Ensemble control of quantum systems by adiabatic evolution

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Workshop “Mathematics for Quantum Technologies”
Nice
04/03/2022

Closed quantum control systems

$$i\frac{d\psi}{dt}(t) = H(u(t))\psi(t), \quad \psi \in \mathcal{H},\ \|\psi\| = 1,$$

with $H(u)$ selfadjoint on the Hilbert space $\mathcal{H}$ for every $u \in U$.
In particular, the flow $\Phi_u(t,s)$ associated with any control $u(\cdot)$ is unitary.
We mostly assume that the system is control affine (or bilinear), i.e.,

$$H(u) = H_0 + \sum_{j=1}^{m} u_j H_j, u = (u_1, \dots, u_m) \in U \subset \mathbb{R}^m.$$

EXAMPLES:

- spin in an electromagnetic field $\psi(t) \in \mathbb{C}^2$, $m = 2$,

$$H_0 = \begin{pmatrix} E & 0 \\ 0 & -E \end{pmatrix}, \quad H_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad H_2 = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

- rotating linear molecule
  $\psi(t) \in L^2(S^1, \mathbb{C})$, $m = 2$, $H_0 = -\partial_\theta^2$, $H_1 = \cos\theta$, $H_2 = \sin\theta$

Slow-varying controls: adiabatic evolution

If the Hamiltonian $[0,1] \ni \tau \mapsto H(\tau)$ smoothly depends on τ and $(\lambda(\tau), \phi(\tau))$ is an eigenpair of $H(\tau)$ with $\lambda(\tau)$ separated from the rest of the spectrum of $H(\tau)$, then the solution ψ_ε of

$$i \frac{d\psi_\varepsilon}{dt}(t) = H(\varepsilon t)\psi_\varepsilon(t)$$

with $\psi_\varepsilon(0) = \phi(0)$ satisfies

$$\|\psi_\varepsilon(1/\varepsilon) - e^{i\theta_\varepsilon}\phi(1)\| < C\varepsilon$$

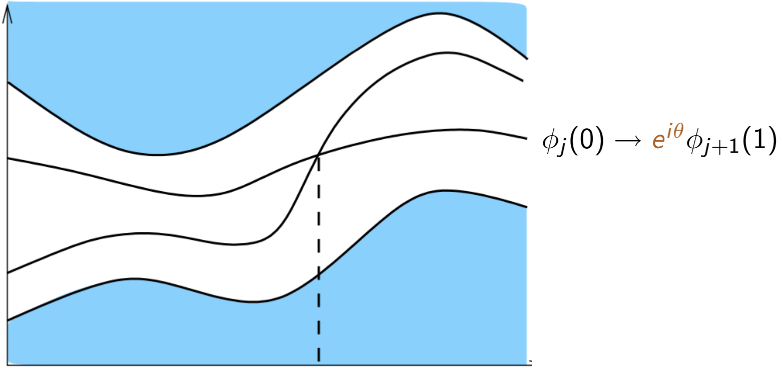
for some $C > 0$ independent on ε and some $\theta_\varepsilon \in \mathbb{R}$.

This gives a constructive motion planning method (Guérin, Jauslin, Yatsenko, Vitanov, Gauthier, Leghtas, Sarlette, Rouchon...):

- regular control laws
- trajectory tracking features (up to phases)
- works both in finite and infinite dimension
- robust motion planning

Eigenvalue crossing

Finer versions of the adiabatic theorem $\longrightarrow$ extension to case $\lambda_j(\bar{\tau}) = \lambda_{j+1}(\bar{\tau})$ at some τ where the intersection is transversal (e.g., [Teufel, 2003])[1]



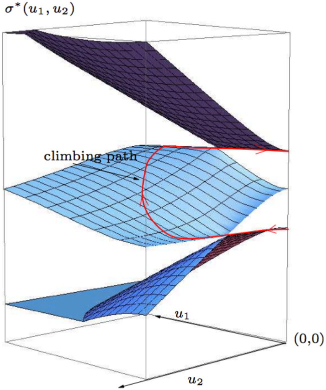
Adiabatic evolution through transversal intersections thus allows to "climb" energy levels

[1] $(\lambda_j)_{j=1}^N$ nondecreasing sequence of eigenvalues of H repeated according to multiplicities. $(\phi_1, \ldots, \phi_N)$ orthonormal basis of associated eigenvectors

