Spectral conditions for the controllability of the Schroedinger equation

Ugo Boscain

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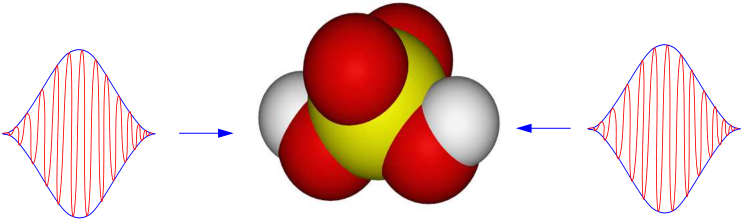
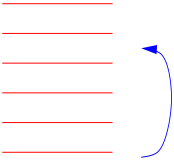


External field(laser, magnetic field)

Quantum System (atom or molecule)

−) to induce chemical reactions
(material science)



EXCITATION

−) to measure the decay --> images
(NMR)

−) to use quantum states as a memory
(quantum computation)

Finite dimensional quantum systems

$$i\frac{d\psi}{dt} = H(\mathbf{u}(t))\psi(t) := (H_0 + \sum_{k=1}^{m} u_k(t)H_k)\psi(t). \qquad (1)$$

$$\psi(t) \in S^{2n-1} \subset \mathbf{C}^n, \quad (u_1(.), \dots u_m(.)) : [0, T] \to \mathbf{U} \subset \mathbf{R}^m,$$

H_k hermitian matrices

If H_0 has eigenvalues $E_1, \dots, E_n$ and $\psi(t) = (\psi_1(t), \dots \psi_n(t)) \in S^{2n-1} \subset \mathbf{C}^n$ then $\|\psi_i\|^2$ is the probability that if we make a measure of energy at time t we get E_i.

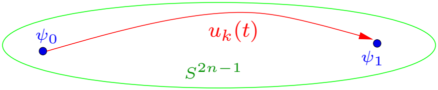
$\rightarrow$examples: spin systems (NMR), Galerkin approximation of molecules etc..

Some of the results extend to infinite dimension, i.e. to systems evolving on an infinite dimensional Hilbert space, e.g. systems of the kind

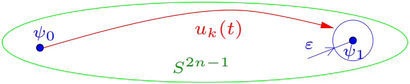
$$i\frac{\partial\psi}{\partial t}(t, x) = (-\Delta + V_0 + \sum_{k=1}^{m} u_k(t)V_k)\psi(t, x).$$

V_k real potentials

Controllability problem: prove that, for every pair of states ψ_0 and ψ_1, there exists controls $u_k(\cdot)$ and a time T such that the solution of the control system with initial condition $\psi(0) = \psi_0$ satisfies $\psi(T) = \psi_1$.



When for every pair of states ψ_0, ψ_1, and $\varepsilon > 0$ there exists controls $u_k(\cdot)$ and a time T such that the solution of the control system with initial condition $\psi(0) = \psi_0$ satisfies $\|\psi(T) - \psi_1\| < \varepsilon$ we say that the system is approximately controllable



REMARK

- in finite dimension sufficient conditions for exact controllability are known from long time (see later).
- in infinite dimension exact controllability is impossible in the natural functional space where the problem is formulated (H^2, see Ball, Marsden, Slemrod).

  $\rightarrow$For exact controllability results in H^d with $d \geq 3$ see Coron, Beauchard, Laurent, Chambrion, and co-autohrs.

finite dim. case for $i\frac{d\psi}{dt} = (H_0 + \sum_{k=1}^{m} u_k(t)H_k)\psi(t)$

As a consequence of the fact that system (1) is the projection of a left-invariant control system on $U(n)$, exact controllability is equivalent to (see D'alessandro's book):

$$\mathrm{Lie}\{-iH(\mathbf{u}) \mid \mathbf{u} \in \mathbf{U}\} \supseteq \begin{cases} \mathrm{su}(n) \text{ if } n \text{ is odd} \\ \mathrm{su}(n) \text{ or } \mathrm{sp}(n/2) \text{ if } n \text{ is even.} \end{cases}$$

