Geometric Methods in Quantum Control

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Quantum Control

Many technologies require the ability to induce a transition from a state to another of a quantum system:

- **Photochemistry** (to induce certain chemical reactions with light);
- **Magnetic Resonance** (in order to exploit spontaneous emission);
- **Realization of Quantum Computers** (to stock information).

To drive a quantum system from one state to another, by designing external fields:

- Lasers;
- X-Rays;
- Magnetic Fields.

Schrödinger equation

$$i\frac{d\psi}{dt} = (-\Delta + V)\psi$$

- $\Omega \subset \mathbb{R}^d$;
- $\psi = \psi(t,x)$ wave function, $\psi(t,\cdot) \in L^2(\Omega)$, $\|\psi(t,\cdot)\|_2 = 1$;
- $-\Delta + V$ Schrödinger operator;
- $V : \Omega \to \mathbb{R}$ uncontrolled potential;

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Controllability

Given ψ_0, ψ_1 of L^2-norm equal to one, find (if there exist) $k \in \mathbb{N}$, $t_1, \dots, t_k > 0$, $u_1, \dots, u_k \in U$ such that

$$\psi_1 = e^{-it_k(-\Delta+V+u_kW)} \circ \cdots \circ e^{-it_1(-\Delta+V+u_1W)}(\psi_0)$$

Examples

Quantum Harmonic oscillator

$$i\frac{\partial\psi(x,t)}{\partial t} = \left(-\frac{\partial^2}{\partial x^2} + x^2 + u(t)x\right)\psi(x,t), \quad x \in \mathbb{R},$$

Potential well

$$i\frac{\partial\psi(x,t)}{\partial t} = \left(-\frac{\partial^2}{\partial x^2} + u(t)x\right)\psi(x,t), \quad x \in (-1,1), \quad \psi(\pm 1,t) = 0.$$

Orientation of a linear bipolar molecule in the plane

$$i\frac{\partial\psi(\theta,t)}{\partial t} = \left(-\frac{\partial^2}{\partial \theta^2} + u(t)\cos(\theta)\right)\psi(\theta,t), \quad \theta \in \mathbb{S}^1$$

- θ rotational degree of freedom of a linear molecule,

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Negative results

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- L^2-approximate controllability by geometric methods
  (Chambrion-Mason-Sigalotti-Boscain [2009]).

Bilinear Schrödinger equation: abstract framework

Let $\mathcal{H}$ be a complex Hilbert space

$$\frac{d}{dt}\psi = A\psi + uB\psi, \quad u \in U. \tag{BSE}$$

We assume that:

- A has discrete spectrum $(i\lambda_k)_{k\in\mathbb{N}}$;
- $A + uB : \mathrm{span}\{\phi_k \mid k \in \mathbb{N}\} \to \mathcal{H}$ is essentially skew-adjoint (not necessarily bounded) for every $u \in U$;
- $\mathcal{H}$ has an Hilbert basis $\Phi = (\phi_k)_{k\in\mathbb{N}}$ made of eigenfunctions of A;
- $\phi_k \in D(B)$ for every $k \in \mathbb{N}$;
- $\langle \phi_j, B\phi_k \rangle = 0$ for $j \neq k$ and $\lambda_j = \lambda_k$.

Definitions

Definition: propagator and solution

$$\Upsilon_T^u(\psi_0) = e^{t_k(A+u_kB)} \circ \cdots \circ e^{t_1(A+u_1B)}(\psi_0)$$

is the **solution** of (BSE) with initial data $\psi_0 \in \mathcal{H}$ associated with the **piecewise constant** control $u = u_1\chi_{[0,t_1)} + u_2\chi_{[t_1,t_1+t_2)} + \cdots$
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Approximate controllability

Given $\varepsilon > 0$, $\psi_0, \psi_1 \in \mathcal{H}$ find $u : [0,T] \to U$ such that

$$\|\Upsilon_T^u(\psi_0) - \psi_1\| < \varepsilon.$$

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Approximate simultaneous controllability

