Which notion of energy for bilinear quantum systems? ⋆

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Abstract: In this note we investigate what is the best L^p-norm in order to describe the relation between the evolution of the state of a bilinear quantum system with the L^p-norm of the external field. Although L^2 has a structure more easy to handle, the L^1 norm is more suitable for this purpose. Indeed for every $p > 1$ it is possible to steer, with arbitrary precision, a generic bilinear quantum system from any eigenstate of the free Hamiltonian to any other with a control of arbitrary small L^p norm. Explicit optimal costs for the L^1 norm are computed on an example.

Keywords: Bilinear systems, quantum systems, distributed parameters systems, optimal control, averaging control.

1. INTRODUCTION

1.1 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 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

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

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.

1.2 Energy for a quantum system

Physically, the energy of a quantum system (1) with wave function ψ is $E(\psi) = \int_\Omega \left[(-\Delta + V)\overline{\psi}\right] \psi \, \mathrm{d}\mu$. The 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 $\psi(t)$. Therefore a natural question is to find an *a priori* relation between the time evolution of the energy of system (1) and properties of the external field represented by u. In particular we address the problem of finding a bound on the energy after the action of an external field. Namely, given an initial condition ψ_0 and a control $u : [0, T] \to \mathbf{R}$ denoting with ψ the solution of (1) with $\psi(0) = \psi_0$ we look for bounds on the energy $E(T)$ in terms of the L^p norm of u

$$\|u\|_{L^p(0,T)} = \left(\int_0^T |u(t)|^p \mathrm{d}t\right)^{\frac{1}{p}},$$

(for some suitable $p > 0$) without computing explicitly the solution $t \in [0, T] \mapsto \psi(t)$.

Many previous works adressed the problem of the optimal control of the system (1) for costs involving the L^2 norm of the control (see for instance Dahleh et al. (1990) or Grivopoulos and Bamieh (2008)). The main reason for the choice of the L^2 norm is the fact that the natural Hilbert structure of L^2 spaces allows to use the powerful tools of Hilbert optimization. It is sometimes believed that there is a natural relation of the L^2 norm of u and the energy of the systems. This note presents a priori bounds on the L^p-norm of the control and shows that, in general, the L^1-norm provides more informations on the evolution of the system than other L^p-norms for $p > 1$. Most of the

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material presented below is classical for finite dimensional conservative bilinear systems. The contribution of the present note is to treat in a rigorous and unified way the case of both finite and infinite dimensional systems.

1.3 Content of the paper

The first part of the paper, Section 2, presents some theoretical tool for bilinear quantum systems. The question of estimation of the energy is reformulated in terms of a problem of optimal control. Relations between the variation of energy of a quantum system and the L^1 norm of the external field are given in Section 3. Finally, explicit computations are presented on an example in Section 4.

2. INFINITE DIMENSIONAL QUANTUM SYSTEMS

2.1 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 (Boussaïd et al., 2011b, 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

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

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 $(-\mathrm{i}\lambda_k)_{k\in\mathbf{N}}$ associated with the sequence $(\phi_k)_{k\in\mathbf{N}}$ of eigenvectors, 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;
(3) for every j, k, $\langle\phi_j, B\phi_k\rangle$ is purely imaginary.

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

For every initial condition ψ_0 in H, for every $u \in L^1(\mathbf{R})$, one can define the solution $t \mapsto \Upsilon^u_t\psi_0$ of (3) as the fixed point solution

$$\Upsilon^u_t\psi_0 = e^{tA}\psi_0 + \int_0^t e^{(t-s)A}u(s)B\Upsilon^u_s\psi_0\,ds$$

see (Reed and Simon, 1980, Theorem). Actually there exists t_0 which only depends on $\|B\|$ and $\|u\|_{L^1}$ such that on can apply the Banach fixed point theorem. As the problem is translation invariant in time one can iterate the above fixed point existence result to obtain global existence.

We have the following continuity result.

Lemma 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, $(\Upsilon^{u_n}_t\psi_0)_{n\in\mathbf{N}}$ converges to $\Upsilon^u_t\psi_0$ as n tends to infinity.