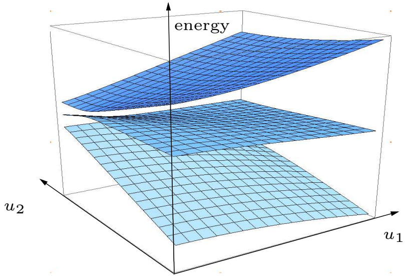
Remarks

- Why the Lie algebra is important? because for a dynamical system where one can use either X or Y, the bracket $[X, Y]$ is the direction that one can approximate by making quick switching between X and Y.
- In general this condition is not easy to check. Many people worked to look for easy verifyable conditions. Typical conditions read:
  - the spectrum of H_0 is non-resonant (e.g. all gaps different)
  - the control matrices couple all eigenstates of H_0.

  See Caponigro, Chambrion, Mason, Sigalotti, Nersesyan, U.B. Mirrahimi

The problem

Consider $\Sigma(\mathbf{u})$=spec$(H_0 + \sum_{k=1}^{m} u_k H_k)$ as function of $\mathbf{u} = (u_1, \dots u_k)$



Is it possible to get controllability results from the knowledge of these surfaces without computing any Lie brackets?

→it seems not obvious, since

- the $\Sigma(u)$ contains information on where you can go by using slow varying controls (by adiabatic theory)
- the brackets contains information on where you can go by using fast controls

Answer to this question for a class of systems

I will consider the following class of systems

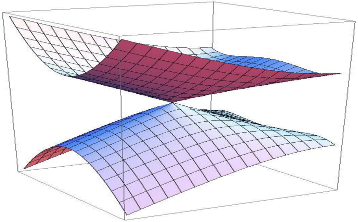
- $m = 2$ i.e.
$$i\frac{d\psi}{dt} = (H_0 + u_1(t)H_1 + u_2(t)H_2)\psi(t).$$
- there exists a basis of $\mathbf{C}^n$ where H_0, H_1, H_2 are real (symmetric)
- $(u_1(.), u_2(.)) : [0, T] \to \mathbf{U}$ connected and containing an an open set

$\to$the hypothesis that we have at least 2 controls is crucial

$\to$the hypothesys that H_0, H_1, H_2 are real can be relaxed by taking $m > 2$

Special features of this class of systems

Eigenvalue intersection are generically conical:



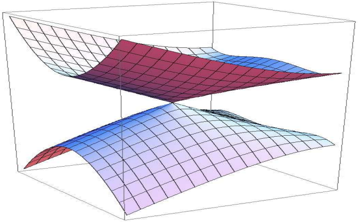
Definition

Let $H(\cdot)$ satisfy hypothesis **(H0)**. We say that $\bar{\mathbf{u}} \in \mathbf{R}^2$ is a *conical intersection* between the eigenvalues λ_j and λ_{j+1} if $\lambda_j(\bar{\mathbf{u}}) = \lambda_{j+1}(\bar{\mathbf{u}})$ has multiplicity two and there exists a constant $c > 0$ such that for any unit vector $\mathbf{v} \in \mathbf{R}^2$ and $t > 0$ small enough we have that

$$\lambda_{j+1}(\bar{\mathbf{u}} + t\mathbf{v}) - \lambda_j(\bar{\mathbf{u}} + t\mathbf{v}) > ct\,. \tag{2}$$

(the presence of eigenvalues intersection will be crucial to get controllability results)

Conical singularities are generic

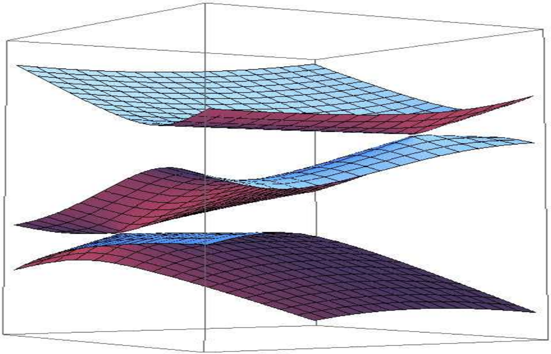


- if there is an eigenvalue intersection then generically it is conical
- conical intersections are “stable” by perturbation of the system