The mechanism of climbing

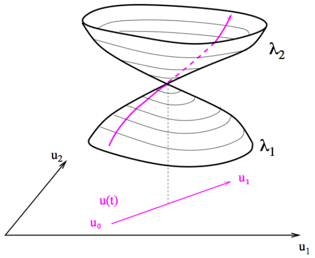
Climbing happens because smooth 1D variations of H lead to smoothly varying eigenpairs even through intersections (Kato–Rellich theorem)

$$\|\psi_\varepsilon(1/\varepsilon) - e^{i\theta_\varepsilon}\phi_{j+1}(1)\| < C\sqrt{\varepsilon}, \quad \psi_\varepsilon(0) = \phi_j(0)$$



Climbing can be repeated in a general control scheme

Conical intersections: transversal in all directions



An intersection $\lambda_j(u) = \lambda_{j+1}(u)$ is conical if it has multiplicity 2 and there exists $c > 0$ such that for any $v \in S^{m-1}$

$$\frac{d}{dt}\bigg|_{t=0^+} \lambda_{j+1}(u + tv) - \lambda_j(u + tv) \geqslant c\,.$$

For Hamiltonians with real matrix elements and $m = 2$ intersections are generically conical (the same for self-adjoint Hamiltonians and $m = 3$): open, dense, and full-measure set of triples (H_0, H_1, H_2) for $\dim \mathcal{H} < \infty$

Spectral conical connectedness and eigenvector controllabillity

The spectrum of $H(\cdot)$ is conically connected if $m = 2$ and

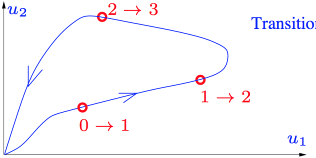
- there exist a conical intersection between each pair of subsequent eigenvalues
- intersection points are distinct and isolated in the plane (u_1, u_2)

Proposition

If the spectrum of $H(\cdot)$ is conically connected then

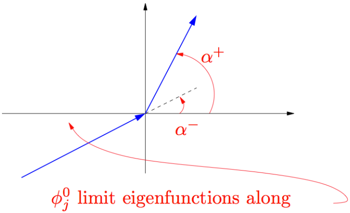
$$\phi_j(u_0) \longrightarrow e^{i\theta}\phi_k(u_1)$$

by adiabatic control



Spreading population occupations is possible by breaking the path [Boscain, Chittaro, Mason, S, TAC, 2012]

$$\phi_j \to e^{i\theta_1} p_1 \phi_j + e^{i\theta_2} p_2 \phi_{j+1}$$



$$p_1 = |\cos(\theta(\alpha_-) - \theta(\alpha_+))| \quad p_2 = |\sin(\theta(\alpha_-) - \theta(\alpha_+))|$$

where $\theta(\alpha)$ is the solution to

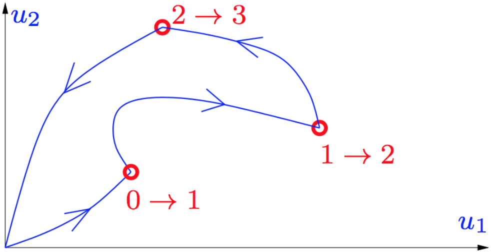
$$\begin{pmatrix}\cos\alpha, \sin\alpha\end{pmatrix} \mathcal{M} \begin{pmatrix}\cos 2\theta(\alpha) \\ \sin 2\theta(\alpha)\end{pmatrix} = 0$$

and by definition

$$\mathcal{M} = \begin{pmatrix} \langle \phi_j^0, H_1 \phi_{j+1}^0 \rangle & \frac{1}{2}(\langle \phi_{j+1}^0, H_1 \phi_{j+1}^0 \rangle - \langle \phi_j^0, H_1 \phi_j^0 \rangle) \\ \langle \phi_j^0, H_2 \phi_{j+1}^0 \rangle & \frac{1}{2}(\langle \phi_{j+1}^0, H_2 \phi_{j+1}^0 \rangle - \langle \phi_j^0, H_2 \phi_j^0 \rangle) \end{pmatrix}$$

(nonsingular if and only if the intersection is conical)

A broken path



Transition between level 0 and a superposition of levels 0,1,2,3

Spectral connectedness by conical intersections implies exact controllability

Let $\mathcal{H} = \mathbb{C}^N$.

