SOME TOPICS IN MODERN QUANTUM CONTROL

Alexander PECHEN

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Geometry & Control
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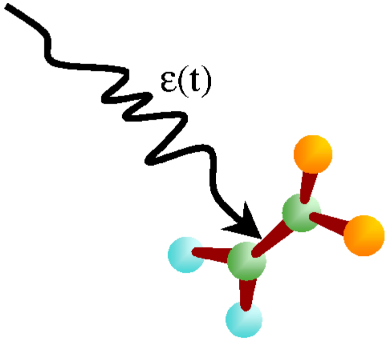
CONTROL OF ATOMS AND MOLECULES



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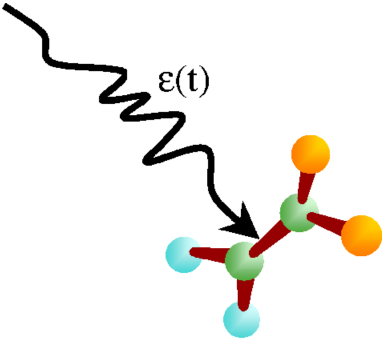

- Laser-assisted control of chemical reactions
- Process generation for quantum information and computing
- Biosensors for detection of small concentrations of molecules

OPTIMAL CONTROL THEORY

OCT (1950–1960): Pontryagin maximum principle (L.S. Pontryagin, V.G. Boltyansky, R.V. Gamkrelidze, E.F. Mishchenko) & Dynamic programming (R. Bellman).

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Quantum control (1970–1980): V.P. Belavkin, P. Brumer, A.G. Butkovskiy, V.F. Krotov, H. Rabitz, S. Rice, M. Shapiro, D.J. Tannor, etc.

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Quantum control (now): Extremely high interest due to many applications. Groups in Princeton, Harvard, Weizmann Institute, MIAN, MSU, RQC, etc.). More than 1300 papers/year.

Nobel Prize 2012 in Physics: D. Wineland and S. Haroche for experimental manipulation of quantum systems.

GENERAL CONTROL PROBLEM

Controlled dynamics: $\dot{x} = f(x, u), \qquad u \in \mathcal{U}$

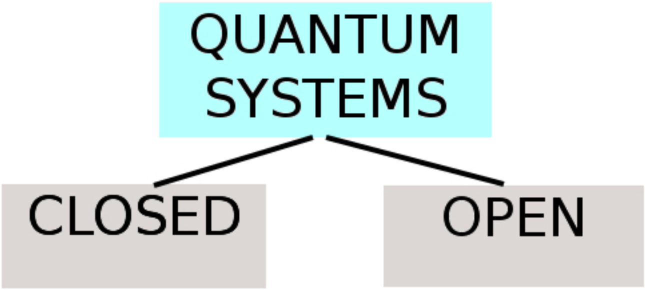
Controllability: For any $x_0, x_1 \in X$ prove existence of such $u \in \mathcal{U}$ that $x_0 \xrightarrow{u} x_1$.

Optimal control: For a given initial state $x_0 \in X$ find control $u \in \mathcal{U}$ which maximizes control objective $\mathscr{F}(x) \to \max\limits_{u \in \mathcal{U}} \mathscr{F}(x)$.

- Hard problems $\Rightarrow$ use numerical algorithms to find optimal controls.
- Efficiency of local algorithms depends on the quantity and properties of local but not global maxima of $\mathscr{F}(x)$.
- Importance of the analysis of all maxima in the landscape of $\mathscr{F}(x(u))$.

OUTLINE OF THIS TALK

- Basic introduction to quantum mechanics
- Control landscapes
  - History
  - Second-order traps for multilevel systems
  - No traps for two-level systems
  - No traps for control of transmission
- Controllability of open quantum systems
- Conclusions



isolated from the environment

interacting with the environment

CLOSED QUANTUM SYSTEMS

Hilbert space $\mathcal{H}$. Examples:

- $\mathcal{H} = \mathbb{C}^n$ — for system with n states;
- $\mathcal{H} = L^2(\mathbb{R}^d)$ — for particle in $\mathbb{R}^d$ ($d = 1, 2, 3$).

State (pure): Wave function $\psi \in \mathcal{H}$, $\|\psi\| = 1$.

Evolution: Schrödinger equation with s.a. Hamiltonian $H(t)$

$$i\frac{d\psi_t}{dt} = H(t)\psi_t, \qquad \psi_{t=0} = \psi_0$$

Unitary transformation:

$$\psi_0 \to \psi_t = U_t\psi_0, \qquad i\frac{dU_t}{dt} = H(t)U_t, \quad U_{t=0} = \mathbb{I}$$

Observables: $\langle \psi_t, O\psi_t \rangle$.

