# Modeling and Control of Quantum Systems 

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## Controllability of bilinear Schrödinger equations ${ }^{1}$

## Schrödinger equation

$$
i \frac{d}{d t}|\psi\rangle=\left(H_{0}+\sum_{k=1}^{m} u_{k} H_{k}\right)|\psi\rangle
$$

## State controllability

For any $\left|\psi_{a}\right\rangle$ and $\left|\psi_{b}\right\rangle$ on the unit sphere of $\mathcal{H}$, there exist a time $T>0$, a global phase $\theta \in[0,2 \pi[$ and a piecewise continuous control $[0, T] \ni t \mapsto u(t)$ such that the solution with initial condition $|\psi\rangle_{0}=\left|\psi_{a}\right\rangle$ satisfies $|\psi\rangle_{T}=e^{i \theta}\left|\psi_{b}\right\rangle$.
${ }^{1}$ See, e.g., Introduction to Quantum Control and Dynamics by D. D'Alessandro. Chapman \& Hall/CRC, 2008.

## Propagator equation:

$$
i \frac{d}{d t} U=\left(H_{0}+\sum_{k=1}^{m} u_{k} H_{k}\right) U, \quad U(0)=\mathbf{1}
$$

We have $|\psi\rangle_{t}=U(t)|\psi\rangle_{0}$.

## Operator controllability

For any unitary operator $V$ on $\mathcal{H}$, there exist a time $T>0$, a global phase $\theta$ and a piecewise continuous control $[0, T] \ni t \mapsto u(t)$ such that the solution of propagator equation satisfies $U_{T}=e^{i \theta} V$.

Operator controllability implies state controllability

$$
\frac{d}{d t} U=\left(A_{0}+\sum_{k=1}^{m} u_{k} A_{k}\right) U
$$

with $A_{k}=H_{k} / i$ are skew-Hermitian. We define

$$
\begin{aligned}
\mathcal{L}_{0} & =\operatorname{span}\left\{A_{0}, A_{1}, \ldots, A_{m}\right\} \\
\mathcal{L}_{1} & =\operatorname{span}\left(\mathcal{L}_{0},\left[\mathcal{L}_{0}, \mathcal{L}_{0}\right]\right) \\
\mathcal{L}_{2} & =\operatorname{span}\left(\mathcal{L}_{1},\left[\mathcal{L}_{1}, \mathcal{L}_{1}\right]\right) \\
\vdots & \\
\mathcal{L}=\mathcal{L}_{\nu} & =\operatorname{span}\left(\mathcal{L}_{\nu-1},\left[\mathcal{L}_{\nu-1}, \mathcal{L}_{\nu-1}\right]\right)
\end{aligned}
$$

## Lie Algebra Rank Condition

Operator controllable if, and only if, the Lie algebra generated by the $m+1$ skew-Hermitian matrices $\left\{-i H_{0},-i H_{1}, \ldots,-i H_{m}\right\}$ is either $s u(n)$ or $u(n)$.

## Exercice

Show that $i \frac{d}{d t}|\psi\rangle=\left(\frac{\omega_{\text {eg }}}{2} \sigma_{z}+\frac{u}{2} \sigma_{x}\right)|\psi\rangle,|\psi\rangle \in \mathbb{C}^{2}$ is controllable.

We consider $H=H_{0}+u H_{1},(|j\rangle)_{j=1, \ldots, n}$ the eigenbasis of $H_{0}$. We assume $H_{0}|j\rangle=\omega_{j}|j\rangle$ where $\omega_{j} \in \mathbb{R}$, we consider a graph $G$ :

$$
V=\{|1\rangle, \ldots,|n\rangle\}, \quad E=\left\{\left(\left|j_{1}\right\rangle,\left|j_{2}\right\rangle\right) \mid 1 \leq j_{1}<j_{2} \leq n,\left\langle j_{1}\right| H_{1}\left|j_{2}\right\rangle \neq 0\right\} .
$$

$G$ amits a degenerate transition if there exist $\left(\left|j_{1}\right\rangle,\left|j_{2}\right\rangle\right) \in E$ and $\left(\left|/_{1}\right\rangle,\left|I_{2}\right\rangle\right) \in E$, admitting the same transition frequencies,

$$
\left|\omega_{j_{1}}-\omega_{j_{2}}\right|=\left|\omega_{l_{1}}-\omega_{l_{2}}\right|
$$

## A sufficient controllability condition

Remove from $E$, all the edges with identical transition frequencies. Denote by $\bar{E} \subset E$ the reduced set of edges without degenerate transitions and by $\bar{G}=(V, \bar{E})$. If $\bar{G}$ is connected, then the system is operator controllable.