Given $\varepsilon > 0$, $\psi^1, \dots, \psi^m \in \mathcal{H}$, $\hat{\Upsilon} \in \mathbf{U}(\mathcal{H})$ find $u : [0, T] \to U$ such that

$$\|\hat{\Upsilon}(\psi^j) - \Upsilon_T^u(\psi^j)\| < \varepsilon \qquad j = 1, \dots, m.$$

Chain of connectedness

$S \subset \mathbb{N}^2$ is a **connectedness chain** for (A, B) if

- $\langle \phi_\alpha, B\phi_\beta \rangle \neq 0$ for every $(\alpha, \beta) \in S$;
- for every $j \leq k \in \mathbb{N}$, there exist $(\alpha_1, \beta_1), \ldots, (\alpha_p, \beta_p)$ in S such that

$$j = \alpha_1, \quad \beta_1 = \alpha_2 \quad \ldots \quad \beta_{p-1} = \alpha_p, \quad \beta_p = k.$$

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Examples:

- Nersesyan [2009]: $S = \{(1, n) \; : \; n \in \mathbb{N}\}$,
- Chambrion et al. [2009]: $S = \{(n, n+1) \; : \; n \in \mathbb{N}\}$.

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A **connectedness chain** for (A, B), S is said to be **non-resonant** if

$$|\lambda_j - \lambda_k| \neq |\lambda_\ell - \lambda_m|$$

for every $(j, k) \in S$, $(\ell, m) \in \mathbb{N}^2$, $\{j, k\} \neq \{\ell, m\}$.

The result

Theorem (Boscain, C., Chambrion, Sigalotti, 2012)

If (A, B) has a non-resonant chain of connectedness, then (A, B) is approximately simultaneously controllable.

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If (A, B) has a non-resonant chain of connectedness containing (j, k), then for every $\varepsilon, \delta > 0$, there exists $u : [0, T] \to [0, \delta]$ such that

$$\|\Upsilon_T^u(\phi_j) - \phi_k\| < \varepsilon \quad \text{et} \quad \|u\|_{L^1} \leq \frac{\pi}{2\nu|\langle \phi_j, B\phi_k \rangle|}.$$

1^{st} step: finite dimensional Galerkin approximation

- Time reparametrization: since $e^{t(A+uB)} = e^{tu\left(\frac{1}{u}A+B\right)}$ then (BSE) become

$$\dot{X} = vAX + BX,$$

- Interaction framework: if $Y = e^{-\int vA}X$, then

$$\dot{Y} = e^{-\int vA}Be^{\int vA}Y$$

$$|\langle \phi_k, Y \rangle| = |\langle \phi_k, X \rangle|, \quad \text{for every } k \in \mathbb{N}$$

- Galerkin approximation: projecting the system on $\mathcal{L}_N = \operatorname{span}\{\phi_1, \ldots, \phi_N\}$ we have

$$\dot{Y} = \left(e^{i(\lambda_j-\lambda_k)\int v}b_{jk}\right)_{j,k=1}^{N} Y, \qquad Y \text{ in } \mathcal{L}_N.$$

2^{nd} step: convexification

We have to study the curve on the torus,

$$\Psi : \omega \mapsto \left(e^{i(\lambda_{j_1} - \lambda_{k_1})\omega}, \ldots, e^{i(\lambda_{j_m} - \lambda_{k_m})\omega} \right) .$$

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Let $\nu \geq \prod_{k=2}^{\infty} \cos\left(\frac{\pi}{2k}\right) = 0.4298...$ then

$$\overline{\mathrm{Conv}\,\Psi([0,\infty))} \supset \nu \mathbb{S}^1 \times \{0\} \times \cdots \times \{0\}.$$

We can realize the transition between the levels j_1 and k_1.