Proof: The function $u \mapsto \Upsilon^u_t\psi_0$ is the limit of the sequence $X^t_n(u)$

$$\begin{cases} X^t_0(u) &= e^{tA}\psi_0 \\ X^t_{n+1}(u) &= e^{tA}\psi_0 + \displaystyle\int_0^t e^{(t-s)A}u(s)BX^s_n(u)\psi_0\,ds \end{cases}.$$

If the convergence is locally uniform for small time, as each of them is continuous with respect to the convergence in law of the distribution associated to the controls u, this concludes the proof. Indeed usual approximation result provides that $\int_0^t u_n(\tau)\mathrm{d}\tau$ converges to $\int_0^t u(\tau)\mathrm{d}\tau$ as n tends to infinity for every t in $\mathbf{R}$ if and only if $\int u_n(\tau)f(\tau)\mathrm{d}\tau$ converges to $\int u(\tau)f(\tau)\mathrm{d}\tau$ as n tends to infinity for every f bounded and continuous. □

2.2 Controllability results

Considerable efforts have been made to study the controllability of (1). It is known, see Turinici (2000), that exact controllability of (1) in H is hopeless in general. With the exception of some very particular examples where Ω is one dimensional, as in Beauchard and Laurent (2010), no description of the attainable set is known. We then consider the notion of approximate controllability.

Definition 2. Let (A, B) satisfy Assumption 1. The system (A, B) is *approximately controllable* if, for every ψ_0, ψ_1 in the unit Hilbert sphere, for every $\varepsilon > 0$, there exists $u_\varepsilon : [0, T_\varepsilon] \to \mathbf{R}$ such that $\|\Upsilon^{u_\varepsilon}_{T_\varepsilon}\psi_0 - \psi_1\| < \varepsilon$.

Various methods have been used to give criterion of approximate controllability of system (1). Nersesyan (2010), Beauchard and Mirrahimi (2009) and Mirrahimi (2009) rely on a Lyapunov approach. Boscain et al. (2012) adopt a more geometrical point of view, centered on the notion of non-degenerate (or non-resonant) transitions.

Definition 3. Let (A, B) satisfy Assumption 1. A pair (j, k) of integers is a *non-degenerate transition* of (A, B) if

(*i*) $\langle\phi_j, B\phi_k\rangle \neq 0$;
(*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 4. Let (A, B) satisfy Assumption 1. A subset S of $\mathbf{N}^2$ is a *non-degenerate chain of connectedness* of (A, B) if

(*i*) for every (j, k) in S, (j, k) is a non-degenerate transition of (A, B)
(*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.

The following sufficient criterion for approximate controllability is the central result of Boscain et al. (2012).

Proposition 5. Let (A, B) satisfy Assumption 1. If (A, B) admits a non-degenerate chain of connectedness, then (A, B) is approximately controllable.

As proved by Mason and Sigalotti (2010) (see also Privat and Sigalotti (2010)), a system (A, B) satisfying Assumption 1 generically admits a non-degenerate chain of connectedness. Hence, approximate controllability is a generic property for systems of the type (3) (see also Nersesyan (2010)).

In Boscain et al. (2012) an extensive (and in some case implicit) use of averaging results has been made. The following result is a generalization of the Rotating Wave Approximation to infinite dimensional systems and can be found in Chambrion (2011).

Proposition 6. Let (A,B) satisfy Assumption 1 and (j,k) be a non-degenerate transition of (A,B). Define $T = 2\pi/|\lambda_j - \lambda_k|$ and $\mathcal{N} = \{(l,m) \in \mathbf{N}^2 | \langle \phi_l, B\phi_m\rangle \neq 0$ and $|\lambda_l - \lambda_m| \in (\mathbf{N}\setminus\{1\})|\lambda_j-\lambda_k|$ and $\{j,k\}\cap\{l,m\}\neq\emptyset\}$. Consider a T-periodic function $u^*:\mathbf{R}\to\mathbf{R}$ satisfying $\int_0^T u^*(t)e^{\mathrm{i}(\lambda_j-\lambda_k)t}\mathrm{d}t \neq 0$ and $\int_0^T u^*(t)e^{\mathrm{i}(\lambda_l-\lambda_m)t}\mathrm{d}t = 0$ for every (l,m) in $\mathcal{N}$ and let

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

Then there exist a sequence $(T_n^*)_{n\in\mathbf{N}}$ such that $T_n^* \in (nT^*-T, nT^*+T)$ and $|\langle \phi_k, \Upsilon^{u^*/n}_{T_n^*}\phi_j\rangle|$ tends to one as n tends to infinity.

2.3 Formulation of an optimal control problem

Let (A,B) satisfy Assumption 1 and admit a non-degenerate chain of connectedness. For every $r>0$, 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 $L^1([0,T_u])\cap L^r([0,T_u])$ 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 eigenstates only when $r=1$. Its proof is given in Section 3.

