Finite dimensional techniques for control of bilinear Schrödinger equations

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Quantum systems

The state of a quantum system evolving in a space (Ω, μ) can be represented by its *wave function* ψ. Under suitable hypotheses, the dynamics for ψ is given by the Schrödinger equation :

$$i\frac{\partial \psi}{\partial t}(x,t) = -\Delta\psi(x,t) + V(x)\psi(x,t)$$

Ω : finite dimensional manifold, for instance a bounded domain of $\mathbf{R^d}$, or $\mathbf{R^d}$, or $SO(3)$,...
$\psi \in L^2(\Omega, \mathbf{C})$: wave function (state of the system)

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The well-posedness is far from obvious. In a first time, we will assume that there exists a unique weak solution $t \mapsto \Upsilon^u_t \psi_0$ with initial condition ψ_0.

Controllability

Exact controllability

ψ_a, ψ_b given. Is it possible to find a control $u : [0, T] \to \mathbf{R}$ such that $\Upsilon^u_T(\psi_a) = \psi_b$?

Approximate controllability

$\epsilon > 0$, ψ_a, ψ_b given. Is it possible to find a control $u : [0, T] \to \mathbf{R}$ such that $\|\Upsilon^u_T(\psi_a) - \psi_b\| < \epsilon$?

Simultaneous approximate controllability

Let $\epsilon > 0$, $\psi_1, \psi_2, \ldots, \psi_p$ in H and $\Psi \in \mathbf{U}(H)$ be given. Is it possible to find a control $u : [0, T] \to \mathbf{R}$ such that $\|\Upsilon^u_T(\psi_j) - \Psi\psi_j\| < \epsilon$ for every $j \leq p$?

A negative result

Theorem (Ball-Marsden-Slemrod, 1982 and Turinici, 2000)

If $\psi \mapsto W\psi$ is bounded, then the reachable set from any point (with L^{1+r} controls) of the control system :

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

has dense complement in the unit sphere.

Non controllability of the harmonic oscillator (I)

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

with $\psi \in L^2(\mathbf{R}, \mathbf{C})$.

Theorem (Mirrahimi-Rouchon, 2004)

The quantum harmonic oscillator is not controllable.

(see also Illner-Lange-Teismann 2005 and Bloch-Brockett-Rangan 2006)

Non controllability of the harmonic oscillator (II)

The Galerkin approximation of order n is controllable (in $U(n)$) :

$$A = -\frac{i}{2}\begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 3 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 2n+1 \end{pmatrix}$$

$$B = -i\begin{pmatrix} 0 & 1 & 0 & \cdots & \cdots & 0 \\ 1 & 0 & \sqrt{2} & \ddots & & \vdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & 0 & \sqrt{n+1} \\ 0 & \cdots & \cdots & 0 & \sqrt{n+1} & 0 \end{pmatrix}$$

Exact controllability for the potential well

$\Omega = (-1/2, 1/2)$

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

Theorem (Beauchard-Coron, 2005)

The system is exactly controllable in the intersection of the unit sphere of L^2 with $H^7_{(0)}$.

Lyapounov techniques

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

Ω is a bounded domain of $\mathbf{R^d}$, with smooth boundary.

Theorem (Nersesyan, 2009)

If

- $\int_\Omega \overline{\phi_1} W \phi_j \neq 0$ *for every* $j \geq 1$ *and*
- $|\lambda_1 - \lambda_j| \neq |\lambda_k - \lambda_l|$ *for every* $j > 1$, $\{1, j\} \neq \{k, l\}$

then the control system is approximately controllable on the unit sphere for H^s norms.

Fixed point theorem

$\Omega = (0,1)$

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

Theorem (Beauchard-Laurent, 2009)

If there exists $C > 0$ such that for every $j \in \mathbf{N}$,

$$|b_{1,j}| > \frac{C}{j^3}$$

then the system is exactly controllable in the intersection of the unit sphere with $H^3_{(0)}$.

Finite dimensional case

If $H = \mathbf{C}^n$, then

$$\dot{x} = (A + u(t)B)x \qquad (\Sigma)$$

can be lifted in $U(n)$ (the set of unitary matrices).