→this is due to the fact that the condition for a symmetric matrix to have a double eigenvalue is of codimension 2.
→it was formalized in [Boscain, F. Chittaro, P. Mason, M. Sigalotti, IEEE TAC, 2012] (for ∞-dim systems), but was essentially known from long time

Definition

We say that the spectrum Σ of $H_0 + u_1 H_1 + u_2 H_2$ is *conically connected* if **all eigenvalue intersections are conical** and for every $j = 1, \ldots, n-1$, there exists a conical intersection $\bar{\mathbf{u}}_j \in \mathbf{U}$ between the eigenvalues λ_j, λ_{j+1}, with $\lambda_l(\bar{\mathbf{u}}_j)$ simple if $l \neq j, j+1$.



The main result

Theorem

Assume that the spectrum Σ is conically connected. Then system is exactly controllable (and hence Lie bracket generating).

→This result is not trivial: It is known how to climb energy levels through eigenvalue intersections to go from one eigenstate to another one, but:

- one arrives to the final state only approximately (because of the adiabatic Theorem);
- controllability among eigenstates is much less than controllability on the full space (all superpositions, with all possible phases, of eigenstates);

→we get the Lie-bracket-generating condition without computing any bracket, but just looking to the spectrum.

A constructive proof in 4 steps

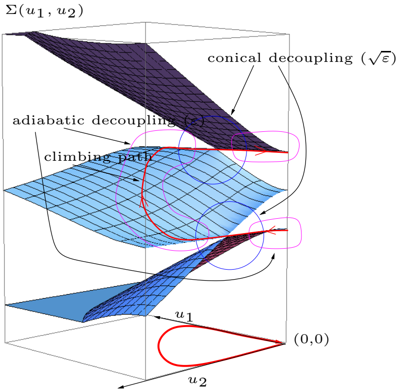
- some of the steps are constructive and interesting by themself
- some steps extends to infinite-dimensional systems

Theorem

For finite dimensional quantum systems, exact controllability is equivalent to approximate controllability

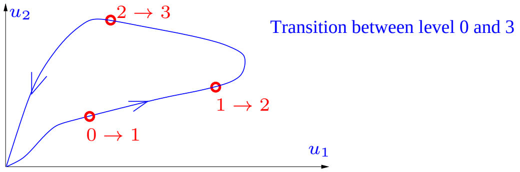
STEP 1: approximate controllability among eigenstates

one can cross the eigenvalue intersections and move between eigenstates at the order $\sqrt{\varepsilon}$.



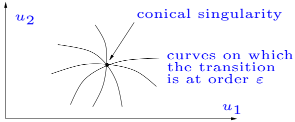
$\rightarrow$"at order ε" means that to obtain a transfer with an error ε, one needs a time $T = C/\varepsilon$.

$\rightarrow$this step cannot be realized with only one control



this idea is very old

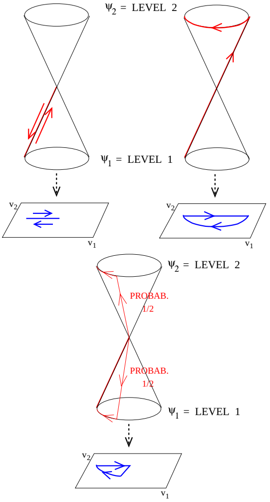
- Born, Fock 1928,
- Dijon school: Jauslin, Guerin, Yatsenko, 2002,
- Teufel, 2003.
- there exists special curves where the conical decoupling is "at order ε" [Boscain, F. Chittaro, P. Mason, M. Sigalotti, IEEE TAC, 2012]



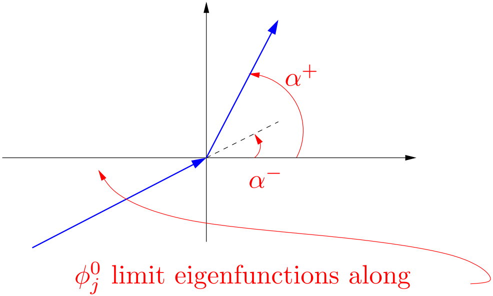
$\rightarrow$this step extends to ∞-dimension
$\rightarrow$this step is constructive

STEP 2: spread controllability (without phases)

By using the adiabatic theory, is it possible to reach some other state than eigenstates?