Example: $m = 2, \lambda_{j_1} - \lambda_{k_1} = 1, \lambda_{j_2} - \lambda_{k_2} = 2,$

$$\mathrm{Conv}\{\Psi(0), \Psi(\pi/2)\} = \left(\frac{1+i}{2}, 0 \right),$$

then

$$\mathrm{Conv}\,\Psi([0,\infty)) \supset \frac{\sqrt{2}}{2}\mathbb{S}^1 \times \{0\}, \qquad \text{and} \quad \frac{\sqrt{2}}{2} > \nu.$$

3^{rd} step: "strong" controllability in $SU(n)$

Thanks to the existence of the chain of connectedness

For every $N \in \mathbb{N}$ the control system

$$\dot{Y} = \left(e^{i(\lambda_j - \lambda_k)\int v} b_{jk}\right)_{j,k=1}^{N} Y, \quad Y \in \mathcal{L}_N,$$

is controllable.

We have more than that

For every N, n and $M(t) \in SU(n)$ we can track, with a tolerance of ε,

$$\left(\begin{array}{c|c|c} M(t) & 0_{n\times N-n} & R(t) \\ \hline 0_{N-n\times n} & 0_{N-n\times N-n} & \cdots \\ \hline \vdots & \vdots & \ddots \end{array}\right)$$

4^{th} and final step: Infinite dimension

The controllability on $SU(n)$ is not sufficient in general.

Counterexample:

Every Galerkin approximation of the quantum harmonic oscillator is controllable but the infinite dimensional system is not controllable.

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In conclusion:

- General controllability result
- Constructive
- With L^1 estimates on the control

Other results

- Approximate controllability with periodic functions (Chambrion 2012) :
  - easy (numerical and physical) implementation of simple transitions
  - no simultaneous controllability
- Approximate simultaneous controllability with Lie algebraic methods (Boscain, C, Sigalotti, 2013) :
  - applies to the multi-input case
  - no constructive proof

Weakly coupled systems

- $i(A + u_1 B_1 + \cdots u_p B_p)$ is bounded from below for every $u \in U$
- λ_j is non-decreasing and unbounded

k-weakly coupled

The system (A, B) is k-weakly coupled if

- $D(|A + uB|^{k/2}) = D(|A|^{k/2})$
- there exists C such that

$$|\Re\langle |A|^k \psi, B\psi\rangle| \leq C|\langle |A|^k \psi, \psi\rangle| \qquad \psi \in D(|A|^k)$$

Examples:

- B is relatively bounded wrt A.
- $iA = -\Delta + V$, $iB = W$ and $V, W \in C^{2k}(\Omega)$, Ω compact.

Growth of the $|A|^{k/2}$-norm

$$\|\psi\|_{k/2} = \||A|^{k/2}\psi\|^2 = |\langle |A|^k \psi, \psi\rangle| = \sum_{n\in\mathbb{N}} \lambda_n^k |\langle \phi_k, \psi\rangle|$$

We want to estimate the growth of the $|A|^{k/2}$-norm

$$\begin{aligned}\left|\frac{d}{dt}\langle |A|^k\psi, \psi\rangle\right| &\leq 2|u(t)||\Re\langle |A|^k\psi, B\psi\rangle| \\ &\leq 2C|u(t)||\langle |A|^k\psi, \psi\rangle|,\end{aligned}$$

by Gronwall's Lemma

$$\|\psi(t)\|_{k/2} \leq e^{2C\|u\|_{L^1}} \|\psi(0)\|_{k/2}.$$

- The regularity of the systems is an obstacle to the exact controllability.

Good Galerkin Approximation

Denote by $X_u^{(N)}$ the propagator of

$$\dot{x} = (A|_{\mathcal{L}_N} + uB|_{\mathcal{L}_N})x \quad x \in \mathcal{L}_N.$$

Theorem (Boussaïd, C, Chambrion, 2012)

Let (A, B) be k-weakly coupled and B be bounded relatively to $|A|^s$, $s < k$. For every $\varepsilon > 0$, $K > 0$, $\psi_0 \in D(|A|^{k/2})$, $s < k$ there exists $N = N(\varepsilon, K, \psi_0)$ such that

$$\|u\|_{L^1} \leq K \implies \|\Upsilon_t^u(\psi_0) - X_u^{(N)}(t)\psi_0\|_s < \varepsilon, \qquad t \geq 0.$$

- A priori estimates in numerical and physical simulations.
- Convergence of controllability strategies:
  - A bang-bang Theorem for weakly coupled systems (Boussaïd, C, Chambrion, 2012);
  - Approximate controllability in norm H^s (Boscain, C, Sigalotti, 2013).

