Controllability of Schrödinger equations and application to quantum rotors

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1: Controllability of finite-dimensional Schrödinger equations
2: Spectral conditions and resonant control
3: Controllability of ∞-dimensional Schrödinger equations

Spectral conditions and resonant control

1. NRCC and controllability
2. Extension to ∞-dimensional systems and harmonic oscillator
3. Conically connected spectra and controllability
4. Resonant control

Non-resonant chain of connectedness (NRCC)

- How to check if $\mathrm{Lie}\{iH_0, iH_1\} = \mathfrak{su}(N)$?
- If $\mathrm{Lie}\{iH_0, iH_1\} = \mathfrak{u}(N)$, find an explicit control steering ψ_0 to ψ_1.

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Let $\{\lambda_k\}_{k=1}^N \subset \mathbb{R}, \{\phi_k\}_{k=1}^N \subset \mathcal{S}^N$ eigenvalues and o.n. eigenvectors of H_0:

$$H_0\phi_k = \lambda_k\phi_k, \quad \langle\phi_k, \phi_j\rangle = \delta_{k,j}.$$

Let $\omega_k := \lambda_{k+1} - \lambda_k$, spectral gaps (or frequencies) of the free system.

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Theorem[1]

Suppose $\omega_k \neq \omega_j$ for every $k \neq j$, and $\langle\phi_j, H_1\phi_k\rangle \neq 0$ iff $k = j \pm 1$. Then $\mathrm{Lie}\{iH_0, iH_1\} = \mathfrak{su}(N)$.

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Proof of the NRCC criterium I

Let $e_{j,k}$ be the $N \times N$ matrix with 1 only on row j and column k, 0 otherwise. Let

$$E_{j,k} = e_{j,k} - e_{k,j}, \quad F_{j,k} = ie_{j,k} + ie_{k,j}, \quad D_{j,k} = ie_{j,j} - ie_{k,k}$$

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$$[E_{j,k}, E_{k,n}] = E_{j,n}, \quad [iH_0, E_{j,k}] = -i(\lambda_j - \lambda_k)F_{j,k}, \quad [E_{j,k}, F_{j,k}] = 2D_{j,k},$$

we are left to prove that $E_{j,j+1} \in \mathrm{Lie}\{iH_0, iH_1\}$ for every $j = 1, \ldots, N-1$.

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$$\mathrm{ad}^n_{iH_0} iH_1 = \sum_{j=1}^{N} (i\omega_j)^n b_j E_{j,j+1},$$

where $\mathrm{ad}_B A = [A, B], \quad \mathrm{ad}^k_B A = [\mathrm{ad}^{k-1}_B A, B].$

Proof of the NRCC criterium II

We thus have

$$\underbrace{\begin{pmatrix} 1 & \dots & 1 \\ i\omega_1 & \dots & i\omega_N \\ \vdots & & \\ (i\omega_1)^{N-1} & \dots & (i\omega_N)^{N-1} \end{pmatrix}}_{=V} \begin{pmatrix} b_1 E_{1,2} \\ b_2 E_{2,3} \\ \vdots \\ b_N E_{N-1,N} \end{pmatrix} = \begin{pmatrix} iH_1 \\ \mathrm{ad}_{iH_0} iH_1 \\ \vdots \\ \mathrm{ad}_{iH_0}^{N-1} iH_1 \end{pmatrix}.$$

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Then V is a ***Vandermonde matrix***, hence

$$\det V = \prod_{1 \leqslant j < k \leqslant N-1} (i\omega_j - i\omega_k) \neq 0,$$

thus V is invertible.

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NRCC in ∞ dimensions

Theorem[2]

Suppose H_0 has purely point spectrum and $H_0 + uH_1$ is self-adjoint for $u > 0$ small enough. Suppose $\omega_k \neq \omega_j$ for every $k \neq j$, and $\langle \phi_j, H_1 \phi_k \rangle \neq 0$ iff $k = j \pm 1$. Then the equation is approximately controllable.

Note that if H_1 is bounded, $H_0 + uH_1$ is self-adjoint for all $u \in \mathbb{R}$, but we can also consider situations in which H_1 is unbounded (e.g., H_0-bounded).

