be non-negative numbers with $0 \leq s < k$. Let (A, B) satisfy Assumption 1 and be k weakly-coupled. Assume that there exist $d > 0$, $0 \leq r < k$ such that $\|B\psi\| \leq d\|\psi\|_{r/2}$ for every ψ in $D(|A|^{r/2})$. 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

$$\|u\|_{L^1} < K \implies \|\Upsilon^u_t(\psi_j) - X^u_{(N)}(t, 0)\pi_N\psi_j\|_{s/2} < \varepsilon,$$

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

D. Construction of control laws

Let (A, B) satisfy Assumption 1, admit a non degenerate chain of connectedness and be k-weakly-coupled, and $\widehat{\Upsilon} \in U(H)$ be a given quantum gate leaving invariant $\mathcal{L}_n = \mathrm{span}(\phi_1, \ldots, \phi_n)$. Proposition 1 asserts that there exists a control u whose associated propagator Υ^u_T is arbitrary close to $\widehat{\Upsilon}$ on $\mathcal{L}_n = \mathrm{span}(\phi_1, \ldots, \phi_n)$. Proposition 2 allows, when imposing a constraint on the L^1-norm of the control, to reduce the problem from the realization of the dynamics Υ^u_t on an infinite dimensional space to the problem of realizing dynamics, $X^u_{(N)}$, on finite dimensional spaces. A large amount of literature is devoted to the motion planning for finite dimensional systems bilinear quantum systems. We refer, for instance, to [12] for an introduction and to [15] for an example of numerical approach.

In the following, we concentrate on the physically relevant case where $\widehat{\Upsilon}$ is a permutation of the eigenstates $\phi_1, \phi_2, \ldots, \phi_n$. It is well known ([13], [19]) that, if (j, k) belongs to a non-degenerate chain of connectedness of $(A^{(N)}, B^{(N)})$, then it is possible to permute ϕ_k and ϕ_j using periodic controls with period $|\lambda_j - \lambda_k|$. This result is known in quantum mechanics as the "Rotating wave approximation" (see also [11] for an infinite dimensional version). It remains, then, to express the given permutation $\widehat{\Upsilon}$ as the (non-commutative) product of the transpositions (j, k), for (j, k) in a non-degenerate chain of connectedness of (A, B).

We present in Sections III and IV two examples of quantum systems (A, B) such that $(1, 2)$ and $(2, 3)$ are in a non-degenerate chain of connectedness of (A, B). We aim to send level 1 to level 3, level 2 to level 1 and level 3 to level 2. With standard algebraic notations, since $(1, 3, 2) = \tau_{23}\tau_{12}$, we realize this quantum gate by first exchanging levels 1 and 2 while leaving level 3 unchanged and then exchanging levels 2 and 3 while leaving level 1 unchanged.

III. The perturbed quantum harmonic oscillator

A. Physical model

The quantum harmonic oscillator is one of the most studied quantum system. The Schrödinger equation reads

$$i\frac{\partial\psi}{\partial t}(x,t) = -\frac{1}{2}\frac{\partial^2\psi}{\partial x^2} + \left(\frac{1}{2}x^2 - u(t)x\right)\psi(x,t), \qquad (3)$$

where $x \in \Omega = \mathbf{R}$. With the notations of (2), $A = -i(-\Delta + x^2)/2$ and $B = ix$.

An Hilbert basis of H made of eigenvectors of A is given by the sequence of Hermite functions $(\phi_n)_{n\in\mathbf{N}}$, associated with the sequence $(-i\lambda_n)_{n\in\mathbf{N}}$ 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:

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

A chain of connectedness for this system is given by $S = \{(n, n+1) \ : \ n \in \mathbf{N}\}$. The chain S is resonant, indeed $|\lambda_{n+1} - \lambda_n| = 1$ for every n in $\mathbf{N}$. As a matter of fact, the system (3) is known to be non-controllable (see [16], [14]).

