

Quantum Optimal Control Landscapes

— a “Simplicity” Theory —

Rebing Wu

**Department of Automation, Tsinghua University
Center for Quantum Information Science and Technology, TNlist**

BIRS Workshop on Quantum Control
Banff, April 5, 2011

Outline

- 1 Motivation
- 2 Basic Concepts
- 3 Topological Analysis of Quantum Control Landscapes
- 4 Open questions
- 5 Concluding Remarks

Schemes for ultrafast laser control

- Frequency-domain approach: Two-pathway interference
- Time-domain approach: Pump-dump, STIRAP
- Optimal design approach: Optimal control theory, leaning control

C. Brif, R. Chakrabarti and H. Rabitz, “Control of quantum phenomena: past, present and future”, *New J. Phys.* 12 075008, 2010.

Achievements

Optimization is supposed to be hard due to

- Limited bandwidth and severe noise in shaped pulses;
- A large number of control parameters.

What have been reported:

- > 1000 excellent simulation results (since 1985);
- ~ 150 successful close-loop experiments (since 1998).

Observations:

- **dramatic enhancement** of the system yield;
- **robust** solutions to noises exist.

Achievements

Optimization is supposed to be hard due to

- Limited bandwidth and severe noise in shaped pulses;
- A large number of control parameters.

What have been reported:

- > 1000 excellent simulation results (since 1985);
- ~ 150 successful close-loop experiments (since 1998).

Observations:

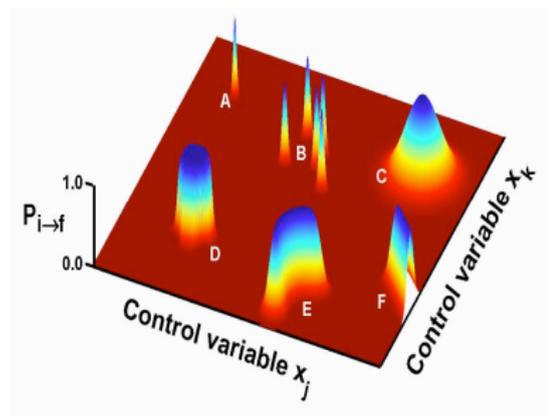
- **dramatic enhancement** of the system yield;
- **robust** solutions to noises exist.

Why is it easy to find a good quantum control?

Quantum Control Landscape: basic concepts

Definition: the graph of the mapping from the **control variables** to the **cost functional**.

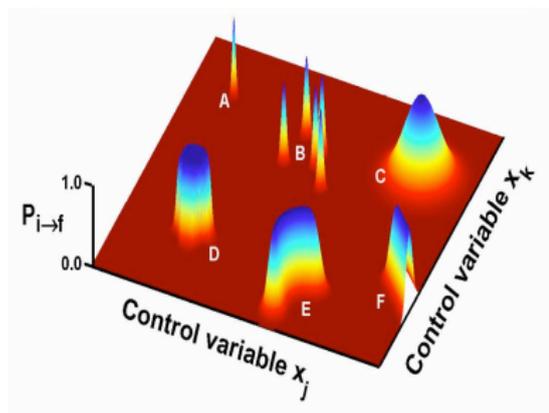
H. Rabitz, M. Hsieh and C. Rosenthal, Science, 303: 1998-2001, 2004;
R. Chakrabarti, H. Rabitz. Quantum control landscapes. Int. Rev. Phys. Chem., 26(4), 2007, 671 - 735.



Quantum Control Landscape: basic concepts

Definition: the graph of the mapping from the **control variables** to the **cost functional**.

H. Rabitz, M. Hsieh and C. Rosenthal, Science, 303: 1998-2001, 2004;
R. Chakrabarti, H. Rabitz. Quantum control landscapes. Int. Rev. Phys. Chem., 26(4), 2007, 671 - 735.



Critical topology: the topology of the set of critical points.

- Distribution of candidate solutions — algorithmic efficiency.
- Multiplicity of optimal solution set — robustness.

What we like...



What we dislike...