[2] Boscain, Caponigro, Chambrion, Sigalotti; A weak spectral condition for the controllability of the bilinear Schrödinger equation with application to the control of a rotating planar molecule. Comm. Math. Phys. 311, pages 423–455, (2012).

Example: Quantum Rotor

Model for a rotating rigid molecule, or a BEC (neglecting Gross-Pitaevskii state-nonlinearity) with control on the depth of the optical lattice:

$$i\partial_t\psi(x,t) = \left[-\partial_x^2 + u(t)\cos(x)\right]\psi(x,t), \quad x \in \mathbb{T}^1 = S^1$$

$$\psi \in \mathcal{S}_{L^2} \subset \mathcal{H} = L_e^2(S^1,\mathbb{C}) = \left\{\psi = \sum_{k=0}^{+\infty} \widehat{\psi}_k\phi_k, \sum_{k=0}^{+\infty} |\widehat{\psi}_k|^2 < \infty\right\},$$

$$H_0 = -\partial_x^2, \quad H_1 = \cos(x), \quad \phi_0 = 1/\sqrt{2\pi}, \quad \phi_k = \cos(kx)/\sqrt{\pi}.$$

and $-\partial_x^2\phi_k = k^2\phi_k$.

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and $-\partial_x^2 \phi_k = k^2 \phi_k$.So $\omega_k = 2k+1$ and $\omega_k \neq \omega_j$ if $k \neq j$. Moreover

$$\langle \phi_j, H_1 \phi_k \rangle = \int_0^{2\pi} cos(jx) cos(x) cos(kx) dx \neq 0 \Leftrightarrow k = j \pm 1.$$

The Theorem implies that this equation is approximately controllable.

Example: Harmonic Oscillator

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

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$$H_0 = -\partial_x^2 + x^2, \quad H_1 = x,$$

$\langle \phi_n, H_1\phi_m \rangle \neq 0$ iff $m = n \pm 1$ but $(-\partial_x^2 + x^2)\phi_n = (n + \frac{1}{2})\phi_n$, hence $\omega_j = \omega_k$ for every $j, k \in \mathbb{N}$.

[3] Rouchon, Mirrahimi: Controllability of quantum harmonic oscillators, IEEE Trans. Automat. Control, 49 (2004), pp. 745–747.

[4] Beauchard, Pozzoli: Examples of small-time controllable Schrödinger equations. Annales Henri Poincaré (2025)

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Theorem[3]

The harmonic oscillator is not approximately controllable. One can only control (in small-time) the average position and momentum of ψ:

$$\langle x(t)\rangle = \langle\psi(t), x\psi(t)\rangle \in \mathbb{R}, \quad \langle p(t)\rangle = \langle\psi(t), i\partial_x\psi(t)\rangle \in \mathbb{R}.$$

For $W(x) \neq x$, (ST-)controllability can hold.[4]

[3] Rouchon, Mirrahimi: Controllability of quantum harmonic oscillators, IEEE Trans. Automat. Control, 49 (2004), pp. 745–747.

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Controlling $\langle x(t) \rangle$ and $\langle p(t) \rangle$ in har. oscillator I

Consider the ansatz

$$\psi(t,x) = e^{i\left(\frac{1}{2}r(t)\cdot x + \theta(t)\right)}\xi(t, x - q(t)).$$

One checks that ψ solves the controlled quantum harmonic oscillator equation iff $(p,q) \in \mathbb{R}^2$ solves the ***controlled classical harmonic oscillator*** equations

$$\begin{cases} \dot{q} = r, \\ \dot{r} = -4q - 2u, \\ (p,q)(0) = (0,0), \end{cases}$$

(where θ is defined by $\theta(t) := \int_0^t \left(|q(s)|^2 - \frac{1}{4}|r(s)|^2\right) ds$, and is an irrelevant global phase) and ξ solves the quantum harmonic oscillator equation ***WITHOUT control***

$$\begin{cases} i\partial_t \xi(t,y) = (-\Delta + y^2)\xi(t,y), \quad (t,y) \in (0,T) \times \mathbb{R}, \\ \xi(0,.) = \psi_0. \end{cases}$$

Controlling $\langle x(t)\rangle$ and $\langle p(t)\rangle$ in har. oscillator II

Hence ψ is completely determined by q, p. Moreover

$$\langle x(t)\rangle = \langle \xi(t), x\xi(t)\rangle + q(t), \quad \langle p(t)\rangle = \langle \xi(t), i\partial_x \xi(t)\rangle - \frac{r(t)}{2},$$

hence $(\langle x(t)\rangle, \langle p(t)\rangle)$ is small-time controllable iff (q, r) is.