Theorem

(Σ) is exactly controllable in $U(n)$ if and only of $\mathrm{Lie}(A, B) = \mathfrak{u}(n) = \{M | \bar{M}^T = -M\}$.

Theorem

If (Σ) is controllable in $U(n)$, the time diameter of $U(n)$ for (Σ) with L^∞ controls is non zero and finite.

Abstract form (rough version)

$$\frac{d\psi}{dt} = A(\psi) + uB(\psi), \qquad u \in U \qquad (A, B, U)$$

with the assumptions

- H complex Hilbert space ;
- $U \subset \mathbf{R}$;

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- A, B skew-adjoint operators on H (not necessarily bounded) ;
- $(\phi_n)_{n\in\mathbf{N}}$ orthonormal basis of H made from eigenvectors of A ;
- $\phi_n \in D(B)$ for every $n \in \mathbf{N}$.

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Under these assumptions

$\forall u \in U, \exists\ e^{t(A+uB)} : H \to H$ group of unitary transformations

Definition of solutions

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

We choose piecewise constant controls

Definition

We call $\Upsilon^u_T(\psi_0) = e^{t_k(A+u_kB)} \circ \cdots \circ e^{t_1(A+u_1B)}(\psi_0)$ *the solution of the system starting from* ψ_0 *associated to the piecewise constant control* $u_1\chi_{[0,t_1]} + u_2\chi_{[t_1,t_1+t_2]} + \cdots$.

Generic controllability results via geometric methods

Definition

$S \subset \mathbf{N}^2$ is a non resonant chain of connectedness of (A, B) if

- *for every $j \leq k$ in $\mathbf{N}$, there exists a sequence $(s_1^1, s_2^1), \ldots, (s_1^p, s_2^p)$ in $S \cap \{1, \ldots, k\}$ such that $s_1^1 = j, s_2^p = k$, $s_2^l = s_1^{l+1}$;*
- *$b_{s_1, s_2} \neq 0$ for every $(s_1, s_2) \in S$*
- *for every (j, k) in $\mathbf{N}^2$, $(s_1, s_2) \in S$, $\{s_1, s_2\} \neq \{j, k\}$ and $|\lambda_{s_1} - \lambda_{s_2}| \neq |\lambda_j - \lambda_k| \Rightarrow b_{j,k} = 0$.*

Theorem (Boscain-Caponigro-Chambrion-Sigalotti, 2011)

If A has simple spectrum and (A, B) admits a non resonant chain of connectedness, then, for every $\delta > 0$, (A, B) is approximately simultaneously controllable by means of controls in $[0, \delta]$.

Non simple spectrum

The result applies also (in a slighty more technical form : there should be no internal coupling inside the degenerate eigenspaces) to operators with non simple spectrum.

$$A = \mathrm{i}\begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 3 \end{pmatrix} B = \mathrm{i}\begin{pmatrix} 0 & 1 & 1 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Estimates of the control

Define $\nu = \prod_{k=2}^{+\infty} \cos\left(\frac{\pi}{2k}\right) \approx 0.43.$

Theorem (Boscain-Caponigro-Chambrion-Sigalotti)

If A has simple spectrum and (A, B) admits a non resonant chain of connectedness containing $(1, 2)$, then, for every $\delta > 0$, for every $\epsilon > 0$, there exists a piecewise constant control $u : [0, T] \to [0, \delta]$ such that

$$\|\Upsilon^u_T(\phi_1) - \phi_2\| < \epsilon \text{ and } \|u\|_{L^1} \leq \frac{\pi}{2\nu|\langle \phi_1, B\phi_2\rangle|}$$

Notice that the bound of the L^1 norm of u does not depend on ϵ.