Control landscape for Observable Preparation

Schrödinger equation for an N -level closed quantum system:

$$\frac{\partial}{\partial t} \rho(t) = \frac{1}{i\hbar} [H_0 - \epsilon(t)\mu, \rho(t)], \quad \rho(t_0) = \rho_0.$$

where $\epsilon(\cdot)$ is the control field. Consider the maximization of $\langle O \rangle$ at $t = T$:

$$J[\epsilon(\cdot)] = \text{Tr}\{\rho[T; \epsilon(\cdot)]O\}, \quad \epsilon(\cdot) \text{ admissible},$$

In principle, what does the landscape look like under unlimited control resources?

Control landscape at a coarse-grained scale

Control landscape at a coarse-grained scale

Projection from the **dynamical control landscape**

$$J[\epsilon(\cdot)] = \text{Tr}\{\rho[T; \epsilon(\cdot)]O\}, \quad \epsilon(\cdot) \text{ admissible}$$

onto the **kinematic control landscapes**:

$$J(\rho) = \text{Tr}(\rho O), \quad \rho \text{ achievable.}$$

$$J(U) = \text{Tr}(U\rho_0 U^\dagger O), \quad U \text{ achievable.}$$

where U is the propagator at $t = T$.

Control landscape at a coarse-grained scale

Projection from the **dynamical control landscape**

$$J[\epsilon(\cdot)] = \text{Tr}\{\rho[T; \epsilon(\cdot)]O\}, \quad \epsilon(\cdot) \text{ admissible}$$

onto the **kinematic control landscapes**:

$$J(\rho) = \text{Tr}(\rho O), \quad \rho \text{ achievable.}$$

$$J(U) = \text{Tr}(U\rho_0 U^\dagger O), \quad U \text{ achievable.}$$

where U is the propagator at $t = T$. In the case that the system is **controllable**

$$J(U) = \text{Tr}(U\rho_0 U^\dagger O), \quad U \in \mathcal{U}(N).$$

Question

Dynamical control landscape

high-dimensional and highly nonlinear.

Kinematic control landscape

lower-dimensional and linear/quadratic.

What can be learned about the **dynamical landscape** from the **kinematic one**?

Landscape Reduction

Landscape Reduction

Suppose that $\epsilon(\cdot)$ is a critical point of $J(\epsilon(\cdot))$:

$$\delta J[\delta\epsilon(\cdot)] = \langle \nabla J(U(T)), \delta U(T) \rangle \equiv 0, \quad \forall \delta\epsilon(\cdot).$$

Landscape Reduction

Suppose that $\epsilon(\cdot)$ is a critical point of $J(\epsilon(\cdot))$:

$$\delta J[\delta\epsilon(\cdot)] = \langle \nabla J(U(T)), \delta U(T) \rangle \equiv 0, \quad \forall \delta\epsilon(\cdot).$$

If $\delta\epsilon(\cdot) \mapsto \delta U(T)$ is surjective (i.e., $\epsilon(\cdot)$ is regular), then $\delta J \equiv 0$
.iff. $\nabla J(U(T)) = 0$,

Landscape Reduction

Suppose that $\epsilon(\cdot)$ is a critical point of $J(\epsilon(\cdot))$:

$$\delta J[\delta\epsilon(\cdot)] = \langle \nabla J(U(T)), \delta U(T) \rangle \equiv 0, \quad \forall \delta\epsilon(\cdot).$$

If $\delta\epsilon(\cdot) \mapsto \delta U(T)$ is surjective (i.e., $\epsilon(\cdot)$ is regular), then $\delta J \equiv 0$
.iff. $\nabla J(U(T)) = 0$,

- $\epsilon(\cdot)$ is critical .iff. $U(T)$ is critical;

Landscape Reduction

Suppose that $\epsilon(\cdot)$ is a critical point of $J(\epsilon(\cdot))$:

$$\delta J[\delta\epsilon(\cdot)] = \langle \nabla J(U(T)), \delta U(T) \rangle \equiv 0, \quad \forall \delta\epsilon(\cdot).$$

If $\delta\epsilon(\cdot) \mapsto \delta U(T)$ is surjective (i.e., $\epsilon(\cdot)$ is regular), then $\delta J \equiv 0$
.iff. $\nabla J(U(T)) = 0$,

- $\epsilon(\cdot)$ is critical .iff. $U(T)$ is critical;
- Moreover, $\epsilon(\cdot)$ is max. (min., saddle) .iff. $U(T)$ is max. (min., saddle).