The dynamics of the 2-qubit system (state $|\psi\rangle \in \mathbb{C}^{2} \otimes \mathbb{C}^{2}$ ) obey

$$
\begin{equation*}
i \frac{d}{d t}|\psi\rangle=\left(H_{0}+u H_{1}\right)|\psi\rangle=\left(Z_{1} Z_{2}+u\left(X_{1}+X_{2}\right)\right)|\psi\rangle \tag{1}
\end{equation*}
$$

with $u \in \mathbb{R}$ as control.
1 Prove that $X_{1} X_{2}$ commutes with $H_{0}$ and with $H_{1}$.
2 Is the system controllable ?
3 Use the spectral basis of $X_{1} X_{2}$ and the decomposition $\operatorname{span}\{|00\rangle,|01\rangle,|10\rangle,|11\rangle\}=$ $\operatorname{span}\{|++\rangle,|--\rangle\} \oplus \operatorname{span}\{|+-\rangle,|-+\rangle\}$ with $|+\rangle=\frac{|0\rangle+|1\rangle}{\sqrt{2}}$,
 separated systems on $\operatorname{span}\{|++\rangle,|--\rangle\}$ and on $\operatorname{span}\{|+-\rangle,|-+\rangle\}$.
4 Prove that one of these sub-systems is controllable and that the other one is not controllable.

Bilinear Schrödinger equation:

$$
i \frac{d}{d t}|\psi\rangle=\left(H_{0}+u(t) H_{1}\right)|\psi\rangle
$$

Control task: to prepare $|\bar{\psi}\rangle$ such that

$$
H_{0}|\bar{\psi}\rangle=\bar{\omega}|\bar{\psi}\rangle .
$$

The states $|\psi\rangle$ and $e^{i \phi}|\psi\rangle$ represent the same physical states
We add a fictitious control:

$$
i \frac{d}{d t}|\psi\rangle=\left(H_{0}+u(t) H_{1}\right)|\psi\rangle+\omega(t)|\psi\rangle
$$

$|\bar{\psi}\rangle$ is a stationary solution for $u(t) \equiv 0$ and $\omega(t) \equiv-\bar{\omega}$.

We look for feedback laws $u(t)=f(|\psi\rangle)$ and $\omega(t)=g(|\psi\rangle)$ such that the solution of

$$
i \frac{d}{d t}|\psi\rangle=\left(H_{0}+f(|\psi\rangle) H_{1}+g(|\psi\rangle)\right)|\psi\rangle
$$

converges asymptotically towards $|\bar{\psi}\rangle$.

## Remark

These feedback laws are calculated off-line and by simulating the closed-loop system and are then applied in open-loop on the real system.

We consider

$$
\mathcal{V}(|\psi\rangle)=\frac{1}{2} \||\psi\rangle-|\bar{\psi}\rangle \|^{2}=1-\Re(\langle\bar{\psi} \mid \psi\rangle)
$$

We have

$$
\frac{d}{d t} \mathcal{V}=-u(t) \Im\langle\bar{\psi}| H_{1}|\psi\rangle-(\omega(t)+\bar{\omega}) \Im(\langle\bar{\psi} \mid \psi\rangle)
$$

Choice of feedback laws

$$
u(t) \equiv a \Im\left(\langle\bar{\psi}| H_{1}|\psi\rangle\right) \quad \text { and } \quad \omega(t) \equiv-\bar{\omega}+b \Im(\langle\bar{\psi} \mid \psi\rangle)
$$

where $a, b>0$.

## LaSalle's invariance principle

## Theorem (Lyapunov function and Lasalle invariance principle)

Take $\Omega \subset \mathbb{R}^{n}$ an open and non-empty subset of $\mathbb{R}^{n}$ and
$\Omega \ni x \mapsto v(x) \in \mathbb{R}^{n}$ continuously differentiable function of $x$. Consider
$\Omega \ni x \mapsto V(x) \in \mathbb{R}$ a continuously differentiable function of $x$ and assume that

1 there exits $c \in \mathbb{R}$ such that the subset $V_{c}=\{x \in \Omega \mid V(x) \leq c\}$ of $\mathbb{R}^{n}$ is compact (bounded and closed) and non-empty.
$2 V$ is a decreasing time function for solutions of $\frac{d}{d t} x=v(x)$ inside $V_{c}$ :

$$
\forall x \in V_{c}, \quad \frac{d}{d t} V(x)=\nabla V(x) \cdot v(x)=\sum_{i=1}^{n} \frac{\partial V}{\partial x_{i}}(x) v_{i}(x) \leq 0
$$