A4: how to compute angles



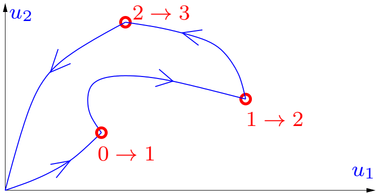
$$p_1 = |\cos(\theta(\alpha_-) - \theta(\alpha_+))| \quad p_2 = |\sin(\theta(\alpha_-) - \theta(\alpha_+))|,$$

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

$$(\cos\alpha, \sin\alpha)\, \mathcal{M}(\phi_i^0, \phi_{i+1}^0) \begin{pmatrix} \cos 2\theta(\alpha) \\ \sin 2\theta(\alpha) \end{pmatrix} = 0.$$

and by definition

$$\mathcal{M}(\phi_i, \phi_{i+1}) = \begin{pmatrix} \langle \phi_i, H_1 \phi_{i+1} \rangle & \frac{1}{2}\left(\langle \phi_{i+1}, H_1 \phi_{i+1} \rangle - \langle \phi_i, H_1 \phi_i \rangle\right) \\ \langle \phi_i, H_2 \phi_{i+1} \rangle & \frac{1}{2}\left(\langle \phi_{i+1}, H_2 \phi_{i+1} \rangle - \langle \phi_i, H_2 \phi_i \rangle\right) \end{pmatrix}.$$

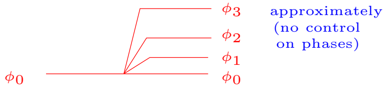


Transition between level 0 and a superposition of levels 0,1,2,3

by making angles at the eigenvalues intersections one can "spread the probability"

→this can be done at order $\sqrt{\varepsilon}$ or at order ε on special curves

→this step is constructive but cannot control the phases



→this step extends to ∞-dimension

STEP 3: spread controllability (with phases)

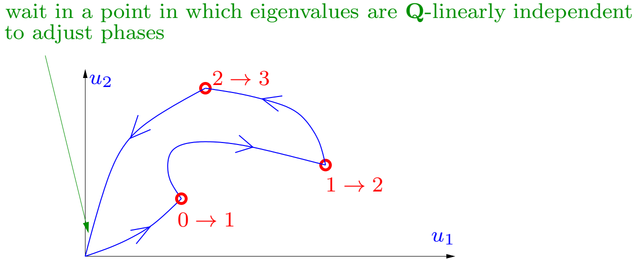
One can control the phases by using the following result:

Lemma

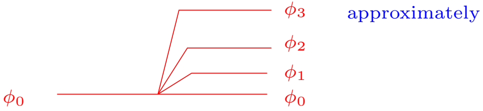
Let Σ be conically connected. Then there exists $\bar{\mathbf{U}} \subset \mathbf{U}$ which is dense and with zero-measure complement in $\mathbf{U}$ such that $\sum_{j=1}^{n} \alpha_j \lambda_j(\bar{\mathbf{u}}) = 0$ with $(\alpha_1, \ldots, \alpha_n) \in \mathbf{Q}^n$ and $\mathbf{u} \in \bar{\mathbf{U}}$ implies $\alpha_1 = \alpha_2 = \cdots = \alpha_n$.

This means that in the space of controls, close to every point there is a value of control for which the eigenvalues are $\mathbf{Q}$-linearly independent (except for the trace).

Hence one can modify a little the path by passing through a point in which the eigenvalues are $\mathbf{Q}$-linearly independent and wait in such a way that the phases take the corrected values (approximately).



$\rightarrow$this step is not really constructive since it is hard to take track of relative phases after an adiabatic path

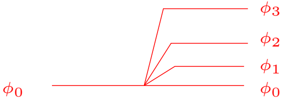


$\rightarrow$this step extends to ∞-dimension

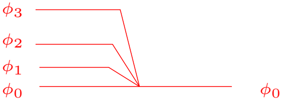
STEP 4: approximate controllability

Since if $u(t)$ send ψ_0 in ψ_1 in time T then $u(T-t)$ send $\bar{\psi}_1$ in $\bar{\psi}_0$