[5] See, e.g., Theorem 1.1 in the book of E. Trélat, Control in Finite and Infinite Dimension.

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Theorem[5]

A n-dim. linear control system $\dot{z} = Az + uB$, $z \in \mathbb{R}^n, u \in \mathbb{R}^m$, is controllable in any time iff its Kalman matrix $(B, AB, ..., A^{n-1}B)$ has rank n.

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We write our 2-dim. system for $z = (q, p)$ in the form

$$\frac{d}{dt}\begin{pmatrix} q \\ r \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & 1 \\ -4 & 0 \end{pmatrix}}_{A} \begin{pmatrix} q \\ r \end{pmatrix} + u \underbrace{\begin{pmatrix} 0 \\ -2 \end{pmatrix}}_{B}.$$

Hence the Kalman matrix $(B, AB) = \begin{pmatrix} 0 & -2 \\ -2 & 0 \end{pmatrix}$ has rank 2.

[5] See, e.g., Theorem 1.1 in the book of E. Trélat, Control in Finite and Infinite Dimension.

Conically connected spectra

Consider the spectrum $\Sigma(u)$ of $H(u) = H_0 + \sum_{j=1}^{m} u_j H_j$ as a function of $u \in \mathbb{R}^m$, $m \geqslant 2$:

$$\mathbb{R}^m \ni u \mapsto \Sigma(u) := \{\lambda_1(u), \ldots, \lambda_N(u)\} \in \mathbb{R}^N,$$

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$$\frac{|t|}{C} \leqslant \lambda_{j+1}(\widetilde{u} + t\eta) - \lambda_j(\widetilde{u} + t\eta) \leqslant C|t|,$$

for any $v \in \mathbb{R}^m$ unit vector and t small enough.

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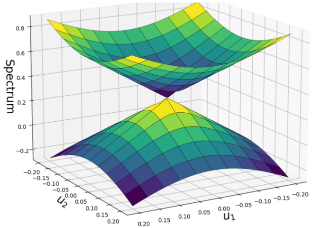
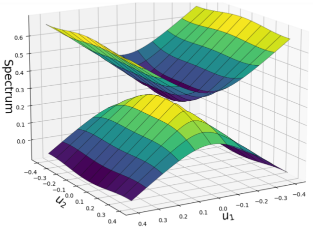
Conically connected spectrum

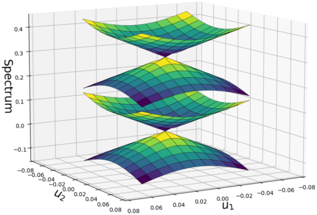
We say that the spectrum $\Sigma(\cdot)$ of $H(\cdot)$ is ***conically connected*** if all eigenvalue intersections are conical and for every j there exists a conical intersection $\widetilde{u}_j$ between λ_j and λ_{j+1}, with $\lambda_l(\widetilde{u}_j)$ simple if $l \neq j, j+1$.



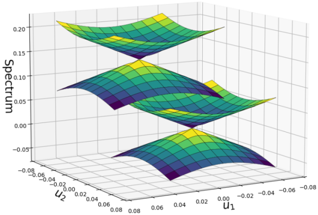
(a) A conical intersection



(b) A semi-conical intersection



(c) Piled-up intersections



(d) Non-piled-up intersections

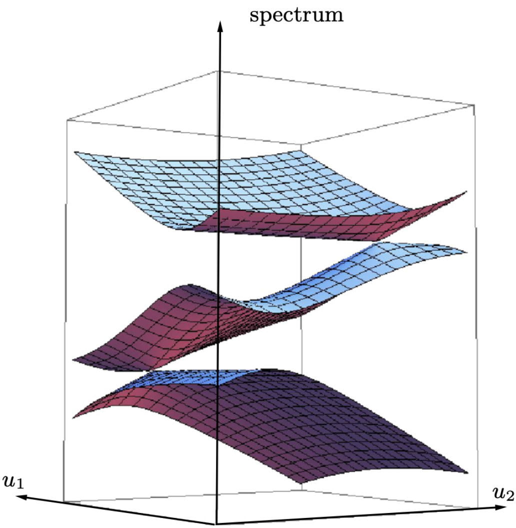


Fig. 2. A conically connected spectrum in the case $m = 2$

CCS implies controllability

Theorem[6] (finite-dimensional case)