Then for any initial condition $x^{0} \in V_{c}$, the solution of $\frac{d}{d t} x=v(x)$ remains in $V_{c}$, is defined for all $t>0$ (no explosion in finite time) and converges towards the largest invariant set included in

$$
\left\{x \in V_{c} \left\lvert\, \frac{d}{d t} V(x)=0\right.\right\} .
$$

## Application to Schrödinger equation

$d \mathcal{V} / d t=0$ and invariance

$$
\begin{aligned}
\Im(\langle\bar{\psi} \mid \psi\rangle) & =0, \\
\Im\left(\langle\bar{\psi}| H_{1}|\psi\rangle\right) & =0, \\
\Re\left(\langle\bar{\psi}|\left[H_{0}, H_{1}\right]|\psi\rangle\right) & =0, \\
\vdots & \\
\Im\left(\langle\bar{\psi}| \operatorname{ad}_{H_{1}}^{2 k} H_{0}|\psi\rangle\right) & =0, \\
\Re\left(\langle\bar{\psi}| \operatorname{ad}_{H_{1}}^{2 k+1} H_{0}|\psi\rangle\right) & =0 .
\end{aligned}
$$

Assume that the spectrum of $H_{0}$ is not $\bar{\omega}$-degenerate: i.e. $H_{0}$ is not degenerate and for any two eigenvalues $\omega_{\alpha} \neq \omega_{\beta}$,

$$
\left|\omega_{\alpha}-\bar{\omega}\right| \neq\left|\omega_{\beta}-\bar{\omega}\right| ;
$$

## $\Omega$-limit set

Intersection of $\mathbb{S}^{2 n-1}$ with $\mathbb{R}|\bar{\psi}\rangle \bigcup_{\alpha} \mathbb{C}\left|\psi_{\alpha}\right\rangle$, where $\left|\psi_{\alpha}\right\rangle$ is any eigenvector of $H_{0}$ non co-linear with $|\bar{\psi}\rangle$ and satisfying $\langle\bar{\psi}| H_{1}\left|\psi_{\alpha}\right\rangle=0$.

## Convergence Analysis

## Theorem

Under the assumption of $H_{0}$ not $\bar{\omega}$-degenerate and mono-photonic transitions to $|\bar{\psi}\rangle\left(\langle\bar{\psi}| H_{1}\left|\psi_{\alpha}\right\rangle \neq 0\right.$ for all eigenvector $\left|\psi_{\alpha}\right\rangle$ of $H_{0}$ ), the $\Omega$-limit set reduces to $\{|\bar{\psi}\rangle,-|\bar{\psi}\rangle\}$. The equilibrium $-|\bar{\psi}\rangle$ is unstable and the attraction region for the equilibrium $|\psi\rangle$ is exactly $\mathbb{S}^{2 n-1} /\{-|\bar{\psi}\rangle\}$.

## Remark

Assumptions of $H_{0}$ not $\bar{\omega}$-degenerate and mono-photonic transitions to $|\bar{\psi}\rangle$

Controllability of linearized system around

$$
(|\psi\rangle, u, \omega)=(|\bar{\psi}\rangle, 0,-\bar{\omega})
$$

Main idea: stabilizing around another reference trajectory, around which the linearized system is controllable.

Reference trajectory:

$$
i \frac{d}{d t}\left|\psi_{r}\right\rangle=\left(H_{0}+u_{r}(t) H_{1}+\omega_{r}(t)\right)\left|\psi_{r}\right\rangle
$$

Same Lyapunov function: $\mathcal{V}(t,|\psi\rangle)=1-\Re\left(\left\langle\psi_{r}(t) \mid \psi\right\rangle\right)$.
Feedback laws:

$$
\begin{aligned}
u(t,|\psi\rangle) & =u_{r}(t)+a \Im\left(\left\langle\psi_{r}(t)\right| H_{1}|\psi\rangle\right), \\
\omega(t,|\psi\rangle) & =\omega_{r}(t)+b \Im\left(\left\langle\psi_{r}(t) \mid \psi\right\rangle\right)
\end{aligned}
$$

## Tracking and quantum gate design

We consider a drift-less propagator dynamics:

$$
i \frac{d}{d t} U=\left(\omega \mathbf{1}+\sum_{k=1}^{m} u_{k} H_{k}\right) U,\left.\quad U\right|_{t=0}=\mathbf{1}
$$

Periodic reference trajectory: $u_{k}^{r}$ and $\omega_{r}$ periodic and odd.

## Main idea

By a Coron's result, as soon as $\operatorname{Lie}\left(H_{1}, \ldots, H_{m}\right)=s u(n)$, one can find reference controls $\omega^{r}$ and $u_{k}^{r}$ around which the linearized system is controllable.

Lyapunov function: $\mathcal{V}\left(U, U^{r}\right)=n-\Re\left(\operatorname{Tr}\left(U^{\dagger} U^{r}\right)\right)$. Feedback laws:

$$
\begin{aligned}
u_{k} & =u_{k}^{r}-a_{k} \Im\left(\operatorname{Tr}\left(U^{\dagger} H_{k} U^{r}\right)\right) \\
\omega & =\omega^{r}-b \Im\left(\operatorname{Tr}\left(U^{\dagger} U^{r}\right)\right)
\end{aligned}
$$

## Remark

The LaSalle's invariance principle also works for time-periodic systems; only one needs to be be careful about the notion of invariance:
A set $S$ is said to be invariant for the time-periodic system $\frac{d}{d t} x=v(x, t)$ if, for all $x_{0} \in S$ there exists a time $t_{0}>0$ such that the solution starting from $x_{0}$ at time $t_{0}$ remains in the set $S$ for all $t \geq t_{0}$.