Example: the rotating molecule

$$i\frac{\partial\psi}{\partial t}(\theta,t) = -\frac{1}{2}\partial_\theta^2\psi(\theta,t) + u(t)\cos(\theta)\psi(\theta,t) \quad \theta\in\mathbb{S}^1$$

- Eigenvalues: $0, i, 4i, 9i, \ldots, k^2 i, \ldots;$
- Control potential

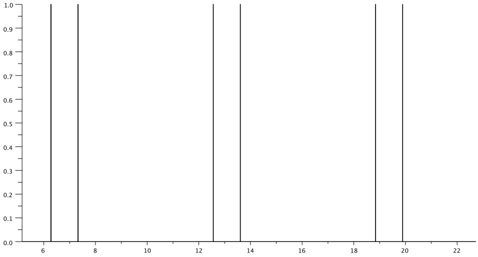
$$B = i\begin{pmatrix} 0 & 1/\sqrt{2} & 0 & \ldots & \\ 1/\sqrt{2} & 0 & 1/2 & 0 & \ldots \\ 0 & 1/2 & 0 & 1/2 & 0 \\ \vdots & 0 & 1/2 & 0 & \ddots \\ & \vdots & 0 & \ddots & \ddots \end{pmatrix}$$

- $\{(k, k\pm 1); k\in\mathbf{N}\}$ is a non-resonant chain of connectedness;
- The system is k-weakly coupled for every k;
- The system is approximately simultaneously controllable in norm H^k for every k

The control algorithm: "Q-track"

Consider the problem of exchanging the states 1 and 2.

- we know, a priori, that $\|u\|_{L^1} = 3$.
- of $N = 14$ then $\|\Upsilon^u_t(\phi_j) - X^u_{(N)}(t,0)\pi_N\phi_j\| < 10^{-3}$, for $j = 1, 2$, and for every $t \in [0, T]$.
- The control $u : [0, T] \to [0, 1]$ is



The control algorithm: “Q-track”

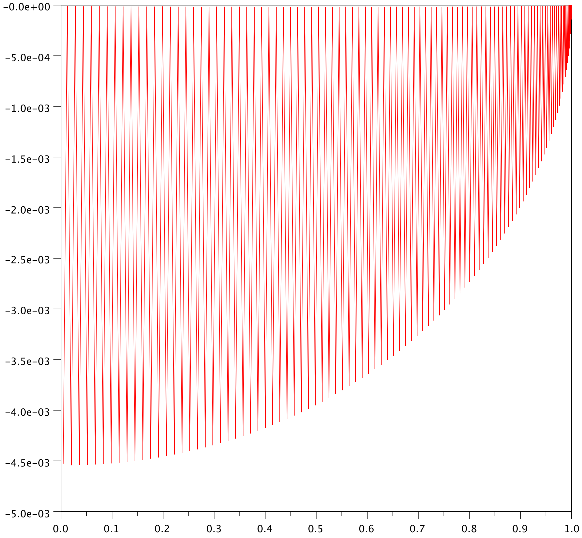
$$\Upsilon_0^u = \begin{pmatrix} 1 & 0 & \cdots & & \\ 0 & 1 & 0 & \cdots & \\ \vdots & 0 & 1 & \ddots & \\ & \vdots & \ddots & \ddots & \end{pmatrix} \to \Upsilon_T^u \approx \begin{pmatrix} 0 & e^{i\theta_1} & 0 & \cdots & \\ e^{i\theta_2} & 0 & 0 & \cdots & \\ 0 & 0 & 1 & \ddots & \\ \vdots & \vdots & \ddots & \ddots & \end{pmatrix}$$