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1. A is skew adjoint with purely discrete spectrum $(\mathrm{i}\lambda_n)_{n\in\mathbf{N}}$;
2. the sequence $(\lambda_n)_{n\in\mathbf{N}}$ takes value in $(0,+\infty)$, is non-decreasing and its only accumulation point is $+\infty$;
3. there exists an Hilbert basis $(\phi_k)_{k\in\mathbf{N}}$ of H such that $A\phi_k = \lambda_k\phi_k$ for every k in $\mathbf{N}$;

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3. there exists an Hilbert basis $(\phi_k)_{k\in\mathbf{N}}$ of H such that $A\phi_k = \lambda_k \phi_k$ for every k in $\mathbf{N}$;
4. for every ψ in $D(A)$, ψ belongs to $D(B)$ and there exists $s_{A,B} < 1/2$ such that $\|B\psi\| \leq \|(\mathrm{i}A)^{s_{A,B}}\psi\|$;
5. for every u in $\mathbf{R}$, $A+uB$ is skew-adjoint, $D(A+uB) = D(A)$ and $D((A+uB)^2) = D(A^2)$;
6. For every interval I containing 0, for every Radon measure u on I, $t \mapsto \mathcal{A}(t) := e^{u([0,t))B} A e^{-u([0,t))B}$ is a family of skew-adjoint operators with common domain $\mathcal{D} = D(A)$ and $\mathcal{A}$ is continuous with bounded variation from I to $\mathcal{B}(\mathcal{D}, H)$;
7. For every Radon measure u, $\sup_{t\in I} \left\|\mathcal{A}(t)^{-1}\right\|_{B(H,D(A))} < +\infty$;

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7. For every Radon measure u, $\sup_{t\in I}\left\|\mathcal{A}(t)^{-1}\right\|_{B(H,D(A))}<+\infty$;
8. there exists $C_{A,B}>0$ such that $|\Im\langle A\psi,B\psi\rangle|\leq C_{A,B}|\langle A\psi,\psi\rangle|$ for every ψ in $D(A)$.

Examples

Most of the academic examples fits within this abstract framework.

- Rotation of a planar molecule, $\Omega = S^1$

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

- (with some work) Harmonic oscillator, $\Omega = \mathbf{R}$

$$\mathrm{i}\frac{\partial \psi}{\partial t} = -\Delta\psi + x^2\psi + u(t)x\psi$$

- Infinite square potential well, $\Omega = (-1, 1)$

$$\mathrm{i}\frac{\partial \psi}{\partial t} = -\Delta\psi + u(t)x\psi$$

Definition of solutions

With these hypotheses, $u \mapsto \Upsilon^u \psi_0$ is defined for every piecewise constant function u. The mapping $u \mapsto \Upsilon^u \psi_0$ admits a unique continuous extension to the set of Radon measures (that includes Dirac masses), endowed with the distance of total variation.

Recall that every L^1_{loc} function u can be associated to a Radon measure μ_u

$$\mu_u(I) = \int_I u(s)\mathrm{d}s = \int_I \mathrm{d}u.$$

Energy propagation

Remark (Boussaïd-Caponigro-TC)

For every $K > 0$, there exists C_K such that for every $T \geq 0$ and for every control u for which $\|u\|_{L^1} < K$, one has

$$|\langle A\Upsilon^u_T(\phi_1), \Upsilon^u_T(\phi_1)\rangle| < C_K.$$

Good Galerkyn approximation

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

Galerkyn approximation of order N, with associated propagator $t \mapsto X_t^{(N),u}$.

Theorem (Good Galerkin Approximation)

For every $\epsilon > 0$, $K \geq 0$, $n \in \mathbf{N}$, there exists $N \in \mathbf{N}$ such that for every $u \in L^1(0,\infty)$

$$\|u\|_{L^1} \leq K \implies \|\Upsilon_t^u(\phi_j) - X_t^{(N),u}\phi_j\| < \epsilon,$$

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

Periodic excitations

$(j,k) \in \mathbf{N}^2$ is uniquely resonant if $\langle \phi_j, B\phi_k \rangle \neq 0$ and

$$\{l,m\} \neq \{j,k\} \Rightarrow \frac{|\lambda_j - \lambda_k|}{|\lambda_l - \lambda_m|} \notin \mathbf{Z}$$

Theorem

Let $u^* : \mathbf{R}^+ \to \mathbf{R}$ be a locally integrable function. Assume that u^* is periodic with smallest period $T = \frac{2\pi}{|\lambda_j - \lambda_k|}$ for some uniquely resonant (j,k). If

$$\int_0^T u^*(\tau) e^{\mathrm{i}(\lambda_j - \lambda_k)\tau} \mathrm{d}\tau \neq 0,$$

then there exists $T^* > 0$ such that the sequence $\left(\left| \langle \phi_k, \Upsilon^{\frac{u^*}{n}}_{nT^*}(\phi_j) \rangle \right| \right)_{n \in \mathbf{N}}$ tends to 1 as n tends to infinity.