## Two optimal control problems

For given $T,\left|\psi_{a}\right\rangle$ and $\left|\psi_{b}\right\rangle$, find the open-loop control $[0, T] \ni t \mapsto u(t)$ such that

$$
\begin{aligned}
& \min _{\substack{\left.u_{k} \in L^{2}([0, T], \mathbb{R}) \\
i \frac{d}{d t}|\psi\rangle\right\rangle=\left(H_{0}+\sum_{k=1}^{m} u_{k} H_{k}\right)|\psi\rangle \\
|\psi\rangle_{t=0} \\
=\left|\psi_{a}\right\rangle,\left|\left\langle\psi_{b} \mid \psi\right\rangle\right|_{t=T}^{2}=1}} \frac{1}{2} \int_{0}^{T}\left(\sum_{k=1}^{m} u_{k}^{2}\right) \\
&
\end{aligned}
$$

Since the initial and final constraints are difficult to satisfy simultaneously from a numerical point of view, consider the second problem where the final constraint is penalized with $\alpha>0$ :

$$
\begin{aligned}
& \min _{\substack{u_{k} \in L^{2}([0, T], \mathbb{R}) \\
i \frac{d}{d t}|\psi\rangle=\left(H_{0}+\sum_{k=1}^{m} u_{k} H_{k}\right)|\psi\rangle \\
|\psi\rangle_{t=0}=\left|\psi_{a}\right\rangle}} \frac{1}{2} \int_{0}^{T}\left(\sum_{k=1}^{m} u_{k}^{2}\right)+\frac{\alpha}{2}\left(1-\left|\left\langle\psi_{b} \mid \psi\right\rangle\right|_{T}^{2}\right) \\
&
\end{aligned}
$$

For two-points problem, the first order stationary conditions read:

$$
\left\{\begin{array}{c}
i \frac{d}{d t}|\psi\rangle=\left(H_{0}+\sum_{k=1}^{m} u_{k} H_{k}\right)|\psi\rangle, t \in(0, T) \\
i \frac{d}{d t}|p\rangle=\left(H_{0}+\sum_{k=1}^{m} u_{k} H_{k}\right)|p\rangle, t \in(0, T) \\
u_{k}=-\Im\left(\langle p| H_{k}|\psi\rangle\right), k=1, \ldots, m, \quad t \in(0, T) \\
|\psi\rangle_{t=0}=\left|\psi_{a}\right\rangle,\left|\left\langle\psi_{b} \mid \psi\right\rangle\right|_{t=T}^{2}=1
\end{array}\right.
$$

For the relaxed problem, the first order stationary conditions read:

$$
\left\{\begin{array}{c}
i \frac{d}{d t}|\psi\rangle=\left(H_{0}+\sum_{k=1}^{m} u_{k} H_{k}\right)|\psi\rangle, t \in(0, T) \\
i \frac{d}{d t}|p\rangle=\left(H_{0}+\sum_{k=1}^{m} u_{k} H_{k}\right)|p\rangle, t \in(0, T) \\
u_{k}=-\Im\left(\langle p| H_{k}|\psi\rangle\right), k=1, \ldots, m, \quad t \in(0, T) \\
|\psi\rangle_{t=0}=\left|\psi_{a}\right\rangle,|p\rangle_{t=T}=-\alpha\left\langle\psi_{b} \mid \psi\right\rangle_{t=T}\left|\psi_{b}\right\rangle
\end{array}\right.
$$

The dynamical system

$$
(\Sigma)\left\{\begin{array}{c}
i \frac{d}{d t}|\psi\rangle=\left(H_{0}+\sum_{k=1}^{m} u_{k} H_{k}\right)|\psi\rangle, t \in(0, T) \\
i \frac{d}{d t}|p\rangle=\left(H_{0}+\sum_{k=1}^{m} u_{k} H_{k}\right)|p\rangle, t \in(0, T) \\
u_{k}=-\Im\left(\langle p| H_{k}|\psi\rangle\right), k=1, \ldots, m, \quad t \in(0, T)
\end{array}\right.
$$

is Hamiltonian with $|\psi\rangle$ and $|p\rangle$ being the conjugate variables. The underlying Hamiltonian function is given by (Pontryaguin Maximum Principle): $\overline{\mathbb{H}}(|\psi\rangle,|p\rangle)=\min _{u \in \mathbb{R}^{m}} \mathbb{H}(|\psi\rangle,|p\rangle, u)$ where

$$
\mathbb{H}(|\psi\rangle,|p\rangle, u)=\frac{1}{2}\left(\sum_{k=1}^{m} u_{k}^{2}\right)+\Im\left(\langle p| H_{0}+\sum_{k=1}^{m} u_{k} H_{k}|\psi\rangle\right) .
$$