We consider a perturbation of this system. Consider the inverse A^{-1} of the operator A. The family $(\phi_n)_{n\in\mathbf{N}}$ is a family of eigenvectors for A^{-1} associated with the eigenvalues $(-i/\lambda_n)_{n\in\mathbf{N}}$. For every $\eta \geq 0$ we set $A_\eta = A + \eta A^{-1}$. Since A and A^{-1} commute then $(\phi_n)_{n\in\mathbf{N}}$ is a family of eigenvectors of A_η associated with the eigenvalues $(-i\lambda_n^\eta)_{n\in\mathbf{N}}$ where $\lambda_n^\eta = \lambda_n + \eta/\lambda_n$. The set S is a non-resonant chain of connectedness for system (A_η, B) for every $\eta > 0$. Indeed $\lambda_{n+1}^\eta - \lambda_n^\eta = 1 - 4\frac{\eta}{4n^2-1}$ and, clearly, $\lambda_{n+1}^\eta - \lambda_n^\eta = \lambda_{m+1}^\eta - \lambda_m^\eta$ if and only if $n = m$.

By Proposition 1 system (A_η, B) is approximately simultaneously controllable. Moreover by [9, Theorem 2.13] we have also an upper bound on the L^1-norm of the control independent of the error. For instance, we can steer approximately the first level ϕ_1 to the second ϕ_2 with a control law of L^1-norm smaller than $5\pi/4$. Another consequence is that a quantum gate for ϕ_1, ϕ_2, and ϕ_3 is approximately reachable, that is for every $\varepsilon > 0$, there exists $t_\varepsilon > 0$ and a piecewise constant function u_ε such that $\|\Upsilon^{u_\varepsilon}_{t_\varepsilon}(\phi_j) - \phi_{\sigma(j)}\| < \varepsilon$ where σ is the 3-cycle exchanging $1, 2$ and 3. Moreover $\|u_\varepsilon\|_{L^1} \leq \pi/2(1 + \sqrt{2}/2)$.

B. Estimates

In the following, we consider only control of L^1-norm less than $K = \pi/2(1 + \sqrt{2}/2)$. The particular tri-diagonal structure of system (A_η, B) is very useful for a priori estimates on the components of the propagator. Indeed if $\|u\|_{L^1} \leq K$, by [10, Remark 6], we have that

$$|\langle\phi_{n+1}, \Upsilon^u_t(\phi_j)\rangle| \leq \frac{(2K)^{n-2}}{(n-2)!}\sqrt{\frac{(2n-3)!}{(n-2)!}}, \qquad (4)$$

for every n in $\mathbf{N}$, $n \geq 3$ and $j = 1, 2, 3$.

We use (4) to find estimates on the size N of the Galerkin approximation whose existence is asserted by Proposition 2. First, let $N \geq j$ and notice that

$$\begin{aligned} \frac{d}{dt}\pi_N \Upsilon^u_t(\phi_j) &= (A^{(N)} + uB_l^{(N)})\pi_N\Upsilon^u_t(\phi_j) \\ &\quad + u(t)\pi_N B(\mathrm{Id} - \pi_N)\Upsilon^u_t(\phi_j). \end{aligned}$$

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

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

Therefore, since $X^u_{(N)}(t,s)$ is unitary and for the tri-diagonal structure of the system we have, for $j = 1, 2, 3$,

$$\begin{aligned} &\|\pi_N\Upsilon^u_t(\phi_j) - X^u_{(N)}(t,s)\phi_j\| \\ &\leq K\|\pi_N B(\mathrm{Id} - \pi_N)\Upsilon^u_t(\phi_j)\| \\ &= K|b_{N,N+1}||\langle\phi_{N+1}, \Upsilon^u_t(\phi_j)\rangle| \\ &= K\sqrt{N}|\langle\phi_{N+1}, \Upsilon^u_t(\phi_j)\rangle| \\ &\leq \frac{2^{N-1}K^{N-1}}{(N-2)!}\sqrt{\frac{(2N-3)!}{(N-3)!}}. \end{aligned}$$

Using $K = \pi/2(1 + \sqrt{2}/2) < 2.69$, it is enough to consider a Galerkin approximation of size $N = 420$ to get $\|\pi_N\Upsilon^u_t(\phi_j) - X^u_{(N)}(t,s)\phi_j\| \leq 10^{-4}$ for $j = 1, 2, 3$.

C. Numerical simulations

In the numerical simulations, we choose $\eta = 1$. To induce the transition between levels 1 and 2, the control law we use is a piecewise constant 4π-periodic function, taking value 1 for $0 \leq t < 5.\,10^{-3}$ and taking value 0 for $5.\,10^{-3} \leq t \leq 4\pi$. We apply this control for 314 periods, that is during a time of 1256π .