Time estimates

$$\lim_{n\to\infty}\left(\left|\langle\phi_k,\Upsilon^{\frac{u^*}{n}}_{nT^*}(\phi_j)\rangle\right|\right)_{n\in\mathbf{N}}=1$$

with

$$T^*=\frac{\pi T}{2|b_{j,k}|\left|\int_0^T u^*(\tau)e^{\mathrm{i}(\lambda_{l_1}-\lambda_{l_2})\tau}\mathrm{d}\tau\right|}$$

Efficiency

L^1 norm needed for the transfer :

$$\underbrace{\frac{\pi}{2|\langle \phi_j, B\phi_k\rangle|}}_{\substack{L^1\text{-norm for a}\\ \text{2 level system}}} \times \underbrace{\frac{\int_0^T |u^*(\tau)| \mathrm{d}\tau}{\left|\int_0^T u^*(\tau) e^{\mathrm{i}(\lambda_j - \lambda_k)\tau} \mathrm{d}\tau\right|}}_{\text{Efficiency}^{-1}}$$

Efficiency for the transition (j, k) :

$$0 \leq \frac{\left|\int_0^T u^*(\tau) e^{\mathrm{i}(\lambda_j - \lambda_k)\tau} \mathrm{d}\tau\right|}{\int_0^T |u^*(\tau)| \mathrm{d}\tau} \leq 1$$

The planar molecule

Let us consider a 2D-planar molecule submitted to a laser

$$i\frac{\partial \psi}{\partial t}(\theta, t) = -\frac{1}{2}\partial_\theta^2 \psi(\theta, t) + u(t)\cos(\theta)\psi(\theta, t) \qquad \theta \in \mathbf{R}/2\pi$$

- The parity of ψ cannot change $\Rightarrow$ no global controllability
- We first look at the odd part
- We try to steer the system from the first odd eigenstate to the second odd eigenstate

Galerkin approximation

$$A = i \begin{pmatrix} 1 & 0 & \dots & \\ 0 & 4 & 0 & \ddots \\ \vdots & \ddots & 9 & \ddots \\ & \vdots & \ddots & 16 \end{pmatrix} \quad B = i \begin{pmatrix} 0 & 1/2 & 0 & \dots \\ 1/2 & 0 & 1/2 & \ddots \\ 0 & 1/2 & 0 & 1/2 \\ \vdots & \ddots & 1/2 & 0 \end{pmatrix}$$

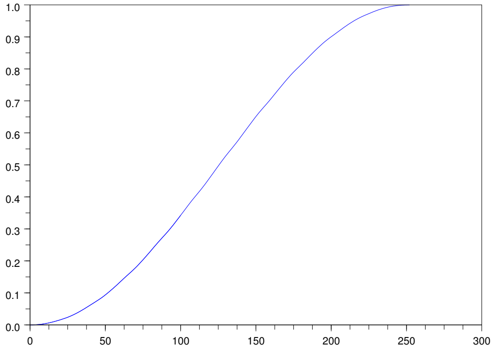
$\{(k, k \pm 1); k \in \mathbf{N}\}$ is a non-resonant chain of connectedness.
$9 - 4 = 5$ is not a multiple of $4 - 1 = 3$ (but $25 - 16 = 9$ is).