Thus for any solutions $(|\psi\rangle,|p\rangle)$ of $(\Sigma)$,

$$
\overline{\mathbb{H}}(|\psi\rangle,|p\rangle)=\Im\left(\langle p| H_{0}|\psi\rangle\right)-\frac{1}{2}\left(\sum_{k=1}^{m} \Im\left(\langle p| H_{k}|\psi\rangle\right)^{2}\right) .
$$

is independent of $t$.
Main difficulty: such systems are not, in general, integrable in the Arnold-Liouville sense.

## Monotone numerical scheme for the relaxed problem $(1)^{2}$

Take an $L^{2}$ control $[0, T] \ni t \mapsto u(t)(\operatorname{dim}(u)=1$ here $)$ and denote by

- $\left|\psi_{u}\right\rangle$ the solution of forward system $i \frac{d}{d t}|\psi\rangle=\left(H_{0}+u H_{1}\right)|\psi\rangle$ starting from $\left|\psi_{\mathrm{a}}\right\rangle$.
- $\left|p_{u}\right\rangle$ the adjoint associated to $u$, i.e. the solution of the backward system $i \frac{d}{d t}\left|p_{u}\right\rangle=\left(H_{0}+u H_{1}\right)\left|p_{u}\right\rangle$ with $\left|p_{u}\right\rangle_{T}=-\alpha P\left|\psi_{u}\right\rangle_{T}, P$ projector on $\left|\psi_{b}\right\rangle$, $P|\phi\rangle \equiv\left\langle\psi_{b} \mid \phi\right\rangle\left|\psi_{b}\right\rangle$.
- $J(u)=\frac{1}{2} \int_{0}^{T} u^{2}+\frac{\alpha}{2}\left(1-\left|\left\langle\psi_{b} \mid \psi_{u}\right\rangle\right|_{T}^{2}\right)$.

Starting from an initial guess $u^{0} \in L^{2}([0, T], \mathbb{R})$, the monotone scheme generates a sequence of controls $u^{\nu} \in L^{2}([0, T], \mathbb{R})$, $\nu=1,2, \ldots$, such that the cost $J\left(u^{\nu}\right)$ is decreasing, $J\left(u^{\nu+1}\right) \leq J\left(u^{\nu}\right)$.
${ }^{2}$ D. Tannor, V. Kazakov, and V. Orlov. Time Dependent Quantum Molecular Dynamics, chapter Control of photochemical branching: Novel procedures for finding optimal pulses and global upper bounds, pages 347-360. Plenum, 1992.

Assume that, at step $\nu$, we have computed the control $u^{\nu}$, the associated quantum state $\left|\psi^{\nu}\right\rangle=\left|\psi_{u^{\nu}}\right\rangle$ and its adjoint $\left|p^{\nu}\right\rangle=\left|p_{u^{\nu}}\right\rangle$. We get their new time values $u^{\nu+1},\left|\psi^{\nu+1}\right\rangle$ and $\left|p^{\nu+1}\right\rangle$ in two steps:
1 Imposing $u^{\nu+1}=-\Im\left(\left\langle p^{\nu}\right| H_{1}\left|\psi^{\nu+1}\right\rangle\right)$ is just a feedback; one get $u^{\nu+1}$ just by a forward integration of the nonlinear Schrödinger equation,

$$
i \frac{d}{d t}|\psi\rangle=\left(H_{0}-\Im\left(\left\langle p^{\nu}\right| H_{1}|\psi\rangle\right) H_{1}\right)|\psi\rangle, \quad|\psi\rangle_{0}=\left|\psi_{a}\right\rangle
$$

that provides $[0, T] \ni t \mapsto\left|\psi^{\nu+1}\right\rangle$ and the new control $u^{\nu+1}$.
2 Backward integration from $t=T$ to $t=0$ of

$$
i \frac{d}{d t}|p\rangle=\left(H_{0}+u^{\nu+1}(t) H_{1}\right)|p\rangle, \quad|p\rangle_{T}=-\alpha\left\langle\psi_{b} \mid \psi^{\nu+1}\right\rangle_{T}\left|\psi_{b}\right\rangle
$$

yields to the new adjoint trajectory $[0, T] \ni t \mapsto\left|p^{\nu+1}\right\rangle$.

Why $J\left(u^{\nu+1}\right) \leq J\left(u^{\nu}\right)$ ?