CONTROL OF CLOSED SYSTEMS

$$H(t) = H_0 + f(t)V, \qquad f \in \mathscr{U}$$

Evolution equation:

$$\frac{dU_t^f}{dt} = -i[H_0 + f(t)V]U_t^f, \qquad U_{t=0}^f = \mathbb{I}$$

Control space $\mathscr{U}$:

E.g., finite energy controls $L^2([0,T])$

Objective functional:

$$\mathscr{F}(f) = \mathcal{F}(U_T^f) \to \max, \qquad \text{where } \mathcal{F} : U(n) \to \mathbb{R}$$

EXAMPLES OF OBJECTIVE FUNCTIONALS

State-to-state transfer:

$$\mathscr{F}_{\mathrm{i}\to\mathrm{f}}(f) = |\langle \psi_{\mathrm{f}}, U_T^f \psi_{\mathrm{i}} \rangle|^2$$

$$\mathcal{F}_{\mathrm{i}\to\mathrm{f}}(U) = |\langle \psi_{\mathrm{f}}, U \psi_{\mathrm{i}} \rangle|^2 (\text{max when } U_T^f \psi_{\mathrm{i}} = e^{i\phi} \psi_{\mathrm{f}})$$

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Average value of observable O:

$$\mathscr{F}_O(f) = \mathrm{Tr}[U_T \rho_0 U_T^\dagger O] = \langle O \rangle_T, \qquad \mathcal{F}_O(U) = \mathrm{Tr}[U \rho_0 U^\dagger O]$$

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Process generation:

$$\mathscr{F}_W(f) = |\mathrm{Tr}(U_T W^\dagger)|^2, \qquad \mathcal{F}_W(U) = |\mathrm{Tr}(U W^\dagger)|^2$$
$$(\text{max when } U_T = e^{i\phi} W)$$

OPEN QUANTUM SYSTEMS

State: density matrix $\rho \in \mathcal{T}(\mathcal{H}) : \rho \geq 0, \mathrm{Tr}\rho = 1.$

$$\mathcal{D} := \{\rho \in \mathcal{T}(\mathcal{H}) \,|\, \rho \geq 0, \mathrm{Tr}\rho = 1\}$$

Dynamics: master equation

$$\dot{\rho}_t = -i[H(t), \rho_t] + \mathscr{L}(\rho_t), \qquad \rho_{t=0} = \rho_0$$

Completely positive transformation:

$$\rho_0 \to \rho_t = \Phi_t(\rho_0), \qquad \Phi_t : \mathcal{D} \to \mathcal{D} \text{ — Kraus map}$$

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CONTROL LANDSCAPE

Algorithms to find optimal controls:

- Global (genetic, etc.)
- Local (gradient, etc.)

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Dynamic control landscape: Graph of $\mathscr{F}$. Its important points:

- Optimal controls: Global maxima of $\mathscr{F}$.
- Traps: Local but not global maxima of $\mathscr{F}$.
- Second-order traps: $\frac{\delta \mathscr{F}}{\delta f} = 0$, $H = \frac{\delta^2 \mathscr{F}}{\delta f^2} \leq 0$, $\mathscr{F}(f) < \mathscr{F}_{\max}$.

Kinematic control landscape: Graph of $\mathcal{F}$.

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Kinematic control landscape: Graph of $\mathcal{F}$.

Goal of the control landscape analysis: find all traps in the landscape.

HISTORY

Conjecture [Rabitz, Hsieh, Rosenthal, Science'04]: Absence of local maxima (traps) for $\mathscr{F}(f)$ for any system dimension n. Not proved!

Theorem [A.P., Tannor, PRL'11]: Trapping behavior for $n \geq 3$-level systems with special symmetries.

Theorem [A.P., Ilyn, PRA'12]: No traps for $\mathcal{F}_{\mathrm{i}\to\mathrm{f}}(u)$ and $\mathcal{F}_W(u)$ (and for much more general objectives) for $n = 2$.

Theorem [de Fouquieres, Schirmer, IDAQP 13]: Traps exist for some systems with $n > 3$.

Theorem [A.P., Tannor, CJC'14]: No traps for transmission $T_E(V)$ ($n = \infty$).

$$\frac{\delta T_E(V)}{\delta V} = 0 \Rightarrow T_E(V) = 1$$

REGULAR and NON-REGULAR CONTROLS

Regular/non-regular controls: The Jacobian of the endpoint map $\chi : \mathscr{U} \to SU(n)$, $\chi(f) = U_T^f$ is full-rank/rank-deficient.

Theorem: A regular control f is critical for $\mathscr{F}(f)$ if and only if $U := U_T^f$ is critical for $\mathcal{F}(U)$ and, moreover, $\mathscr{F}$ and $\mathcal{F}$ at regular controls have identical numbers of positive and negative Hessian eigenvalues.