- The error

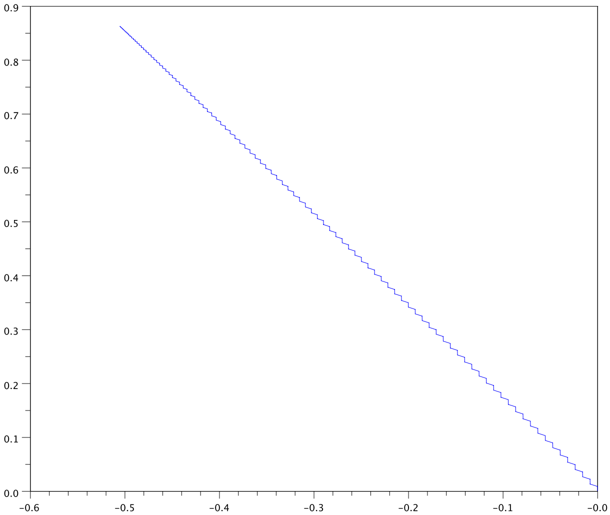
$$\| |\langle \phi_j, \Upsilon_t^u(\phi_2) \rangle| - \langle \phi_j, \phi_1 \rangle \| < \varepsilon \quad \| |\langle \phi_j, \Upsilon_t^u(\phi_1) \rangle| - \langle \phi_j, \phi_2 \rangle \| < \varepsilon$$

  is $\varepsilon = O(1/T)$
- for $N = 14$, $T = 624$ we have $\varepsilon = 7 * 10^{-3}$.

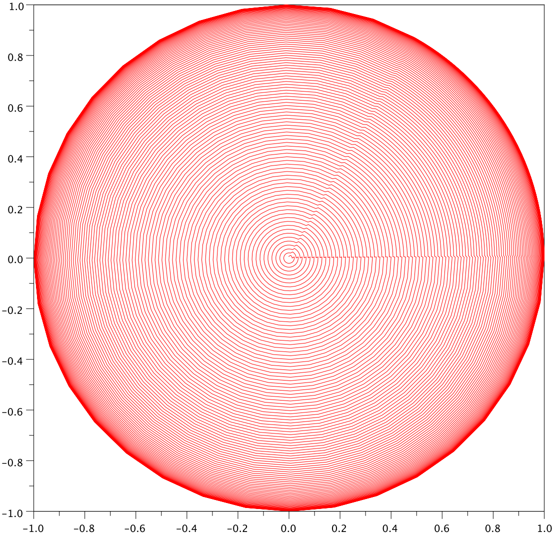
$$\langle \phi_1, \Upsilon_t^u(\phi_1) \rangle$$



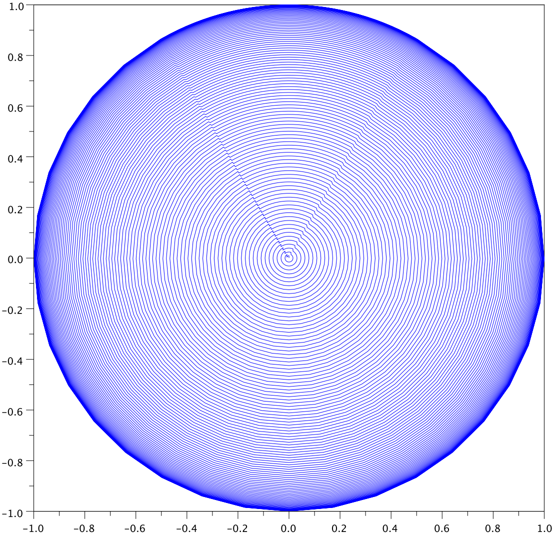
$$\langle \phi_1, \Upsilon_t^u(\phi_2) \rangle$$