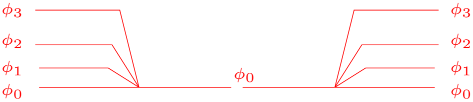
If you are able to do



you are also able to do



Then you are able to do



We have approximate controllability

$\rightarrow$this step extends to ∞-dimension

STEP 5: approximate controllability implies exact controllability

Theorem

Consider the system

$$i\dot{\psi}(t) = H(\mathbf{u}(t))\psi(t). \tag{3}$$

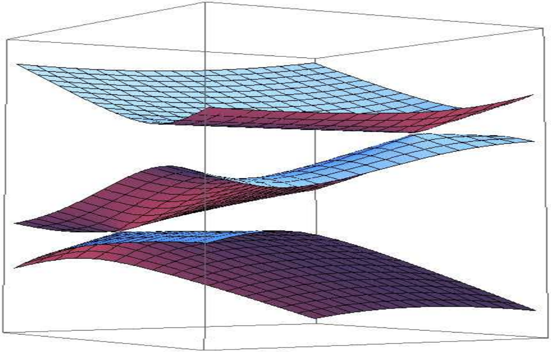
where $\psi : [0, T] \to S^{2n-1} \subset \mathbf{C}^n$, $\mathbf{u}(\cdot) : [0, T] \to \mathbf{U} \subset \mathbf{R}^m$, $H(\mathbf{u})$, $\mathbf{u} \in \mathbf{U}$, *are* $n \times n$ *Hermitian matrices. Then it is approximately controllable if and only it is exactly controllable.*

→even for a nonlinear dependence on the control

→here $H(\mathbf{u})$ can be complex (Hermitian)
→this step does not extend to ∞-dimension

Conclusions

If you see a spectrum like that:



then

- in finite dimension we get exact controllability (i.e. Lie Bracket generated)
- in infinite dimension we get approximate controllability

thanks

Extensions

Both in finite and infinite dimension, the fact that the spectrum is conically connected implies that:

- close to every point in the space of controls, there is a value of control for which the eigenvalues are $\mathbf{Q}$-linearly independent;
- controls couple every pair of eigenspaces.

In finite dimension

using the following

Theorem (see for instance Caponigro, Chambrion, Sigalotti, B., CMP2012)

Consider the control system

$$i\dot{g} = (H_0 + \sum_{1}^{m} u_i H_i)g, \quad g \in U(n) \textit{ (resp. } SU(n) \textit{ if } Trace(H_i) = 0\textit{)}$$

If the differences among eigenvalues of H_0 are all different and the controls couple every eigenstate of H_0 then the system is exactly controllable in $U(n)$ (resp. $SU(n)$). Some degeneracies are also admitted under additional hypotheses.

we get (in a non-constructive way)

conically connected $\Rightarrow$ exact controllability (i.e. LBG) on the group

In infinite dimension

using the following

Theorem (Caponigro, Chambrion, Sigalotti, B., CMP 2012)

Consider the control system

$$i\dot{\psi} = (H_0 + \sum_{1}^{m} u_i H_i)\psi, \quad \psi \in S \in \mathcal{H}$$

H_i *self adjoint + technical hypotheses on the domains*

If the differences among eigenvalues of H_0 *are all different and the controls couple every eigenstate of* H_0 *then the system is approximate controllable for the density matrix. Some degeneracies are also admitted under additional hypotheses.*

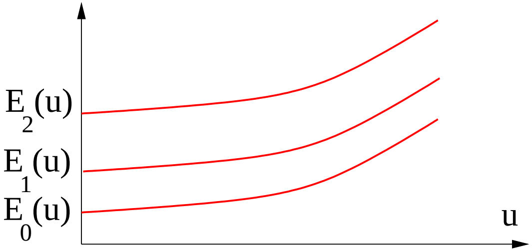
we get (in a non-constructive way)

conically connected $\Rightarrow$ approximate controllability for the density matrix

Thanks

A1: the adiabatic theory

The adiabatic theory states that if $H(u(t))$ is very slow and $\psi(x,0) = \phi_n$
$\psi(x,t) \sim \phi_n(u(t))$ (in the L^2 norm, up to phases)



A1: the adiabatic Theorem (rougher form)

- $\lambda(u_1, u_2)$ be an eigenvalue of $H(u_1, u_2)$ depending continuously on (u_1, u_2)
- for every $u_1, u_2 \in K$ (K compact subset of $\mathbf{R}^2$), $\lambda(u_1, u_2)$ is simple.