To induce the transition between levels 2 and 3, the control law we use is a piecewise constant $12\pi/5$-periodic function, taking value 1 for $0 \leq t < 5.\,10^{-3}$ and taking value 0 for $5.\,10^{-3} \leq t < 12\pi/5$. We apply this control for 222 periods.

The simulations are done on a Galerkin approximation of size 420, which guarantees $\|\pi_N\Upsilon^u_t(\phi_j) - X^u_{(N)}(t,s)\phi_j\| \leq 10^{-4}$ for $j = 1, 2, 3$. At final time T, the resulting propagator is such that $|\langle\Upsilon^u_T\phi_1, \phi_3\rangle| > 0.998$, $|\langle\Upsilon^u_T\phi_2, \phi_1\rangle| > 0.999$ and $|\langle\Upsilon^u_T\phi_3, \phi_2\rangle| > 0.999$. The time evolution of the moduli of the first coordinates of $\Upsilon^u_t(\phi_j)$ for $j = 1, 2, 3$ is depicted in Figures 1, 2, and 3.

All the computations were done using the free software NSP, see [17]. The source code for the simulation is available at [1]. The total computation time is less than 4 minutes on a standard desktop computer.

IV. Particle in a box

A. Physical model

We consider now the case of a particle confined in $(0, \pi)$. This model has been extensively studied by several authors in the last few years and it has been the first quantum system for which a positive controllability result has been obtained. Beauchard proved exact controllability in some dense subsets of L^2 using Coron's return method (see [4], [6] for a precise statement). Nersesyan obtained approximate controllability

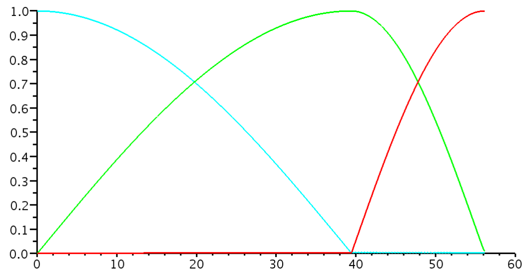

Fig. 1. Time evolution of the moduli of the first three coordinates of $\Upsilon^u_t \phi_1$ in the case of the perturbed harmonic oscillator. First coordinate in blue, second coordinate in green, third coordinate in red. For the sake of readability, time scale is 1:100, total duration around 5500.

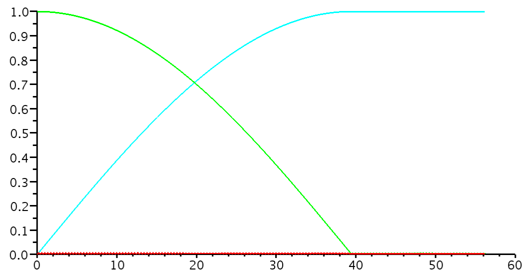

Fig. 2. Time evolution of the moduli of the first three coordinates of $\Upsilon^u_t \phi_2$ in the case of the perturbed harmonic oscillator. First coordinate in blue, second coordinate in green, third coordinate in red. Time scale is 1:100.

results using Lyapunov techniques. In the following, we extend these controllability results to simultaneous controllability and provide some estimates of the L^1-norm of the controls achieving simultaneous controllability.

The Schrödinger equation writes

$$i\frac{\partial \psi}{\partial t} = -\frac{1}{2}\frac{\partial^2 \psi}{\partial x^2} - u(t)x\psi(x,t) \tag{6}$$

with boundary conditions $\psi(0,t) = \psi(\pi,t) = 0$ for every $t \in \mathbf{R}$.

In this case $\mathcal{H} = L^2\left((0,\pi),\mathbb{C}\right)$ endowed with the Hermitian product $\langle \psi_1, \psi_2 \rangle = \int_0^\pi \overline{\psi_1(x)}\psi_2(x)dx$. The operators A and B are defined by $A\psi = i\frac{1}{2}\frac{\partial^2\psi}{\partial x^2}$ for every ψ in $D(A) = (H_2 \cap H_0^1)\left((0,\pi),\mathbb{C}\right)$, and $B\psi = ix\psi$. An Hilbert basis of H is $(\phi_k)_{k\in\mathbf{N}}$ with $\phi_k : x \mapsto \sin(kx)/\sqrt{2}$. For every k, $A\phi_k = -ik^2/2\phi_k$.