Landscape Reduction

Suppose that $\epsilon(\cdot)$ is a critical point of $J(\epsilon(\cdot))$:

$$\delta J[\delta\epsilon(\cdot)] = \langle \nabla J(U(T)), \delta U(T) \rangle \equiv 0, \quad \forall \delta\epsilon(\cdot).$$

If $\delta\epsilon(\cdot) \mapsto \delta U(T)$ is surjective (i.e., $\epsilon(\cdot)$ is regular), then $\delta J \equiv 0$
.iff. $\nabla J(U(T)) = 0$,

- $\epsilon(\cdot)$ is critical .iff. $U(T)$ is critical;
- Moreover, $\epsilon(\cdot)$ is max. (min., saddle) .iff. $U(T)$ is max. (min., saddle).

Conclusion: critical topology preserved from the **dynamical** to the **kinematic** picture if **all admissible controls are regular**.

Conditions for kinematic landscape critical points

Take the parametrization $U \rightarrow Ue^{isA}$ in $\mathcal{U}(N)$ for any $A^\dagger = A$ and take the derivative of J :

$$\left. \frac{dJ}{ds} \right|_{s=0} = \text{Tr}(iA[U\rho_0 U^\dagger, O]) = 0, \quad \forall A^\dagger = A.$$

Critical Condition: $[U\rho_0 U^\dagger, O] = 0$.

In particular, when ρ and O are nondegenerate, the critical U simultaneously diagonalizes $\rho(T)$ and O .^a

^aH. Rabitz, M. Hsieh, C. Rosenthal, J. Chem. Phys., 124, 204107 (2006).

Conditions for kinematic landscape critical points

Take the parametrization $U \rightarrow Ue^{isA}$ in $\mathcal{U}(N)$ for any $A^\dagger = A$ and take the derivative of J :

$$\left. \frac{dJ}{ds} \right|_{s=0} = \text{Tr}(iA[U\rho_0 U^\dagger, O]) = 0, \quad \forall A^\dagger = A.$$

Critical Condition: $[U\rho_0 U^\dagger, O] = 0$.

In particular, when ρ and O are nondegenerate, the critical U simultaneously diagonalizes $\rho(T)$ and O .^a

^aH. Rabitz, M. Hsieh, C. Rosenthal, J. Chem. Phys., 124, 204107 (2006).

Critical topology of kinematic control landscapes

Critical topology of kinematic control landscapes

Further Hessian analysis shows that:

- Only one local maximum submanifold;

Critical topology of kinematic control landscapes

Further Hessian analysis shows that:

- Only one local maximum submanifold;
- One minimum and a number ($< N!$) of saddle submanifolds;

Critical topology of kinematic control landscapes

Further Hessian analysis shows that:

- Only one local maximum submanifold;
- One minimum and a number ($< N!$) of saddle submanifolds;
- Degeneracies in ρ_0 and O lead to **fewer** and **larger** critical submanifolds. (R. Wu, H. Rabitz and M. Hsieh, J. Phys. A., 41, 015006, 2008)

Critical topology of kinematic control landscapes

Further Hessian analysis shows that:

- Only one local maximum submanifold;
- One minimum and a number ($< N!$) of saddle submanifolds;
- Degeneracies in ρ_0 and O lead to **fewer** and **larger** critical submanifolds. (R. Wu, H. Rabitz and M. Hsieh, J. Phys. A., 41, 015006, 2008)

Conclusion:

- **no false traps** (local suboptima) exist to impede the search for optimal controls;

Critical topology of kinematic control landscapes

Further Hessian analysis shows that:

- Only one local maximum submanifold;
- One minimum and a number ($< N!$) of saddle submanifolds;
- Degeneracies in ρ_0 and O lead to **fewer** and **larger** critical submanifolds. (R. Wu, H. Rabitz and M. Hsieh, J. Phys. A., 41, 015006, 2008)

Conclusion:

- **no false traps** (local suboptima) exist to impede the search for optimal controls;
- Robustness of optimal controls on the “flat top” (maximum submanifold).

Control landscape for unitary gate fidelity

Fidelity defined as the distance from a desired quantum gate:

$$J(U) = \|U - W\|^2 = 2N - 2\operatorname{Re}\operatorname{Tr}(W^\dagger U), \quad U \in \mathcal{U}(N).$$

Critical condition: $W^\dagger U = U^\dagger W$.