REGULAR CONTROLS: NO TRAPS

Theorem: Regular controls are not traps for $\mathscr{F}_O$ and $\mathscr{F}_W$ (kinematic landscape is trap free).[1]

Theorem: Function $\mathcal{F}(U) := \mathrm{Tr}[UAU^\dagger B]$, where A, B are two $n \times n$ matrices, has exactly one maximum and one minimum value.

- J. von Neumann (1937): A, B — symmetric non-degenerate, $U \in U(n)$.
- R. Brockett (1989): A, B — symmetric non-degenerate, $U \in O(n)$.
- H. Rabitz, M. Hsieh, C. Rosenthal (*Science*'04 and subsequent works): any $A \geq 0$ and Hermitian B.

Conjecture: There are no traps in the dynamic landscape.

[1] H. Rabitz, M. Hsieh, C. Rosenthal (*Science*'04 and subsequent works): any $A \geq 0$ and Hermitian B.

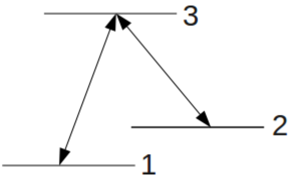
NON-REGULAR CONTROLS: SECOND-ORDER TRAPS

Non-regular controls were shown to exist. Can they be traps?

Theorem: If $V_{ij} = 0$ for some $i \neq j$ in the eigenbasis $|i\rangle$ of H_0, then there exist ρ_0 and O for which the control $f(t) \equiv 0$ is a second-order trap of $\mathscr{F}_O$ (the result is generalized to any constant control).[2]

This results "show mathematically that the situation is more complicated" [than the original conjecture].[3]

Example: Λ-system.



[2]A.N. Pechen, D.J. Tannor, "Are there traps in quantum control landscapes?", *Phys. Rev. Lett.* **106**, 120402 (2011).

[3]Yeston J. Look Out for Traps. *Science* **332**, 514 (2011).

FIRST RESULT: NO TRAPS FOR $n = 2$

Theorem: Consider two-level quantum system with evolution

$$i\frac{d}{dt}U_t^f = [H_0 + f(t)V]U_t^f$$

where $H_0, V \in \mathbb{C}^{2\times 2}$. Assume $H_0, V, [H_0, V]$ generate Lie algebra $su(2)$. Then for sufficiently large T all maxima of $\mathscr{F}_{i\to f}(f) = |\langle\psi_f, U_T^f\psi_i\rangle|^2$ and $\mathscr{F}_W(f) = |\mathrm{Tr}(U_T^f W^\dagger)|^2$ (and of much more general functionals) are global.[4]

More details: Talk by Nikolay Il'in today at 12:00.

[4] Pechen A.N., Il'in N.B. Trap-free manipulation in the Landau-Zener system. *Phys. Rev. A* **86**, 052117 (2012).

CONTROL OF TRANSMISSION: NO TRAPS FOR $n = \infty$

Control of transmission of particle through potential barrier $V(x)$.

Formulation. Stationary Schrödinger equation ($E = k^2 > 0$):

$$\left[\frac{d^2}{dx^2} + V(x)\right]\psi = E\psi, \qquad V \in L^1(\mathbb{R}) \cap C_c(\mathbb{R})$$

- Incoming + reflected waves on the left:
  $$\psi(x) = e^{ikx} + A(k)e^{-ikx}, \; x \to -\infty$$
- Transmitted wave on the right: $\psi(x) = B(k)e^{ikx}$, $x \to +\infty$

Transmission coefficient $T_E(V) = |B(k)|^2$. $V(x)$ — **control**.

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[5] A.N. Pechen, D.J. Tannor, Canadian J. of Chemistry **92**, 157 (2014). Thanks to Misha Ivanov (MIPT).

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- Transmitted wave on the right: $\psi(x) = B(k)e^{ikx}$, $x \to +\infty$

Transmission coefficient $T_E(V) = |B(k)|^2$. $V(x)$ — control.

Theorem: No traps for transmission coefficient $T_E(V)$.[5]

$$\frac{\delta T_E(V)}{\delta V} = 0 \Rightarrow T_E(V) = 1$$

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OPEN QUANTUM SYSTEMS

Evolution of an open quantum system is driven by master equation:

$$\frac{d\rho_t}{dt} = -i[H_0 + Vf(t), \rho_t] + \mathscr{L}_f(\rho_t), \qquad \rho_{t=0} = \rho_0$$

Unitary transformation of state is replaced by a Kraus map:

$$\rho_0 \to \rho_T = \Phi(\rho_0) = \sum_{i=1}^{n^2} K_i \rho_0 K_i^\dagger, \qquad \sum_{i=1}^{n^2} K_i^\dagger K_i = \mathbb{I}.$$

Each Φ is a point on the complex Stiefel manifold $S_n(\mathbb{C}^{n^3})$

$$\Phi \to S = (K_1; \ldots; K_{n^2}), \qquad S^\dagger S = \mathbb{I}\,.$$

REGULAR CONTROLS: NOT TRAPS

Control objective for an open quantum system is:

$$\mathscr{F}_O(u) = \mathrm{Tr}[\rho_T O] \longleftarrow \mathcal{F}_O(S) = \mathrm{Tr}\left[S\rho S^\dagger(\mathbb{I}_{n^2} \otimes O)\right]$$

Theorem: The function $\mathcal{F}_O(S)$ on the Stiefel manifold $S_n(\mathbb{C}^{n^3})$ has as critical points only global maxima/minima and saddles (all are found).[6]

Conclusion: Regular controls for open quantum systems also can not be traps.