Theorem (Boscain, Gauthier, Rossi, S., CMP, 2015)

If the spectrum of $H(\cdot)$ is conically connected, then $\mathrm{Lie}\{iH(u) \mid u \in \mathbb{R}^2\} \subset \mathrm{u}(N)$ contains $\mathrm{su}(N)$. In particular every logical gate can be obtained by choosing a suitable control.

- by measuring the spectrum of $H(\cdot)$ one can “read” Lie algebraic properties
- spirit of the proof:
  - conical connectedness + analyticity $\Longrightarrow$ at almost every $\bar{u}$ the spectrum is rationally independent and there is no invariant linear subspace
  - a Vandermonde argument on matrices written in the eigenbasis of $H(\bar{u})$ allows to conclude

Ensemble controllability

$$i\dot{\psi}(t) = H^\alpha(u(t))\psi(t)$$

α time-independent parameter, u control, each $H^\alpha(u)$ self-adjoint.
$(\lambda_j^\alpha(u))_{j=1}^N$ nondecreasing sequence of eigenvalues of $H^\alpha(u)$ repeated according to multiplicities.
$(\phi_1^\alpha(u), \ldots, \phi_N^\alpha(u))$ orthonormal basis of associated eigenvectors

Definition

The system is ensemble approximately controllable between eigenstates if for every $\varepsilon > 0$, $j, k \in \{1, \ldots, N\}$ and $u_0, u_1 \in \mathrm{U}$ such that $\lambda_j^\alpha(u_0)$ and $\lambda_k^\alpha(u_1)$ are simple for every α, there exists $u : [0, T] \to \mathrm{U}$ such that for every α the solution with initial condition $\psi^\alpha(0) = \phi_j^\alpha(u_0)$ satisfies $\|\psi^\alpha(T) - e^{i\theta}\phi_k^\alpha(u_1)\| < \varepsilon$.

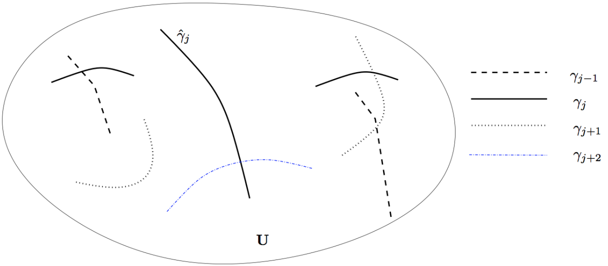
Typical case: $u = 0$ represents free Hamiltonian and one seeks to steer $\phi_j^\alpha(0)$ towards $\phi_k^\alpha(0)$

Ensemble eigenvalue crossing

$$\gamma_j = \{u \in \mathsf{U} \mid \exists \alpha \in [\alpha_0, \alpha_1] \text{ such that } \lambda_j^\alpha(u) = \lambda_{j+1}^\alpha(u)\}$$

Assumption A_j. The set $\mathsf{U} \setminus (\gamma_{j-1} \cup \gamma_j \cup \gamma_{j+1})$ is pathwise connected and there exist connected component $\hat{\gamma}_j$ of γ_j and $\beta_j : [\alpha_0, \alpha_1] \to \mathsf{U}$ smooth embedding such that

- $\hat{\gamma}_j = \beta_j([\alpha_0, \alpha_1]) \subset \mathsf{U} \setminus (\gamma_{j-1} \cup \gamma_{j+1})$
- For every $\alpha \in [\alpha_0, \alpha_1]$, λ_j^α has a conical intersection at $\beta_j(\alpha)$.