Let $m \geqslant 2$. If $\Sigma(\cdot)$ is conically connected, the Schrödinger equation for the propagator (hence, for the state) is controllable.

The Theorem is false if $m = 1$: e.g.,
$H_0 = \mathrm{diag}(0, 1, 2), H_1 = \mathrm{diag}(1, 1, 0)$. The spectrum of $H(u)$ is $\Sigma(u) = \{u, u + 1, 2\}$, hence is conically connected, but clearly $\mathrm{Lie}\{iH_0, iH_1\}$ contains only diagonal matrices hence is not $\mathfrak{su}(3)$.

[6] Boscain, Gauthier, Rossi, Sigalotti; Approximate Controllability, Exact Controllability, and Conical Eigenvalue Intersections for Quantum Mechanical Systems. Commun. Math. Phys. (2014)

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Theorem (infinite-dimensional case)

Let $m \geqslant 2$. Suppose that H_0 has purely point spectrum and that $H(u)$ is self-adjoint for all $u \in \mathbb{R}^m$. If $\Sigma(\cdot)$ is conically connected, the Schrödinger equation for the state is approximately controllable.

[6] Boscain, Gauthier, Rossi, Sigalotti; Approximate Controllability, Exact Controllability, and Conical Eigenvalue Intersections for Quantum Mechanical Systems. Commun. Math. Phys. (2014)

Example: Eberly-Law model[7]

$$H(u,v) = \begin{pmatrix} E_0 & \alpha_0 u & 0 & 0 & 0 & \cdots \\ \alpha_0 u & E_1 & \beta_0 v & 0 & 0 & \cdots \\ 0 & \beta_0 v & E_2 & \alpha_1 u & 0 & \cdots \\ 0 & 0 & \alpha_1 u & E_3 & \beta_1 v & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

Eigenvalues intersections happen only if $u = 0$ or $v = 0$.

[7] Eberly, Law: Arbitrary Control of a Quantum Electromagnetic Field, Phys. Rev. Lett. 76 (1996)

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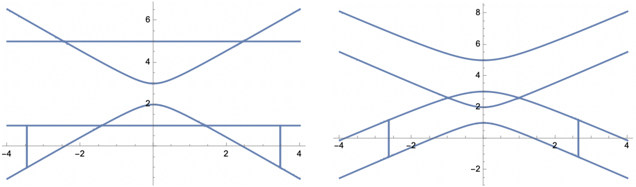
Eigenvalues intersections happen only if $u = 0$ or $v = 0$.

- $E_0 = 1, E_1 = 2, E_2 = 3, E_3 = 5, \alpha_0 = \alpha_1 = \beta_0 = 1$: conically connected spectrum, hence controllable.



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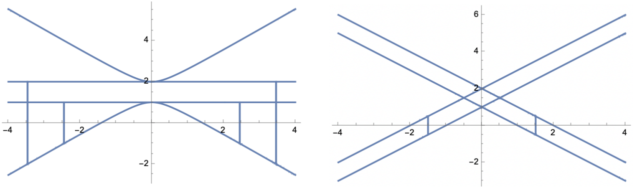
Eigenvalues intersections happen only if $u = 0$ or $v = 0$.

- $E_0 = E_1 = 1, E_2 = E_3 = 2, \alpha_0 = \alpha_1 = \beta_0 = 1$: intersections are not conical, and pile up. The controllability analysis is more delicate[8].



[8] Liang, Boscain, Sigalotti; Controllability of quantum systems having weakly conically connected spectrum. SIAM J. Control Optim. (2025)

1 NRCC and controllability

2 Extension to ∞-dimensional systems and harmonic oscillator

3 Conically connected spectra and controllability

4 Resonant control

Resonant control for eigenstates transfer

There is an averaging technique for realizing eigenstate transfer.