Let $\phi(u_1, u_2)$ be the corresponding eigenvector (defined up to a phase). Consider a path $(u_1, u_2) : [0, 1] \to K$ and its reparametrization $(u_1^\varepsilon(t), u_2^\varepsilon(t)) = (u_1(\varepsilon t), u_2(\varepsilon t))$, defined on $[0, 1/\varepsilon]$.

Then the solution $\psi_\varepsilon(t)$ of the equation $i\frac{d\psi_\varepsilon}{dt} = (H_0 + u_1^\varepsilon(t)H_1 + u_2^\varepsilon(t)H_2)\psi_\varepsilon(t)$ with initial condition $\psi_\varepsilon(0) = \phi(u_1(0), u_2(0))$ satisfies

$$\left\| \psi_\varepsilon\left(1/\varepsilon\right) - e^{i\vartheta}\phi\left(u_1^\varepsilon\left(1/\varepsilon\right), u_2^\varepsilon\left(1/\varepsilon\right)\right) \right\| \leq C\varepsilon \tag{4}$$

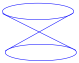
for some $\vartheta = \vartheta(\varepsilon) \in \mathbf{R}$.

- This means that, if the controls are slow enough, then, up to phases, the state of the system follows the evolution of the eigenstates of the time-dependent Hamiltonian.
- The constant C depends on the gap between the eigenvalue λ and the other eigenvalues.

A3: why a trajectory passing through a conical singularity induce a transition?: the two level case

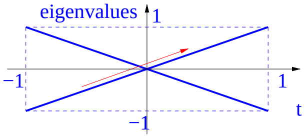
Two level systems:

$$i\begin{pmatrix}\dot\psi_1\\ \dot\psi_2\end{pmatrix}=\begin{pmatrix}u_1 & u_2\\ u_2 & -u_1\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix},\quad \lambda_\pm=\sqrt{u_1^2+u_2^2}$$



Let us take $u_1=t$, $t\in[-1,1]$, $u_2=0$

$$i\begin{pmatrix}\dot\psi_1\\ \dot\psi_2\end{pmatrix}=\begin{pmatrix}t & 0\\ 0 & -t\end{pmatrix}\begin{pmatrix}\psi_1\\ \psi_2\end{pmatrix},\quad \begin{array}{lcl}\psi_1(-1)=1 & & |\psi_1(1)|=1\\ \psi_2(-1)=0 & \Rightarrow & |\psi_2(1)|=0\\ \Rightarrow\lambda=-1 & & \Rightarrow\lambda=+1\end{array}$$



→For generic two level systems there is an exact climb (on special curves)

→On straight lines (or on generic smooth curves) the transition is of order $\sqrt{\varepsilon}$

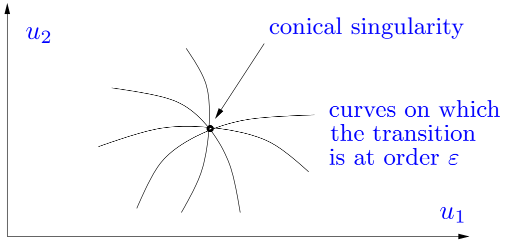
higher dimensional systems: Effective Hamiltonian

By adiabatic theory, at the order ε the dynamics is given by:

$$H_{eff}(\tau) = \begin{pmatrix} \lambda_\alpha(\tau) & 0 \\ 0 & \lambda_\beta(\tau) \end{pmatrix} + i\varepsilon \begin{pmatrix} 0 & \langle \dot{\phi}_\alpha(\tau), \phi_\beta(\tau) \rangle \\ \langle \dot{\phi}_\alpha(\tau), \phi_\beta(\tau) \rangle & 0 \end{pmatrix}$$

$\rightarrow$For a smooth curve passing through a conical intersection the term in $i\varepsilon$ give a contribution of order $\sqrt{\varepsilon}$ [Teufel 2003] (adiabatic theorem gives a decoupling at the order ε, far from singularities)

$\rightarrow$on the special curves $\begin{cases} \dot{u}_1 = -\langle \phi_i, V_2 \phi_{i+1} \rangle \\ \dot{u}_2 = \langle \phi_i, V_1 \phi_{i+1} \rangle \end{cases}$ the term in $i\varepsilon$ vanish and hence the climb is of order ε (the same as the adiabatic approximation).