Proposition 7. $\mathcal{C}_1$ is a distance on the set $\{\phi_j, j\in\mathbf{N}\}$. For $r>1$, $\mathcal{C}_r$ is equal to zero on $\{(\phi_j,\phi_k), j,k\in\mathbf{N}\}$.

2.4 Weakly-coupled systems

Definition 8. Let k be a positive number and let (A,B) satisfy Assumption 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 $c_{(A,B)}$ such that, for every ψ in $D(|A|^k)$, $|\Re\langle |A|^k\psi, B\psi\rangle| \leq c_{(A,B)}|\langle |A|^k\psi,\psi\rangle|$.

The notion of weakly-coupled systems is closely related to the growth of the $|A|^{k/2}$-norm $\langle |A|^k\psi,\psi\rangle$. For $k=1$, this quantity is the expected value of the energy of the system.

Proposition 9. (Boussaïd et al., 2011b, Proposition 2) Let (A,B) be k-weakly-coupled. Then, for every $\psi_0 \in D(|A|^{k/2})$, $K>0$, $T\geq 0$, and u in $L^1([0,\infty))$ for which $\|u\|_{L^1}<K$, one has $\|\Upsilon^u_T(\psi_0)\|_{k/2} \leq e^{c(A,B)K}\|\psi_0\|_{k/2}$.

For every N in $\mathbf{N}$, we define $\mathcal{L}_N$ the linear space spanned by $\phi_1,\phi_2,\dots,\phi_N$ and $\pi_N : H\to H$, the orthogonal projection onto $\mathcal{L}_N$

$$\pi_N(\psi) = \sum_{k=1}^{N}\langle\phi_k,\psi\rangle\phi_k.$$

The compressions of order N of A and B are the finite rank operators $A^{(N)} = \pi_N A_{\restriction \mathcal{L}_N}$ and $B^{(N)} = \pi_N B_{\restriction\mathcal{L}_N}$. The Galerkin approximation of (3) at order N is the infinite dimensional system

$$\frac{\mathrm{d}}{\mathrm{d}t}x = A^{(N)}x + u(t)B^{(N)}x. \tag{4}$$

Since $\mathcal{L}_N$ is invariant by (4), one may also consider (4) as a finite-dimensional system, whose propagator is denoted by $X^u_{(N)}(t,s)$.

Proposition 10. (Boussaïd et al., 2011b, Proposition 4) Let k and s be non-negative numbers with $0\leq s<k$. Let (A,B) 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

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

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

Remark 1. An interesting feature of Propositions 9 and 10 is the fact that the bound of the $|A|^{k/2}$ norm of the solution of (3) or the bound on the error between the infinite dimensional system and its finite dimensional approximation only depends on the L^1 norm of the control, not on the time.

3. PROOF OF PROPOSITION 7

3.1 Lower bounds for the L^1 norm

Proposition 11. Let (A,B) satisfy Assumption 1. For every j,k in $\mathbf{N}$ such that $B\phi_j\neq 0$, for every locally integrable $u:[0,T]\to\mathbf{R}$,

$$\|u\|_{L^1(0,T)} \geq \frac{\big||\langle\phi_j,\phi_k\rangle| - |\langle\phi_j,\Upsilon^u_T\phi_k\rangle|\big|}{\|B\phi_j\|}.$$

Proof: Let j,k in $\mathbf{N}$. For every locally integrable $u:[0,T]\to\mathbf{R}$, define $y : u\mapsto e^{-At}\Upsilon^u_t\phi_k$. For almost every t, y is differentiable with respect to t and $\frac{\mathrm{d}y}{\mathrm{d}t} = u(t)e^{-At}Be^{At}y$. In particular,

$$\left|\left\langle \phi_j, \frac{\mathrm{d}y}{\mathrm{d}t}\right\rangle\right| \leq |u(t)|\|B\phi_j\|.$$

This concludes the proof of Proposition 11. □

A consequence of Proposition 11 is that $\mathcal{C}_1(\phi_j,\phi_k)$ is bounded away from zero as soon as $j\neq k$.

3.2 Upper bound for the L^1 norm

In order to give an upper bound for $\mathcal{C}_1(\phi_j,\phi_k)$ when (j,k) is a non-degenerate transition of (A,B), we come back to Proposition 6. In the case where $\mathcal{N}$ is finite, Boscain et al. (2012) give an explicit construction of a piecewise constant u^* with value in $[0,1]$ and satisfying the assumptions of Proposition 6 such that, for every n in $\mathbf{N}$,

$$\left\|\frac{u^*}{n}\right\|_{L^1(0,T_n^*)} \leq \frac{5\pi}{4|\langle\phi_j,B\phi_k\rangle|}.$$

More details about the choice of u^* when (A,B) is weakly-coupled are given by (Boussaïd et al., 2011a, Section III-C). Let us just mention that the choice $u^*: t\mapsto \cos(|\lambda_j - \lambda|t)$ guarantees

$$\left\|\frac{u^*}{n}\right\|_{L^1(0,T_n^*)} \leq \frac{2}{|\langle\phi_j,B\phi_k\rangle|}$$

for every n in $\mathbf{N}$.