For every j,k in $\mathbf{N}$,

$$b_{jk} := \langle \phi_j, B\phi_k \rangle = \begin{cases} (-1)^{j+k}\frac{2jk}{(j^2-k^2)^2} & \text{if } j-k \text{ odd} \\ 0 & \text{otherwise.} \end{cases}$$

Despite numerous degenerate transitions, the system is approximately simultaneously controllable (see [9, Section 7]).

B. *Estimates*

Using Proposition 2 to estimate the error done when replacing infinite dimensional system by its Galerkin approximation one finds, for $\|u\|_{L^1} = 9\pi/16$ (see [10, Remark 4], with $K = 9\pi/16$, $d = \pi$, $k = 1$, $r = 1$, $c_1(A,B) \leq \pi + 2$, $\varepsilon = 10^{-3}$), that if $N > 1.6\ 10^7$, then

$$\|\pi_N \Upsilon^u_t \phi_1 - X^u_{(N)}(t,0)\phi_1\| \leq 10^{-3}.$$

This estimation is definitely too rough to allow easy numerical simulations: matrix $B^{(10^7)}$ has about $5\ 10^{13}$ non-zeros entries, the numerical simulations at such scale are difficult without large computing facilities. We have to go more into details to obtain finer estimates.

Assume that, for some N in $\mathbf{N}$ and $\eta > 0$, the control $u : [0,T] \to \mathbf{R}$ is such that, for every t in $[0,T]$,

$$\|X^u_{(N)}(t,0)\pi_3 - \pi_3 X^u_{(N)}(t,0)\| \leq \eta.$$

We have

$$\begin{aligned} &\pi_3 X^u_{(N)}(t,s) - X^u_{(N)}(t,s)\pi_3 \\ &= \pi_3 X^u_{(N)}(t,0)X^u_{(N)}(0,s) - X^u_{(N)}(t,0)X^u_{(N)}(0,s)\pi_3 \\ &= X^u_{(N)}(t,0)(\pi_3 X^u_{(N)}(0,s) - X^u_{(N)}(0,s)\pi_3) \\ &\quad + (\pi_3 X^u_{(N)}(t,0) - X^u_{(N)}(t,0)\pi_3)X^u_{(N)}(0,s) \end{aligned}$$

so that

$$\|\pi_3 X^u_{(N)}(t,s) - X^u_{(N)}(t,s)\pi_3\| \leq 2\eta. \tag{7}$$

Projecting (5) on the first 3 components we have, for $j = 1,2,3$, that

$$\begin{aligned} &\|\pi_3 \Upsilon^u_t(\phi_j) - \pi_3 X^u_{(N)}(t,0)\phi_j\| \\ &\leq \int_0^t \|\pi_3 X^u_{(N)}(t,s)\pi_N B(\mathrm{Id} - \pi_N)\Upsilon^u_s(\phi_j)\||u(s)|\mathrm{d}s \\ &\leq \int_0^t \|X^u_{(N)}(t,s)\pi_3 B(\mathrm{Id} - \pi_N)\Upsilon^u_s(\phi_j)\||u(s)|\mathrm{d}s \\ &\quad + \int_0^t \|(\pi_3 X^u_{(N)}(t,s) - X^u_{(N)}(t,s)\pi_3)\|\|B\||u(s)|\mathrm{d}s \\ &\leq \left(\int_0^T |u(t)|\mathrm{d}t\right)(\|\pi_3 B(\mathrm{Id} - \pi_N)\| \\ &\quad + 2\|B\| \sup_t \|\pi_3 X^u_{(N)}(t,0) - X^u_{(N)}(t,0)\pi_3)\|). \end{aligned} \tag{8}$$

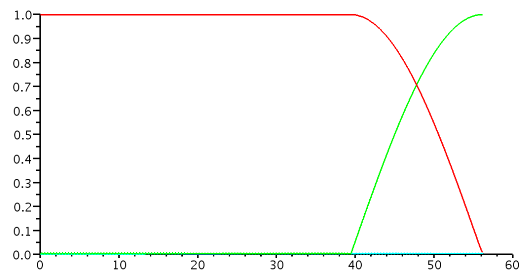

Fig. 3. Time evolution of the moduli of the first three coordinates of $\Upsilon^u_t \phi_3$ in the case of the perturbed harmonic oscillator. First coordinate in blue, second coordinate in green, third coordinate in red. Time scale is 1:100.