Approximate-exact controllability on the group

Approximate and exact controllability on the group $SU(n)$ are equivalent. This is a direct consequence of the following result,

Theorem

If an everywhere dense subgroup H of a simple Lie group G of dimension larger than 1 contains an analytic arc, then $H = G$.

Let us apply this theorem to our system,

$$\begin{cases} \dot{g} = M(u)\, g, \\ y(0) = Id. \end{cases} \tag{5}$$

Let (5) be approximately controllable. Then, the orbit from the identity is an everywhere dense subgroup H of $SU(n)$. Any trajectory of (5) with constant u is an analytic arc, contained in H. Then $H = SU(n)$, i.e., the orbit is the whole group. Since we are in the compact case, we have that the accessible set coincides with the orbit, i.e., that system (5) is exactly controllable.

Conical intersections are generic for $m = 2, 3$ (finite dimension)

Let us first consider the case $m = 2$. Let sym(n) be the set of all $n \times n$ symmetric real matrices. Then, generically with respect to the pair (H_1, H_2) in sym$(n) \times$ sym(n) (i.e., for all (H_1, H_2) in an open and dense subset of sym$(n) \times$ sym(n)), for each $\mathbf{u} = (u_1, u_2) \in \mathbb{R}^2$ and $\lambda \in \mathbf{R}$ such that λ is a multiple eigenvalue of $H_0 + u_1 H_1 + u_2 H_2$, the eigenvalue intersection $\mathbf{u}$ is conical. Moreover, each conical intersection $\mathbf{u}$ is structurally stable, in the sense that small perturbations of H_0, H_1 and H_2 give rise, in a neighborhood of $\mathbf{u}$, to conical intersections for the perturbed H.
In the case $m = 3$, let Herm(n) be the space of $n \times n$ Hermitian matrices. Then, generically with respect to the triple (H_1, H_2, H_3) in Herm$(n)^3$, for each $\mathbf{u} = (u_1, u_2, u_3) \in \mathbb{R}^3$ and $\lambda \in \mathbf{R}$ such that λ is a multiple eigenvalue of $H_0 + u_1 H_1 + u_2 H_2 + u_3 H_3$, the eigenvalue intersection $\mathbf{u}$ is conical. Structural stability also holds, in the same sense as above.

Conical intersections are generic in infinite dimension

Conical intersections are generic in the reference case where $\mathcal{H} = L^2(\Omega, \mathbf{C})$, $H_0 = -\Delta + V_0 : D(H_0) = H^2(\Omega, \mathbf{C}) \cap H_0^1(\Omega, \mathbf{C}) \to L^2(\Omega, \mathbf{C})$, $H_1 = V_1$, $H_2 = V_2$, with Ω a bounded domain of $\mathbf{R}^d$ and $V_j \in \mathcal{C}^0(\Omega, \mathbf{R})$ for $j = 0, 1, 2$. Indeed, generically with respect to the pair (V_1, V_2) in $\mathcal{C}^0(\Omega, \mathbf{R}) \times \mathcal{C}^0(\Omega, \mathbf{R})$ (i.e., for all (V_1, V_2) in a countable intersection of open and dense subsets of $\mathcal{C}^0(\Omega, \mathbf{R}) \times \mathcal{C}^0(\Omega, \mathbf{R})$), for each $\mathbf{u} \in \mathbb{R}^2$ and $\lambda \in \mathbf{R}$ such that λ is a multiple eigenvalue of $H_0 + u_1 H_1 + u_2 H_2$, the eigenvalue intersection $\mathbf{u}$ is conical. Moreover, each conical intersection $\mathbf{u}$ is structurally stable, in the sense that small perturbations of V_0, V_1 and V_2 give rise, in a neighbourhood of $\mathbf{u}$, to conical intersections for the perturbed H.