In any case, (A,B) being weakly-coupled or not, this guarantees that, for every j,k in $\mathbf{N}$, $\mathcal{C}_1(\phi_j,\phi_k)<+\infty$ as long as (j,k) is a non degenerate chain of connectedness.

3.3 Symmetry of $\mathcal{C}_1$

The fact that $\mathcal{C}_1$ is symmetric is a consequence of the so-called time reversibility of (3). Let $T>0$, $x_0\in H$, $u\in L^1([0,T],\mathbf{R})$. We define $x:[0,T]\to H$ by $x(t)=\Upsilon^u_t x_0$, $v:t\mapsto u(T-t)$ and $y:[0,T]\to H$ the solution of $y'=-(A+v(t)B)y$ such that $y(0)=x(T)$ and $z:[0,T]\to H$ by $z(t)=y(T-t)$ for every $0\le t\le T$. The mapping z is differentiable almost everywhere and, for almost every t, $z'(t)=(A+u(t)B)z(t)$. Since $z(T)=x(T)$, one has $y(T)=z(0)=x(0)$.

This proves that the L^1 cost needed to steer $x(0)$ to $x(T)$ with the system (A,B) is less or equal to the L^1 cost needed to steer $x(T)$ to $x(0)$ with the system $(-A,-B)$.

In the basis $(\phi_k)_{k\in\mathbf{N}}$, the infinite dimensional matrices of A and B have purely imaginary entries. Hence, if y satisfies $y'=-(A+uB)y$, then $s:t\mapsto\sum_k\overline{\langle\phi_k,y(t)\rangle}\phi_k$ satisfies $s'=(A+uB)s$. If $y(0)=\phi_k$, then $s(0)=y(0)$ since all the coordinates of $y(0)$ in the basis $(\phi_k)_{k\in\mathbf{N}}$ are real. The same holds for $y(T)=s(T)$ is $y(T)=\phi_j$. In other words, the L^1 cost needed to steer ϕ_j to ϕ_k with the system (A,B) is less or equal to the L^1 cost needed to steer ϕ_k to ϕ_j with the system (A,B), and $\mathcal{C}_1$ is symmetric.

3.4 L^r norms with $r>1$

Proposition 12. Let (A,B) satisfy Assumption 1 and admit a non-degenerate chain of connectedness. If $r>1$, then, for every j,k in $\mathbf{N}$, $\mathcal{C}_r(\phi_j,\phi_k)=0$.

Proof: It is enough to consider (j,k) in a non-degenerate chain of connectedness of (A,B). The result is then a consequence of Proposition 6, since, for every n in $\mathbf{N}$,

$$\begin{aligned}\left\|\frac{u^*}{n}\right\|^r_{L^r(0,T^*_n)}&=\frac{1}{n^r}\int_0^{T^*_n}|u^*(t)|^r\mathrm{d}t\\&\le\frac{1}{n^r}\int_0^{nT^*+T}|u^*(t)|^r\mathrm{d}t\\&\le\frac{1}{n^r}\int_0^{(n\lceil\frac{T^*}{T}\rceil+1)T}|u^*(t)|^r\mathrm{d}t\\&\le\frac{n}{n^r}\left(\frac{T^*}{T}+2\right)\int_0^T|u^*(t)|^r\mathrm{d}t,\end{aligned}$$

which tends to zero as n tends to infinity. □

4. 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, Salomon and Turinici (2005); Boscain et al. (2009, 2012)).

4.1 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

$$\mathrm{i}\frac{\partial\psi}{\partial t}(t,\theta)=-\Delta\psi(t,\theta)+u(t)\cos(\theta)\psi(t,\theta),\qquad(5)$$

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 invariant under the dynamics of (5), hence no global controllability is to be expected in H.

We 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 with 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 (Boussaïd et al., 2011b, Section III.C)).

The Galerkin approximations of A and B of order N are $A^{(N)}=-\mathrm{i}\,\mathrm{diag}(1,2^2,\ldots,N^2)$ and

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

4.2 Computation of $\mathcal{C}_1(\phi_1,\phi_2)$

Our aim is to compute the minimal L^1 norm needed to approximately transfer the wave function from the first eigenspace to the second one. Precisely, we will prove

Proposition 13. $\mathcal{C}_1(\phi_1,\phi_2)=\pi$.