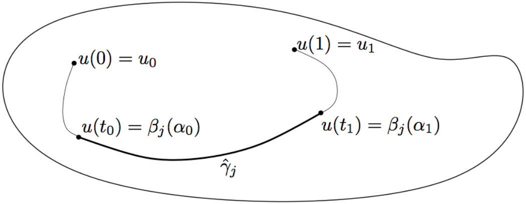


Adiabatic evolution through an ensemble eigenvalue crossing

Lemma

Let $(\alpha, u) \mapsto H^\alpha(u)$ *smooth and satisfying* A_j*. Take* $u_0, u_1 \in \mathrm{U} \setminus (\gamma_{j-1} \cup \gamma_j \cup \gamma_{j+1})$ *and a* $u : [0,1] \to \mathrm{U}$ $\mathcal{C}^3$ *satisfying* $u(0) = u_0$, $u(1) = u_1$, $\dot{u}(t) \neq 0$ *for every* $t \in [0,1]$, $u|_{[t_0,t_1]}$ *reparameterization of* β_j *for some* $0 < t_0 < t_1 < 1$, $u(t) \notin \gamma_{j-1} \cup \gamma_j \cup \gamma_{j+1}$ *for every* $t \notin [t_0, t_1]$.
Then $\exists C > 0$ *such that* $\forall \alpha \in [\alpha_0, \alpha_1]$ *and* $\forall \varepsilon > 0$ *the solution* ψ_ε^α *of* $i\dot{\psi}_\varepsilon^\alpha = H^\alpha(u(\varepsilon t))\psi_\varepsilon^\alpha$ *with initial condition* $\psi_\varepsilon^\alpha(0) = \phi_j^\alpha(u_0)$ *satisfies*

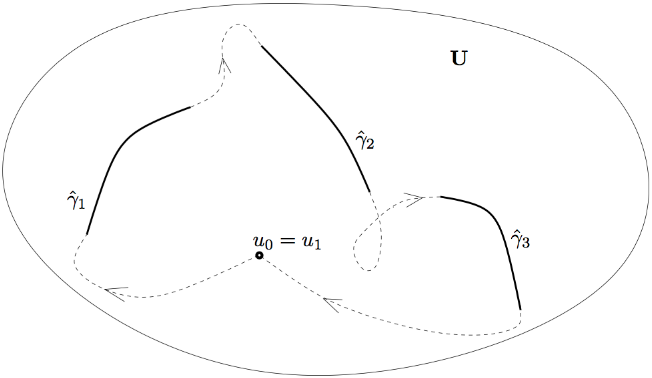
$$\|\psi_\varepsilon^\alpha(1/\varepsilon) - e^{i\theta}\phi_{j+1}^\alpha(u_1)\| < C\sqrt{\varepsilon}$$



Ensemble approximate controllability

Corollary (Augier, Boscain, S, SICON, 2018)

Let $(\alpha, u) \mapsto H^\alpha(u)$ be smooth and satisfy A_j for every $j = 1, \ldots, N-1$. Then the system is ensemble approximately controllable between eigenstates.



Example: spin system

$$i\frac{d}{dt}\begin{pmatrix}\psi_1^\alpha \\ \psi_2^\alpha\end{pmatrix} = \begin{pmatrix} E+\alpha & \Omega(t) \\ \Omega^*(t) & -E-\alpha \end{pmatrix}\begin{pmatrix}\psi_1^\alpha \\ \psi_2^\alpha\end{pmatrix}.$$

We want to steer $\phi_1^\alpha(0) = (1,0)$ to $\phi_2^\alpha(0) = (0,1)$, $\forall \alpha \in [\alpha_0, \alpha_1]$
The eigenvalues of the Hamiltonian are simple for every value of $\alpha \in [\alpha_0, \alpha_1]$ and $\Omega \in \mathbb{C} \Longrightarrow$ time-dependent change of variables (interaction picture)
$\Omega(t) = u_1(t)e^{-i(2Et+\Delta(t))}$ and $\psi^\alpha(t) = U(t)\Phi^\alpha(t)$ with

$$U(t) = \begin{pmatrix} e^{-iEt} & 0 \\ 0 & e^{i(Et+\Delta(t))} \end{pmatrix}.$$

Transformed equation:

$$i\frac{d}{dt}\begin{pmatrix}\Phi_1^\alpha \\ \Phi_2^\alpha\end{pmatrix} = \begin{pmatrix} \alpha & u_1(t) \\ u_1(t) & -\alpha+u_2(t) \end{pmatrix}\begin{pmatrix}\Phi_1^\alpha \\ \Phi_2^\alpha\end{pmatrix}.$$

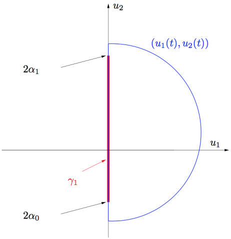
with $u_2(t) = \frac{d\Delta}{dt}(t)$

Example: spin system

A_1 is satisfied: the matrix $H^\alpha(u_1,u_2) = \begin{pmatrix} \alpha & u_1 \\ u_1 & -\alpha + u_2 \end{pmatrix}$ has conical intersections on

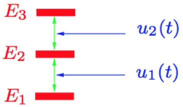
$$\gamma_1 = \{(0, 2\alpha) \in \mathbb{R}^2 \mid \alpha \in [\alpha_0, \alpha_1]\} = \{0\} \times [2\alpha_0, 2\alpha_1]$$

The controls used to achieve the adiabatic transition can be taken as in figure and apply to the original system since $U(t)$ preserves (up to phases) $(1,0)$ and $(0,1)$.