- Because we have the identity for any open-loop controls $u$ and $v$.

$$
\begin{aligned}
& J(u)-J(v)=-\frac{\alpha}{2}\left(\left\langle\psi_{u}-\psi_{v}\right| P\left|\psi_{u}-\psi_{v}\right\rangle\right)_{T} \\
&+\frac{1}{2}\left(\int_{0}^{T}(u-v)\left(u+v+2 \Im\left(\left\langle p_{v}\right| H_{1}\left|\psi_{u}\right\rangle\right)\right)\right) .
\end{aligned}
$$

■ If $u=-\Im\left(\left\langle p_{v}\right| H_{1}\left|\psi_{u}\right\rangle\right)$ for all $t \in[0, T)$, we have

$$
J(u)-J(v)=-\frac{\alpha}{2}\left(\left\langle\psi_{u}-\psi_{v}\right| P\left|\psi_{u}-\psi_{v}\right\rangle\right)_{T}-\frac{1}{2}\left(\int_{0}^{T}(u-v)^{2}\right)
$$

and thus $J(u) \leq J(v)$.
■ Take $v=u^{\nu}, u=u^{\nu+1}$ : then $\left|p_{v}\right\rangle=\left|p^{\nu}\right\rangle,\left|\psi_{v}\right\rangle=\left|\psi^{\nu}\right\rangle$,
$\left|p_{u}\right\rangle=\left|p^{\nu+1}\right\rangle$ and $\left|\psi_{u}\right\rangle=\left|\psi^{\nu+1}\right\rangle$.

## Monotone numerical scheme for the relaxed problem (4)

## Proof of

$$
J(u)-J(v)=-\frac{\alpha}{2}\left(\left\langle\psi_{u}-\psi_{v}\right| P\left|\psi_{u}-\psi_{v}\right\rangle\right)_{T}+\frac{1}{2}\left(\int_{0}^{T}(u-v)\left(u+v+2 \Im\left(\left\langle p_{v}\right| H_{1}\left|\psi_{u}\right\rangle\right)\right)\right) .
$$

## Start with

Hermitian product of $i \frac{d}{d t}\left(\left|\psi_{u}\right\rangle-\left|\psi_{v}\right\rangle\right)=\left(H_{0}+v H_{1}\right)\left(\left|\psi_{u}\right\rangle-\left|\psi_{v}\right\rangle\right)+(u-v) H_{1}\left|\psi_{u}\right\rangle$ with $\left|p_{v}\right\rangle$ :

$$
\left\langle p_{v} \left\lvert\, \frac{d\left(\psi_{u}-\psi_{v}\right)}{d t}\right.\right\rangle=\left\langle p_{v}\right| \frac{H_{0}+v H_{1}}{i}\left|\psi_{u}-\psi_{v}\right\rangle+\left\langle p_{v}\right| \frac{(u-v) H_{1}}{i}\left|\psi_{u}\right\rangle .
$$

Integration by parts (use $\left|\psi_{v}\right\rangle_{0}=\left|\psi_{u}\right\rangle_{0},\left|p_{v}\right\rangle_{T}=-\alpha P\left|\psi_{v}\right\rangle_{T}$ and $\frac{d}{d t}\left\langle p_{v}\right|=-\left\langle p_{v}\right|\left(\frac{H_{0}+v H_{1}}{i}\right)$ ):

$$
\begin{aligned}
\int_{0}^{T}\left\langle p_{v} \left\lvert\, \frac{d\left(\psi_{u}-\psi_{v}\right)}{d t}\right.\right\rangle=\left\langle p_{v} \mid \psi_{u}-\psi_{v}\right\rangle_{T} & -\left\langle p_{v} \mid \psi_{u}-\psi_{v}\right\rangle_{0}-\int_{0}^{T}\left\langle\left.\frac{d p_{v}}{d t} \right\rvert\, \psi_{u}-\psi_{v}\right\rangle \\
& =-\alpha\left\langle\psi_{v}\right| P\left|\psi_{u}-\psi_{v}\right\rangle_{T}+\int_{0}^{T}\left\langle p_{v}\right| \frac{H_{0}+v H_{1}}{i}\left|\psi_{u}-\psi_{v}\right\rangle
\end{aligned}
$$

Thus $-\alpha\left\langle\psi_{v}\right| P\left|\psi_{u}-\psi_{v}\right\rangle_{T}=\int_{0}^{T}\left\langle p_{v}\right| \frac{(u-v) H_{1}}{i}\left|\psi_{u}\right\rangle$ and
$\alpha \Re\left(\left\langle\psi_{v}\right| P\left|\psi_{u}-\psi_{v}\right\rangle_{T}\right)=-\int_{0}^{T} \Im\left(\left\langle p_{v}\right|(u-v) H_{1}\left|\psi_{u}\right\rangle\right)$. Finally we have

$$
J(u)-J(v)=-\frac{\alpha}{2}\left(\left\langle\psi_{u}-\psi_{v}\right| P\left|\psi_{u}-\psi_{v}\right\rangle\right)_{T}+\frac{1}{2}\left(\int_{0}^{T}(u-v)\left(u+v+2 \Im\left(\left\langle p_{v}\right| H_{1}\left|\psi_{u}\right\rangle\right)\right)\right) .
$$