Numerical simulations

Good Galerkyn approximation

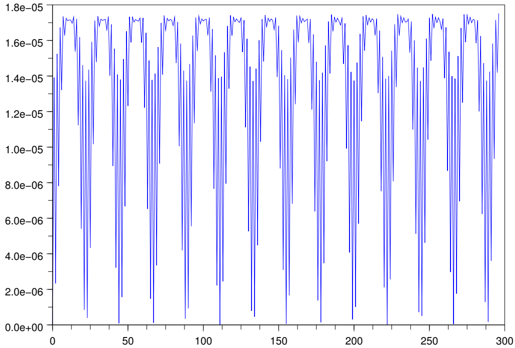
The error done when replacing the original system by its Galerkyn approximation of order 22 is smaller than $\epsilon = 10^{-7}$ when $\|u\|_{L_1} \leq 13/3$ and initial condition is ϕ_1.

Results (I)



Evolution 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 ($Eff_{1\to 2} \approx 88\%$).

Results (II)



Evolution 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 ($Eff_{1\to 2} = 0$).

Efficiencies

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%

Asymptotically, precision is $\sim \frac{K}{n}$. (Numerically, much better for small n.)

Even eigenstates

We consider next the Hilbert space of even functions on the torus.

$$A = i\begin{pmatrix} 0 & 0 & \dots & \\ 0 & 1 & 0 & \ddots \\ \vdots & \ddots & 4 & \ddots \\ & \vdots & \ddots & 9 \end{pmatrix} \quad B = i\begin{pmatrix} 0 & 1/\sqrt{2} & 0 & \dots \\ 1/\sqrt{2} & 0 & 1/2 & \ddots \\ 0 & 1/2 & 0 & 1/2 \\ \vdots & \ddots & 1/2 & 0 \end{pmatrix}$$

$\{(k, k \pm 1); k \in \mathbf{N}\}$ is a non-resonant chain of connectedness.
$4 - 1 = 3$ is a multiple of $1 - 0 = 1$.

Control via periodic excitations

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

We have to find a 1-periodic shape such that

- the efficiency for the transition $(1, 2)$ is as large as possible
- the efficiency for the transition $(2, 3)$ is zero

The control given explicitly by Boscain, Caponigro, TC, Sigalotti has efficiencies $\frac{\sqrt{3}}{2}$ and 0.

Multiple resonant transitions

To kill the transition $(2, 3)$, one had to multiply the efficiciency of the transition to be kept by $\cos(\pi/6)$.

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Remember ν ?

$$\nu = \prod_{k=2}^{+\infty} \cos\left(\frac{\pi}{2k}\right) \approx 0.43$$

Result

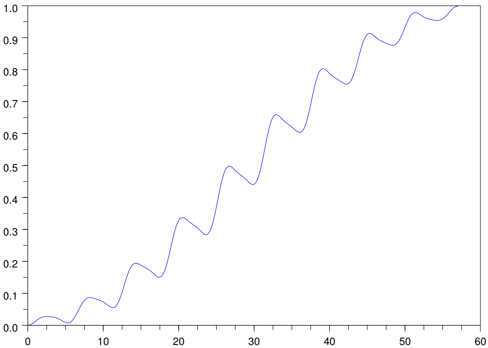

Figure: Modulus of the second coordinate with control $u^* : t \mapsto \frac{1}{20}\left(2\cos^2\left(\frac{t}{2}\right) + \cos^2\left(\frac{t-\pi/3}{2}\right) + \cos^2\left(\frac{t+\pi/3}{2}\right)\right)$. Theoretical efficiencies for transition $(1,2)$ and $(2,3)$ are $3/8 = 37.5\%$ and 0. Numerical efficiencies are 38% and 5.10^{-4}.

Concluding remarks

Geometric control theory provides effective methods

- to investigate various notions (including density matrices) of *approximate* controllability of a bilinear system with discrete spectrum ;
- to design efficient control ;
- to provide precise estimates for the analysis/simulations.

But it is unable (up to now)

- to provide *exact* controllability results of bilinear system with discrete spectrum ;
- to provide controllability results for the propagator.

Future directions

- Time estimates with large controls

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- Continuous spectrum

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- Time estimates with large controls
- Continuous spectrum
- Non linear equations

Questions

- Does it really make sense ? (allowable shapes, time scale, ...)
- What is the physical meaning of $\|u\|_{L_1} = \int |u|$?
- Do you know examples of bilinear systems with discrete spectrum ?