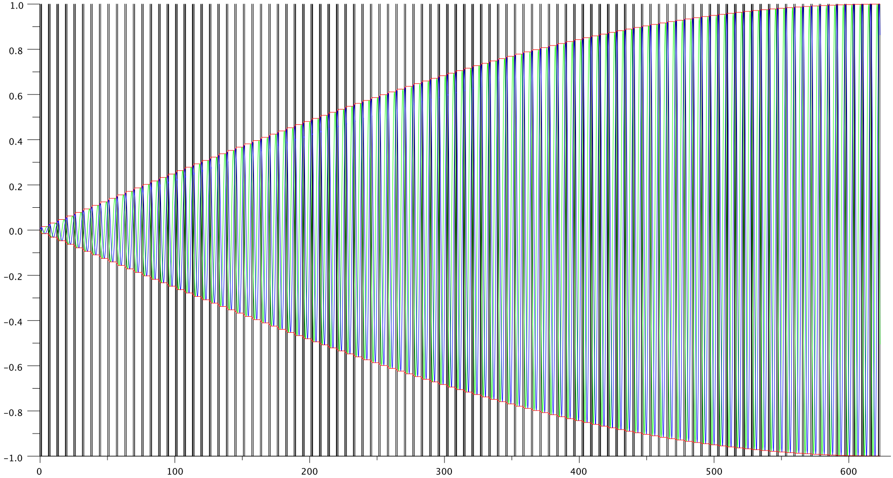
$\langle \phi_2, \Upsilon_t^u(\phi_2) \rangle$



$$\langle \phi_2, \Upsilon_t^u(\phi_1) \rangle$$



$\langle \phi_2, \Upsilon_t^u(\phi_1) \rangle$: time evolution $t \in [0, T]$



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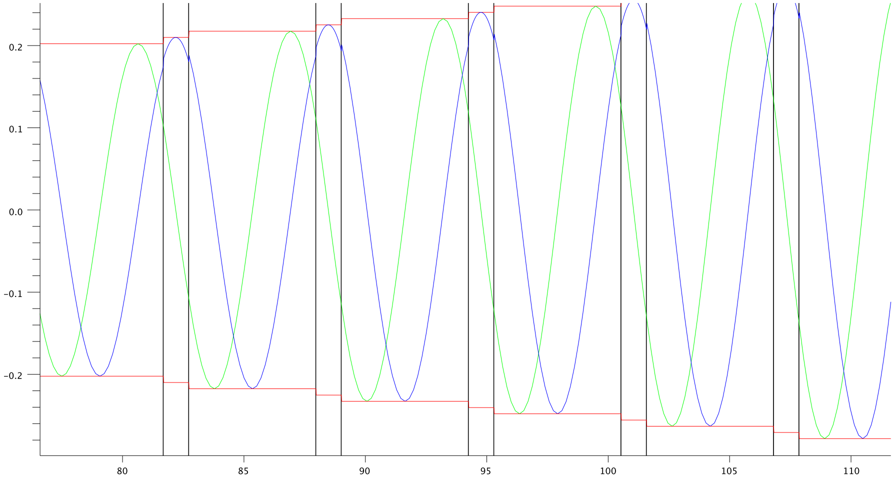
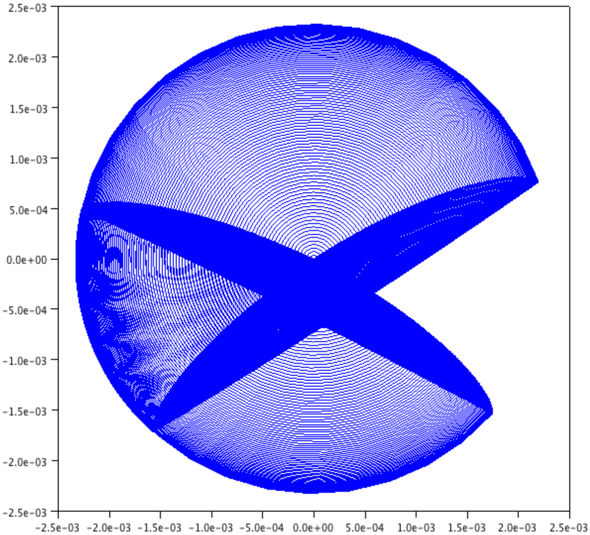


$$\langle \phi_2, \Upsilon_t^u(\phi_4) \rangle$$



$$\langle \phi_{10}, \Upsilon_t^u(\phi_2) \rangle$$