For given $T, a_{k} \geq 0$ and $b_{k} \geq 0\left(\sum_{k=1}^{n} a_{k}^{2}=\sum_{k=1}^{n} b_{k}^{2}=1\right)$,

$$
\begin{aligned}
& \min _{\mathbf{u}_{k, l} \in L^{2}([0, T], \mathbb{C}),(k, l) \in I} \quad \frac{1}{2} \int_{0}^{T}\left(\sum_{(k, l) \in I}\left|\mathbf{u}_{k \mid}\right|^{2}\right) \\
& i \frac{d}{d t}|\psi\rangle=\left(\sum_{(k, l) \in I} \mu_{k} \mathbf{u}_{k l}|k\rangle\langle I|\right)|\psi\rangle, \\
& |\langle k \mid \psi\rangle|_{t=0}^{2}=a_{k}^{2},|\langle k \mid \psi\rangle|_{t=T}^{2}=b_{k}^{2}, k=1, \ldots, n
\end{aligned}
$$

admits the same minimal cost as the following reduced problem

$$
\begin{gathered}
\min _{v_{k, I} \in L^{2}([0, T], \mathbb{R}), v_{k l}=-v_{l, k},(k, l) \in I} \\
\frac{d}{d t}|\phi\rangle=\left(\sum_{(k, l) \in I} \mu_{k l} v_{k l}|k\rangle\langle I|\right)|\phi\rangle \\
\left.\langle k \mid \phi\rangle\right|_{t=0}=a_{k},\langle k \mid \phi\rangle_{t=T}=b_{k}, k=1, \ldots, n
\end{gathered}
$$

where the components of $|\psi\rangle=|\phi\rangle$ remain real, the $\mathbf{u}_{k l}$ 's are purely imaginary, $\mathbf{u}_{k l}=i v_{k l}\left(v_{k l} \in \mathbb{R}\right.$ with $\left.v_{k l}=-v_{l k}\right)$.
${ }^{3}$ U. Boscain and G. Charlot. Resonance of minimizers for $n$-level quantum systems with an arbitrary cost. ESAIM COCV, 10:593-614,2004.

■ Go back to resulting optimal physical controls $\left(\mathbf{u}_{k l}=i v_{k l}\right)$ :

$$
\mathbf{u}_{k l}(t) e^{i\left(\omega_{k}-\omega_{l}\right) t}+\mathbf{u}_{k l}^{*}(t) e^{-i\left(\omega_{k}-\omega_{l}\right) t}=-2 v_{k l}(t) \sin \left(\left(\omega_{k}-\omega_{l}\right) t\right)
$$

- They are in resonance with the frequency transition between $|k\rangle$ and $|\Lambda\rangle$. They contain only amplitude modulations (up to a $\pi$ phase-shift since $v_{k l}$ can pass through zero).
■ For drift-less quantum systems

$$
i \frac{d}{d t}|\psi\rangle=\left(\sum_{(k, l) \in I} \mu_{k l} \mathbf{u}_{k l}|k\rangle\langle I|\right)|\psi\rangle
$$

population transfer minimizing the $L^{2}$ control norm is achieved by resonant controls $\mathbf{u}_{k l}=i v_{k l}$ with $v_{k l} \in \mathbb{R}$ (the reduction of the problem to a real case of half dimension).

Associated to any $\theta=\left(\theta_{1}, \theta_{2}, \ldots, \theta_{n}\right)$ consider

$$
|\psi\rangle \mapsto\left|\psi^{\theta}\right\rangle=\left(\sum_{k=1}^{n} e^{i \theta_{k}}|k\rangle\langle k|\right)|\psi\rangle, \quad \mathbf{u}_{k l} \mapsto \mathbf{u}_{k l}^{\theta}=e^{i\left(\theta_{k}-\theta_{l}\right)} \mathbf{u}_{k l} .
$$

These transformations leave unchanged cost and constraints of

$$
\begin{aligned}
& \min _{\mathbf{u}_{k, I} \in L^{2}([0, T], \mathbb{C}),(k, l) \in I} \quad \frac{1}{2} \int_{0}^{T}\left(\sum_{(k, l) \in I}\left|\mathbf{u}_{k k}\right|^{2}\right) . \\
& i \frac{d}{d t}|\psi\rangle=\left(\sum_{(k, l) \in I} \mu_{k} \mathbf{u}_{k l}|k\rangle\langle I|\right)|\psi\rangle, \\
& |\langle k \mid \psi\rangle|_{t=0}^{2}=a_{k}^{2},|\langle k \mid \psi\rangle|_{t=T}^{2}=b_{k}^{2}, k=1, \ldots, n
\end{aligned}
$$