[6] A. Pechen, D. Prokhorenko, R. Wu, H. Rabitz, *J. Phys. A: Math. Theor.* **41**, 045205 (2008); R. Wu, A. Pechen, H. Rabitz, M. Hsieh, B. Tsou, *J. Math. Phys.* **49**, 022108 (2008).

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CONTROLLABILITY

Definition System $\dot{x} = f(f, x)$ is controllable on X if for any initial and target states $x_0, x_1 \in X$ there exists f which steers x_0 into x_1.

Closed quantum systems: Controllablity on the set of pure states ($x = \psi$): controllable if Lie algebra $\mathrm{Lie}(H_0, V)$ isomorphic to $su(n)$ (or $sp(n/2)$ for even n).

Open quantum systems: Controllability on the set of all density matrices ($x = \rho$, $X = \mathcal{D}$): uncontrollable if $\mathscr{L} = \mathrm{const}$.[7]

[7] C. Altafini, Phys. Rev. A (2003).

USE OF ENGINEERED ENVIRONMENTS

No need to assume $\mathscr{L} = \mathrm{const}!$

- Incoherent control A.P., H. Rabitz *PRA'06*
- Preparing entangled states; S. Diehl, A. Micheli, A. Kantian, B. Kraus, H. P. Buchler, P. Zoller, *Nat.Phys.'08*; H. Weimer, M. Müller, I. Lesanovsky, P. Zoller, H.P. Büchler, A Rydberg quantum simulator, *Nat.Phys.'10*
- Improving quantum computation; F. Verstraete, M. Wolf, J. Cirac, *Nat.Phys.'09*.
- Inducing multiparticle entanglement dynamics; J.T. Barreiro, P. Schindler, O. Ghne, T. Monz, M. Chwalla, C.F. Roos, M. Hennrich, R. Blatt, *Nat.Phys.'10*.
- Quantum metrology of open dynamical systems: Precision limits through environment control (L. Davidovich).

COMPLETE CONTROLLABILITY IF $\mathscr{L} = \mathscr{L}_{n_\omega(t)}$

Consider open system under action of coherent control plus incoherent control (engineered environment):[8]

$$\frac{d\rho_t}{dt} = -i[H_0 + Vf(t), \rho_t] + \mathcal{L}_{n_\omega(t)}(\rho_t)$$

$$\mathcal{L}_{n_\omega}(\rho) = \sum_{i<j} A_{ij}[(n_{ij}+1)L_{ij}(\rho) + n_{ij}L_{ji}(\rho)]$$

$$L_{ij}(\rho) = 2\rho_{jj}P_i - P_j\rho - \rho P_j, \quad A_{ij} \geq 0$$

Theorem Under some assumptions such system is approximately controllable in $\mathcal{D}$.[9]

[8] A. Pechen, H. Rabitz, *Phys. Rev. A* **73**, 062102 (2006).

[9] A. Pechen, *Phys. Rev. A* **84**, 042106 (2011).

PROOF

Proof: Fix $\rho_{\mathrm{i}}, \rho_{\mathrm{f}} \in \mathcal{D}$. Our goal is to show the existence of f, n_ω such that

$$\rho_{\mathrm{i}} \xrightarrow{f, n_\omega} \rho_{\mathrm{f}} = \sum p_i P_{\phi_i}$$

- Incoherent control: engineered environment with spectral density $n_{ij} = p_j/(p_i - p_j)$:

$$\rho_{\mathrm{i}} \xrightarrow{n_{\omega_{ij}}} \tilde{\rho} = \sum p_i P_{e_i}$$

- Coherent control: $e_i \xrightarrow{f} \phi_i$. Then

$$\tilde{\rho} \xrightarrow{f} U^f_T \tilde{\rho} U^{f\dagger}_T = \rho_{\mathrm{f}}$$

CONCLUSIONS

Control landscapes:

- $n = 2$ and $n = \infty$: no traps.
- $2 < n < \infty$: sometimes trapping behavior.

Controllability:

- Can be realized with coherent and incoherent controls.

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- A. Pechen, D. Tannor, *Phys. Rev. Lett.* **106**, 120402 (2011).
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Thank you!