[9] Chambrion; Periodic excitations of bilinear quantum systems. Automatica 48, 9, Pages 2040-2046 (2012).

[10] Caponigro, Sigalotti; Exact controllability in projections of the bilinear Schrödinger equation. SIAM J Control Optim 56, 4, pp. 2901=2920 (2018).

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Theorem[9] (frequency absorption)

Suppose $\langle \phi_k, H_1 \phi_j \rangle \neq 0$. Take a periodic control law ($T = 2\pi / |\lambda_j - \lambda_k|$)

$$u^{\varepsilon}(t) = \frac{1}{\langle \phi_k, i H_1 \phi_j \rangle} \frac{\pi}{2} \frac{\varepsilon}{T} \cos(|\lambda_j - \lambda_k| t).$$

If all other spectral gaps ω of H_0 satisfies $\omega \neq |\lambda_j - \lambda_k|$, then

$$\lim_{\varepsilon \to 0} \| \psi(T/\varepsilon, u^{\varepsilon}, \phi_j) - e^{i\theta} \phi_k \|_{\mathcal{H}} = 0,$$

(for some irrelevant global phase $\theta(\epsilon) \in \mathbb{R}$).

We sketch the proof in finite dimensions, but the statement holds also in infinite dimensions when H_0 has purely point spectrum[10]. Note that this control law is bounded (uniformly w.r.t. ε).

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Interaction picture

Let $A = -iH_0, B = -iH_1$. Consider $\phi(t) = e^{-tA}\psi(t)$ where

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

Then,

$$\frac{d}{dt}\phi(t) = u(t)e^{-tA}Be^{tA}\phi(t).$$

Hence, if we control ϕ towards an eigenstate ϕ_k, we are also controlling ψ towards ϕ_k (modulo an irrelevant global phase $e^{it\lambda_k}$).

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Notice also that, by computing the exponential series,

$$\exp(tE_{j,k}) = \cos(t)(e_{j,j} + e_{k,k}) + \sin(t)E_{j,k},$$

hence $\exp(\frac{\pi}{2}E_{j,k})\phi_j = E_{j,k}\phi_j = -\phi_k$ swaps the eigenstates ϕ_j and ϕ_k. It thus suffices to show that we are controlling the propagator towards $\exp(\frac{\pi}{2}E_{j,k})$.

Averaging

We need to study, as $\varepsilon \to 0$,

$$\phi(T/\varepsilon, u_\varepsilon, \phi_j) = \exp\left(\frac{1}{\langle \phi_k, B\phi_j\rangle}\frac{\pi}{2}\frac{\varepsilon}{T}\int_0^{T/\varepsilon} \cos(|\lambda_j - \lambda_k|t) e^{-tA} B e^{tA} dt\right)\phi_j.$$

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We note that

$$\begin{aligned}
&\frac{\varepsilon}{T}\int_0^{T/\varepsilon}\langle \phi_m, \cos(|\lambda_j - \lambda_k|t)e^{-tA}Be^{tA}\phi_n\rangle dt \\
=&\langle \phi_m, B\phi_n\rangle \frac{\varepsilon}{T}\int_0^{T/\varepsilon} e^{i(\lambda_n - \lambda_m)t}\cos(|\lambda_j - \lambda_k|t)dt \\
\xrightarrow[\varepsilon\to 0]{}& \begin{cases} \langle \phi_n, B\phi_m\rangle, & |\lambda_n - \lambda_m| = |\lambda_j - \lambda_k| \\ 0, & \text{otherwise} \end{cases}
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\end{aligned}$$

By hypothesis, $|\lambda_n - \lambda_m| = |\lambda_j - \lambda_k|$ only if $(m, n) = (j, k)$ or (k, j). So, $\varepsilon \to 0$,

$$\exp\left(\frac{1}{\langle \phi_k, B\phi_j\rangle}\frac{\pi}{2}\frac{\varepsilon}{T}\int_0^{T/\varepsilon} \cos(|\lambda_j - \lambda_k|t)e^{-tA}Be^{tA}dt\right)\phi_j \to \exp\left(\frac{\pi}{2}E_{j,k}\right)\phi_j = -\phi_k.$$

Thanks for your attention!