By skew-adjointness, $\|\pi_3 B(\mathrm{Id}-\pi_N)\| = \|(\mathrm{Id}-\pi_N)B\pi_3\|$. This last quantity tends to zero, and we are able to give estimates of the convergence rate. Indeed,

$$\begin{aligned}\|(\mathrm{Id}-\pi_N)B\phi_1\|^2 &\leq \sum_{k>N}\left|\frac{2k}{(k-1)^2(1+k)^2}\right|^2\\ &\leq 4\sum_{k>N}\frac{1}{(k-1)^6}\\ &\leq \frac{1}{(N-2)^5}.\end{aligned}$$

Similarly,

$$\begin{aligned}\|(\mathrm{Id}-\pi_N)B\phi_2\|^2 &\leq \frac{\sqrt{2}}{(N-3)^5}\\ \|(\mathrm{Id}-\pi_N)B\phi_3\|^2 &\leq \frac{2}{(N-4)^5}.\end{aligned}$$

The procedure to induce a given transformation, up to a given tolerance $\varepsilon > 0$, on the space $\mathrm{span}\{\phi_1,\phi_2,\phi_3\}$ is the following:

1) Use estimates given in [9] to give an a priori upper bound K on the L^1-norm of the control.
2) From K and ε, find N such that $K\|\pi_3 B(\mathrm{Id}-\pi_N)\| \leq \varepsilon/2$.
3) In the finite dimensional space $\mathrm{span}\{\phi_1,\ldots,\phi_N\}$, consider the bilinear system $\dot{x} = (A^{(N)} + uB^{(N)})x$ and find a control u achieving the desired transition up to $\varepsilon/(2K)$ and such that $\|u\|_{L^1} \leq K$. This can be done using standard averaging procedures (see for instance [18]).
4) Use (8) to get an upper bound of the distance of the trajectories of (Σ_N) and the actual infinite dimensional system.

C. Numerical simulations

We illustrate the above procedure on an example. Fix $\varepsilon = 7\ 10^{-2}$. We would like to find $u : [0,T] \to \mathbf{R}$ such that $|\langle\phi_3, \Upsilon^u_T\phi_1\rangle| > 1-\varepsilon$, $|\langle\phi_1, \Upsilon^u_T\phi_2\rangle| > 1-\varepsilon$ and $|\langle\phi_2, \Upsilon^u_T\phi_3\rangle| > 1-\varepsilon$ at final time T. For this example, we are not interested in the respective phases but the method can easily be generalized to address this point (see Section IV-D below).

From [9], the transition can be achieved with controls of L^1-norm smaller than $5\pi/4(9/8+25/24)$. Using controls with better efficiencies (as described in [11]), we can use controls with L^1-norm smaller than $2(9/8+25/4) = 13/3$.

Using the above estimates, one sees that if $N = 20$, then

$$K\|\pi_3 B(\mathrm{Id}-\pi_N)\| \leq \frac{13}{3}\frac{\sqrt{2}}{(N-4)^{5/2}} \leq 6\ 10^{-3}.$$

Finally, we set $T = 138$ and we define u by

$$u(t) = \begin{cases}\cos(3t)/20, & t\in[0,72]\\ \cos(5t)/20, & t\in(72,138].\end{cases} \tag{9}$$

Notice that $\int_0^T |u(t)|\mathrm{d}t \leq 13/3$. One checks numerically that $\|\pi_3 X^u_{(20)}(t,0) - X^u_{(20)}(t,0)\pi_3\| \leq 1.3\ 10^{-3}$ for $t \leq 138$.

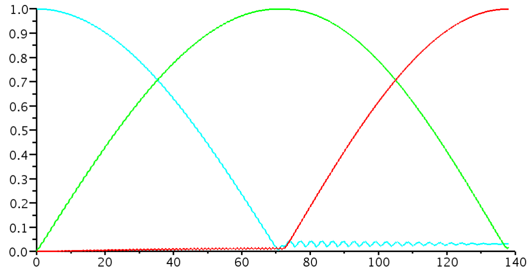

Fig. 4. Time evolution of the moduli of the first three coordinates of $\Upsilon^u_t\phi_1$ in the case of the potential well. First coordinate in blue, second coordinate in green, third coordinate in red.

