Geometric Methods in Quantum Control

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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;
- \( V : \Omega \rightarrow \mathbb{R} \) uncontrolled potential;
Bilinear Schrödinger equation

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**Controllability**

Given \( \psi_0, \psi_1 \) of \( L^2 \)-norm equal to one, find (if there exist) \( k \in \mathbb{N}, t_1, \ldots, t_k > 0, u_1, \ldots, u_k \in U \) such that

\[ \psi_1 = e^{-it_k(-\Delta+V+u_kW)} \circ \ldots \circ e^{-it_1(-\Delta+V+u_1W)}(\psi_0) \]
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

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

\( \theta \) rotational degree of freedom of a linear molecule,
Controllability results

**Negative results**

- non-exact controllability in the unit sphere of $L^2(\Omega)$
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  (Mirrahimi [2006], Ito-Kunisch [2009], Nersesyan [2009]);
- $L^2$-approximate controllability by geometric methods
  (Chambrion-Mason-Sigelotti-Boscain [2009]).
Let $\mathcal{H}$ be a complex Hilbert space

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

We assume that:

- $A$ has discrete spectrum $(i\lambda_k)_{k \in \mathbb{N}}$;
- $A + uB : \text{span}\{\phi_k \mid k \in \mathbb{N}\} \to \mathcal{H}$ 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 $\lambda_j = \lambda_k$. 
**Definition: propagator and solution**

\[
Υ^u_T(ψ_0) = e^{tk(A+u_kB)} \circ \ldots \circ e^{t_1(A+u_1B)}(ψ_0)
\]

is the **solution** of \((BSE)\) with initial data \(ψ_0 ∈ H\) associated with the **piecewise constant** control \(u = u_1χ[0,t_1) + u_2χ[t_1,t_1+t_2) + \cdots\)

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\(\Upsilon_t^u\) is the propagator of \((BSE)\) associated with \(u\).

Approximate controllability

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

\[ \| \Upsilon^u_T(\psi_0) - \psi_1 \| < \varepsilon. \]
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Approximate simultaneous controllability

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

\[ \| \hat{\Upsilon}(\psi^j) - \Upsilon^u_T(\psi^j) \| < \varepsilon \quad j = 1, \ldots, m. \]
$S \subset \mathbb{N}^2$ 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]: $S = \{(1, n) : n \in \mathbb{N}\}$,
- Chambrión et al. [2009]: $S = \{(n, n + 1) : n \in \mathbb{N}\}$.
Chain of connectedness

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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., Chambrión, Sigalotti, 2012)

If \((A, B)\) has a non-resonant chain of connectedness, then \((A, B)\) is approximately simultaneously controllable.
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Theorem (Boscain, C., Chambrión, Sigalotti, 2012)

If \((A, B)\) has a non-resonant chain of connectedness containing \((j, k)\), then for every \(\varepsilon, \delta > 0\), there exists \(u : [0, T] \rightarrow [0, \delta]\) 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\textsuperscript{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
  \[
  \dot{X} = vX + BX,
  \]

- 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 $\mathcal{L}_N = \text{span}\{\phi_1, \ldots, \phi_N\}$ we have
  \[
  \dot{Y} = \left(\frac{e^{i(\lambda_j-\lambda_k)\int v b_{jk}}}{N}\right)_{j,k=1}^{N} Y, \quad Y \text{ in } \mathcal{L}_N.
  \]
We have to study the curve on the torus,

\[ \Psi : \omega \mapsto (e^{i(\lambda_{j1} - \lambda_{k1})\omega}, \ldots, e^{i(\lambda_{jm} - \lambda_{km})\omega}) . \]
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$$\Psi : \omega \mapsto \left(e^{i(\lambda_{j_1} - \lambda_{k_1})\omega}, \ldots, e^{i(\lambda_{j_m} - \lambda_{k_m})\omega}\right).$$

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

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

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

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

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

then

$$\text{Conv}\Psi([0, \infty)) \supset \frac{\sqrt{2}}{2} S^1 \times \{0\}, \quad \text{and} \quad \frac{\sqrt{2}}{2} > \nu.$$
3rd step: “strong” controllability in $SU(n)$

Thanks to the existence of the chain of connectedness

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

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

is controllable.

We have more than that

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

$$
\begin{pmatrix}
M(t) & 0_{n \times N-n} & R(t) \\
0_{N-n \times n} & 0_{N-n \times N-n} & \cdots \\
\vdots & \vdots & \ddots \\
\end{pmatrix}
$$
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 (Chambiron 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 $u \in U$
- $\lambda_j$ 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

\[ |\Re\langle|A|^k\psi, B\psi\rangle| \leq C|\langle|A|^k\psi, \psi\rangle| \quad \psi \in D(|A|^k) \]

Examples:

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

\[ \left| \frac{d}{dt} \langle |A|^k \psi, \psi \rangle \right| \leq 2 |u(t)| \| \Re \langle |A|^k \psi, B \psi \rangle \| \]

\[ \leq 2C |u(t)| \| \langle |A|^k \psi, \psi \rangle \| \]

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.
Denote by $X^{(N)}_u$ 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

$$\|u\|_{L^1} \leq K \implies \|\Upsilon^u_t(\psi_0) - X^{(N)}_u(t)\psi_0\|_s < \varepsilon, \quad t \geq 0.$$ 

- 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

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

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

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

- \{(k, k \pm 1); k \in \mathbb{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 \(k\)
Consider the problem of exchanging the states 1 and 2.

- we know, a priori, that $\|u\|_{L^1} = 3$.
- If $N = 14$ then $\|\mathcal{Y}_t^u(\phi_j) - X_{(N)}^u(t, 0)\pi_N\phi_j\| < 10^{-3}$, 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”

\[ \Upsilon^u_0 = \begin{pmatrix} 1 & 0 & \cdots & 0 & \cdots \\ 0 & 1 & 0 & \cdots \\ \vdots & 0 & 1 & \ddots \\ \vdots & \ddots & \ddots & \ddots \end{pmatrix} \rightarrow \Upsilon^u_T \approx \begin{pmatrix} 0 & e^{i\theta_1} & 0 & \cdots \\ e^{i\theta_2} & 0 & 0 & \cdots \\ 0 & 0 & 1 & \ddots \\ \vdots & \vdots & \ddots & \ddots \end{pmatrix} \]

The error

\[ \|\langle \phi_j, \Upsilon^u_t(\phi_2) \rangle - \langle \phi_j, \phi_1 \rangle\| < \varepsilon \quad \|\langle \phi_j, \Upsilon^u_t(\phi_1) \rangle - \langle \phi_j, \phi_2 \rangle\| < \varepsilon \]

is \( \varepsilon = O(1/T) \)

for \( N = 14, T = 624 \) we have \( \varepsilon = 7 \times 10^{-3} \).
$\langle \phi_1, \Upsilon^u_t(\phi_1) \rangle$
$\langle \phi_1, \Upsilon^u_t(\phi_2) \rangle$
$\langle \phi_2, \Upsilon^u_t(\phi_2) \rangle$
$\langle \phi_2, \mathcal{Y}_t^u(\phi_1) \rangle$
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$\langle \phi_2, \gamma^u_t(\phi_4) \rangle$
\langle \phi_{10}, \Upsilon_t^u(\phi_2) \rangle