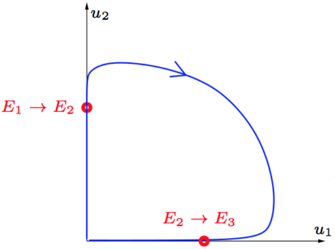


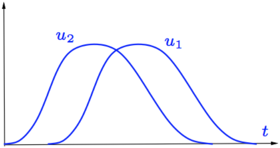
$$\Omega(\varepsilon t) = u_1(\varepsilon t) e^{-i(2Et + \frac{1}{\varepsilon}\int_0^{\varepsilon t} u_2(s)ds)} \quad t \in \left[0, \frac{1}{2\varepsilon}\right]$$

Example: the STIRAP processes



$$i\frac{d}{dt}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix} = \begin{pmatrix} E_1 & u_1(t) & 0 \\ u_1(t) & E_2 & u_2(t) \\ 0 & u_2(t) & E_3 \end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix}, \quad u_1(t), u_2(t) \text{ real controls}$$





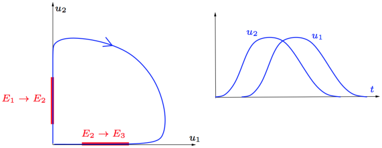
the conunterintuitive strategy is a consequence of the presence of conical intersections

STIRAP with parameters

$$i\frac{d}{dt}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix}=\begin{pmatrix}\alpha_1 E_1 & \beta_1 u_1 & 0\\ \beta_1 u_1 & \alpha_2 E_2 & \beta_2 u_2\\ 0 & \beta_2 u_2 & \alpha_3 E_3\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\end{pmatrix}$$

Here $\alpha_1, \alpha_2, \alpha_3, \beta_1, \beta_2 > 0$ and $\alpha_1 E_1 < \alpha_2 E_2 < \alpha_3 E_3$

The same strategy is working for the whole family of systems



- Often only some parameters are responsible for "perturbing" eigenvalue intersections
- This explains why the counterintuitive strategy is so robust

Adiabatic control with a single scalar control

In principle it does not work, since once we cross an eigenvalue intersection, we should cross it in the opposite sense to get to the initial value of u.

Creation of new control parameters by rotating wave approximation: the trajectories of

$$i\dot{\psi}(t) = \begin{pmatrix} E & u(t) \\ u(t) & -E \end{pmatrix} \psi(t)$$

with

$$u(t) = 2\varepsilon t v(\varepsilon t) \cos(2Et + \Delta(\varepsilon t)), \quad t \in [0, T/\varepsilon]$$

approximate, for $\varepsilon \to 0$, the rescaled solution $(s = \varepsilon t)$ of

$$i\dot{\phi}(s) = \begin{pmatrix} -\Delta'(s)/2 & v(s) \\ v(s) & \Delta'(s)/2 \end{pmatrix} \phi(s)$$

up to a change of rotating frame.

Issue for adiabatic control: double time scale

Adiabatic control with a single scalar control [Robin, Augier, Boscain, S, JDE, to appear]

By combining rotating wave approximation and adiabatic control we can induce ensemble eigenvector controllability for

$$i\dot{\psi}(t) = \begin{pmatrix} \alpha E & \beta u(t) \\ \beta u(t) & -\alpha E \end{pmatrix} \psi(t)$$

with respect to $(\alpha, \beta) \in [\alpha_0, \alpha_1] \times [\beta_0, \beta_1]$ with $0 < \alpha_0 < \alpha_1$, $0 < \beta_0 < \beta_1$ provided that

$$3\alpha_0 > \alpha_1.$$

Moreover (but less constructive): ensemble approximate controllability between elements of $C^0([\alpha_0, \alpha_1] \times [\beta_0, \beta_1], S^3)$ and also in terms of logical gates, extending previous results by Li–Khaneja and Beauchard–Coron–Rouchon to the case $u(t) \in \mathbb{R}$ (instead of $\mathbb{C}$)