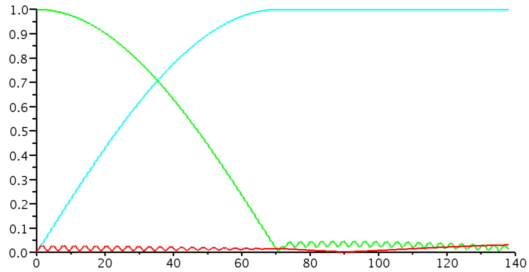

Fig. 5. Time evolution of the moduli of the first three coordinates of $\Upsilon^u_t\phi_2$ in the case of the potential well. First coordinate in blue, second coordinate in green, third coordinate in red.

From (7), we get, for every $t, s \leq T$

$$\|\pi_3 X^u_{(N)}(t,s) - X^u_{(N)}(t,s)\pi_3\| \leq 2.6\ 10^{-3}.$$

From (8), we have, for $j = 1,2,3$,

$$\begin{aligned}\|\pi_3\Upsilon^u_t(\phi_j) - \pi_3 X^u_{(N)}(t,0)\phi_j\| &\leq \frac{13}{3}(6\ 10^{-3} + 8.2\ 10^{-3})\\ &\leq 6.1\ 10^{-2}.\end{aligned}$$

Conclusion follows from the numerical computations

$$\begin{aligned}|\langle\phi_3, X^u_{(20)}(T,0)\phi_1\rangle| &\approx 0.99924\\ |\langle\phi_1, X^u_{(20)}(T,0)\phi_2\rangle| &\approx 0.99943\\ |\langle\phi_2, X^u_{(20)}(T,0)\phi_3\rangle| &\approx 0.99949.\end{aligned}$$

In particular, note that the accuracy in the controllability process is significantly higher than the a priori estimates.

The evolutions with respect to the time of the moduli of the first coordinates of $X^u_{(20)}\phi_k$ for $k = 1,2,3$ are represented in Figures 4, 5, and 6.

All the computations were done using the free software NSP, see [17]. The source code for the simulation is available at [2]. The total computation time is less than 4 minutes on a standard desktop computer.

D. Possible improvements

If one is interested not only in the modulus but also in the respective phases of the final points, it is enough to replace the functions $t \mapsto \cos(3t)/20$ and $t \mapsto \cos(5t)/20$ in (9) by

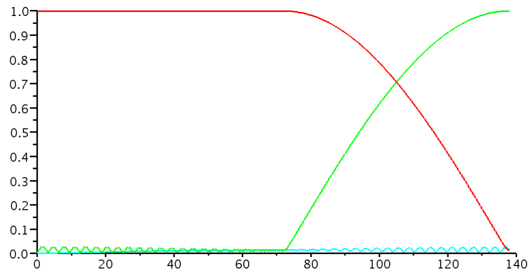

Fig. 6. Time evolution of the moduli of the first three coordinates of $\Upsilon_t^u \phi_3$ in the case of the potential well. First coordinate in blue, second coordinate in green, third coordinate in red.

$t \mapsto \cos(3t + \theta_1)/20$ and $t \mapsto \cos(5t + \theta_2)/20$ respectively, where θ_1 and θ_2 are suitable phases.

In order to get higher accuracy in the approximation (i.e. a smaller ε), it is enough to replace the functions $t \mapsto \cos(3t)/20$ and $t \mapsto \cos(5t)/20$ above by the functions $t \mapsto \cos(3t)/L$ and $t \mapsto \cos(5t)/L$ with L large enough. The price to pay for a higher precision is the increasing of the time needed for the transfer.

V. Conclusion and future works

We have shown how it was possible to implement a quantum gate consisting in a permutation of the first eigenstates on two types of infinite dimensional quantum oscillators. Our method provides rigorous estimates and permits numerical simulations that can be run on standard desktop computers.

A limitation of our models is that the Schrödinger equation neglects decoherence. This approximation may be justified for time small with respect to the relaxation time of the quantum system. Future works may focus on the optimization of the time of implementation.

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