Proof: The transition $(1,2)$ is non-degenerate. Proposition 6 applies with $\mathcal{N}=\emptyset$. For every η in $(0,1)$, we define u^η, the $2\pi/3$ periodic function defined by

$$\begin{cases}u^\eta(x)=1&\text{for }\ 0<x<\eta\\u^\eta(x)=0&\text{for }\ \eta\le x\le 2\pi/3.\end{cases}$$

Proposition 6 states that, defining $T^*=\dfrac{\pi^2}{\left|\sin\left(\frac{3\eta}{2}\right)\right|}$, there exists a sequence $(T^*_n)_{n\in\mathbf{N}}$ such that $T^*_n\in(nT^*-2\pi/3,nT^*+2\pi/3)$ and $|\langle\phi_2,\Upsilon^{u^\eta/n}_{T^*_n}\phi_1\rangle|$ tends to one as n tends to infinity.

One computes, for every n in $\mathbf{N}$,

$$\left\|\frac{u^\eta}{n}\right\|_{L^1(0,T^*_n)}\le\frac{\eta}{\left|\sin\left(\frac{3\eta}{2}\right)\right|}\frac{3\pi}{2}.$$

This last quantity tends to π as η tends to zero. This proves that $\mathcal{C}_1(\phi_1,\phi_2) \le \pi$.

For every locally integrable control u, we define $y_1 : t \mapsto \langle \phi_1, \Upsilon^u_t \phi_1\rangle$ and $y_2 : t \mapsto \langle \phi_2, \Upsilon^u_t \phi_1\rangle$. The function $t \mapsto |y_1(t)|^2$ is absolutely continuous, and, for almost every t,

$$\frac{\mathrm{d}}{\mathrm{d}t}|y_1(t)|^2 = 2\Re(y_1'(t)\bar{y}_1(t)) = u(t)\Re(y_2(t)\bar{y}_1(t)).$$

Hence,

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}|y_1(t)|^2\right| \le |y_2(t)||y_1(t)||u(t)|,$$

or

$$-|u(t)| \le \frac{\frac{\mathrm{d}}{\mathrm{d}t}|y_1(t)|^2}{\sqrt{|y_1|^2}\sqrt{1-|y_1(t)|^2}} \le |u(t)|$$

Integrating between 0 and T, one gets

$$2\left|\arctan\left(\sqrt{\frac{1}{|y_1(T)|^2}-1}\right)\right| \le \|u\|_{L^1(0,T)},$$

and, provided $\|u\|_{L^1(0,T)} < \pi$,

$$\sqrt{\frac{1}{|y_1(T)|^2}-1} \le \tan\left(\frac{\|u\|_{L^1(0,T)}}{2}\right).$$

Finally, $|y_1(T)| \ge \cos\left(\frac{\|u\|_{L^1(0,T)}}{2}\right)$ and

$$|y_2(T)| \le \sqrt{1-|y_1(t)|^2} \le \sin\left(\frac{\|u\|_{L^1(0,T)}}{2}\right).$$

If $(u_n)_{n\in\mathbf{N}}$ is a sequence of locally integrable functions and $(T_n)_{n\in\mathbf{N}}$ is a sequence of positive numbers such that $|\langle \phi_2, \Upsilon^{u_n}_{T_n}\phi_1\rangle|$ tends to one, then $\liminf_n \|u_n\|_{L^1(0,T_n)} \ge \pi$, hence $\mathcal{C}_1(\phi_1,\phi_2) \ge \pi$. This concludes the proof of Proposition 13. $\square$

5. CONCLUSION AND PERSPECTIVES

5.1 Conclusion

We introduced a variational principle associated with a bilinear quantum system. For $p \ge 1$, we gave some estimate of the L^p norm of the control needed to steer the system from an eigenstate of the free Hamiltonian to another. In particular, for generic bilinear quantum systems, it is possible to steer any eigenstate of the free Hamiltonian to any neighborhood of any other eigenstate with arbitrary small L^2 norm of the control.

5.2 Future works

The estimates given for the L^1 norm only depend on the control potential B (and not on the eigenvalues of the free Hamiltonian A as long as the transition stay non-degenerate). It is possible that L^p costs, with $p < 1$, are physically more relevant. A new approach would be needed to study this case since our methods do not provide any information about the L^p norm of the control needed to steer an energy level to another in the case $p < 1$.

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