that coincides with

$$
\begin{gathered}
\min _{\mathbf{u}_{k, I} \in L^{2}([0, T], \mathbb{C}),(k, l) \in I} \quad \frac{1}{2} \int_{0}^{T}\left(\sum_{(k, l) \in I}\left|\mathbf{u}_{k \mid}\right|^{2}\right) . \\
i \frac{d}{d t}|\psi\rangle=\left(\sum_{(k, l) \in I} \mu_{k \mid} \mathbf{u}_{k l}|k\rangle\langle l|\right)|\psi\rangle, \\
\langle k \mid \psi\rangle\rangle_{t=0}=a_{k},|\langle k \mid \psi\rangle|_{t=T}^{2}=b_{k}^{2}, k=1, \ldots, n
\end{gathered}
$$

■ Set $\psi_{k}=\langle k \mid \psi\rangle$ and $\mathbf{z}_{k l}=\psi_{k} \psi_{l}^{*}: \frac{d}{d t}\left(\left|\psi_{k}\right|^{2}\right)=\sum_{l \mid(k, l) \in I} \mu_{k l} \frac{\mathbf{u}_{k l} \mathbf{z}_{k \mid}^{*}-\mathbf{u}_{k \mid}^{*} \mathbf{z}_{k l}}{i}$ Evolution of the direction of $\psi_{k}$ in the complex plane is governed by

$$
\psi_{k}^{*} \frac{d}{d t} \psi_{k}-\psi_{k} \frac{d}{d t} \psi_{k}^{*}=\sum_{l \mid(k, l) \in l} \mu_{k l} \frac{\mathbf{u}_{k \mid} \mathbf{z}_{k l}^{*}+\mathbf{u}_{k \mid}^{*} \mathbf{z}_{k l}}{i}
$$

■ For $(k, I) \in I$ set $v_{k \mid}(t)= \begin{cases}0, & \text { if } \mathbf{z}_{k \mid}(t)=0 ; \\ \frac{\mathbf{u}_{k \mid}(t) \mathbf{z}_{k \mid}^{*}(t)-\mathbf{u}_{k}^{*}(t) \mathbf{z}_{k \mid}(t)}{2 i\left|\mathbf{z}_{k \mid}(t)\right|}, & \text { if } \mathbf{z}_{k \mid}(t) \neq 0 ;\end{cases}$
■ We have $v_{k l}=-v_{\mid k}$ since $\mathbf{u}_{k l}^{*}=\mathbf{u}_{\mid k}$ and $z_{k l}^{*}=z_{\mid k}$. Moreover $\left|v_{k \mid}\right| \leq\left|\mathbf{u}_{k \mid}\right|$. Thus each $v_{k l}$ belongs to $L^{2}([0, T], \mathbb{R})$ and the solution $|\phi\rangle$ of $\frac{d}{d t} \phi_{k}=\sum_{l \mid(k, l) \in I} \mu_{k l} v_{k l} \phi_{l}, \phi_{k}(0)=a_{k}, \quad k=1, \ldots, n$ coincides with $\phi_{k}=\left|\psi_{k}\right|$.
■ To summarize: starting from complex controls $\mathbf{u}_{k l} \in L^{2}([0, T], \mathbb{C})$ satisfying the constraints of the full problem, we have constructed real controls $v_{k l} \in L^{2}([0, T], \mathbb{C})$ satisfying the constraints of the reduced problem; the cost associated to $\mathbf{u}_{k l}$ is larger than the cost associated to $v_{k l}$ since $\left|v_{k l}\right| \leq\left|u_{k l}\right|$.

Lect. 1 (Oct. 4) Introduction on LKB Photon-Box: control issues for classical and quantum oscillators (creation/annihilation operator, coherent state).
Part 1, open-loop control of Schrödinger systems:
Lect. 2 (Oct. 11) RWA and multi-frequency averaging; 2-level system (half spin) and Jaynes-Cummings model (spin-spring)
Lect. 3 (Oct. 25) Law-Eberly method for trapped ions; adiabatic invariance and control.
Lect. 4 (Nov. 22) Controllability, Lyapounov control and optimal control
Part 2, closed-loop control of open quantum systems:
Lect. 5 (Nov. 29) Measurement and quantum trajectories (discrete time, Kraus operators, LKB-photon box)
Lect. 6 (Dec. 6) Feedback stabilization (Photon-box, quantum filter, Lyapunov, separation principle, delay compensation)
Lect. 7 (Dec. 13) Quantum trajectories (continuous time with Poisson process, Lindblad operators, time/scale reduction, synchronization loop on a $\Lambda$-system)
Lect. 8 (Dec. 14) Quantum trajectories (continuous time with Wiener process, homodyn detection, Lyapunov feedback stabilization of entangled states).