- only one local minimal submanifold;

Control landscape for unitary gate fidelity

Fidelity defined as the distance from a desired quantum gate:

$$J(U) = \|U - W\|^2 = 2N - 2\operatorname{Re}\operatorname{Tr}(W^\dagger U), \quad U \in \mathcal{U}(N).$$

Critical condition: $W^\dagger U = U^\dagger W$.

- only one local minimal submanifold;
- one maximal and $N - 1$ saddle submanifolds;

Control landscape for unitary gate fidelity

Fidelity defined as the distance from a desired quantum gate:

$$J(U) = \|U - W\|^2 = 2N - 2\operatorname{Re}\operatorname{Tr}(W^\dagger U), \quad U \in \mathcal{U}(N).$$

Critical condition: $W^\dagger U = U^\dagger W$.

- only one local minimal submanifold;
- one maximal and $N - 1$ saddle submanifolds;
- the topology is universal for all $W \in \mathcal{U}(N)$.

Control landscape for unitary gate fidelity

Fidelity defined as the distance from a desired quantum gate:

$$J(U) = \|U - W\|^2 = 2N - 2\operatorname{Re}\operatorname{Tr}(W^\dagger U), \quad U \in \mathcal{U}(N).$$

Critical condition: $W^\dagger U = U^\dagger W$.

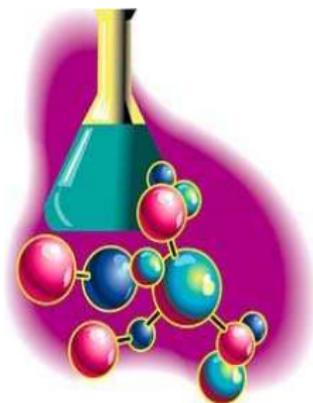
- only one local minimal submanifold;
- one maximal and $N - 1$ saddle submanifolds;
- the topology is universal for all $W \in \mathcal{U}(N)$.

Conclusion: **no false traps**(local suboptima) exist to impede the search for optimal controls.

How about open quantum systems?

In reality, environmental interactions are always present:

$$H = H_S \otimes \mathbb{I}_\lambda + \mathbb{I}_N \otimes H_E + H_{SE}$$



Kinematic Control Landscape for Open Quantum Systems

Definition

$$J(\{K_j\}) = \sum_j \text{Tr}(K_j \rho_0 K_j^\dagger O), \quad \sum_{j=1}^{\lambda} K_j^\dagger K_j = \mathbb{I}_N.$$

Kinematic Control Landscape for Open Quantum Systems

Definition

$$J(\{K_j\}) = \sum_j \text{Tr}(K_j \rho_0 K_j^\dagger O), \quad \sum_{j=1}^{\lambda} K_j^\dagger K_j = \mathbb{I}_N.$$

Assumptions

- all Kraus maps are achievable;
- all admissible controls are regular.

Landscape Lifting for $J(\{K_j\}) = \sum_j \text{Tr}(K_j \rho_0 K_j^\dagger O)$

Landscape Lifting for $J(\{K_j\}) = \sum_j \text{Tr}(K_j \rho_0 K_j^\dagger O)$

The equity $\sum_j K_j^\dagger K_j = \mathbb{I}_N$ implies that the following K is the first N columns of some enlarged unitary matrix:

$$K = \begin{pmatrix} K_1 \\ \vdots \\ K_\lambda \end{pmatrix} = U \begin{pmatrix} I_N \\ \vdots \\ 0_N \end{pmatrix}, \quad U = \begin{pmatrix} K_1 & \cdots & * \\ \vdots & \vdots & * \\ K_\lambda & \cdots & * \end{pmatrix}$$

Landscape Lifting for $J(\{K_j\}) = \sum_j \text{Tr}(K_j \rho_0 K_j^\dagger O)$

The equity $\sum_j K_j^\dagger K_j = \mathbb{I}_N$ implies that the following K is the first N columns of some enlarged unitary matrix:

$$K = \begin{pmatrix} K_1 \\ \vdots \\ K_\lambda \end{pmatrix} = U \begin{pmatrix} I_N \\ \vdots \\ 0_N \end{pmatrix}, \quad U = \begin{pmatrix} K_1 & \cdots & * \\ \vdots & \vdots & * \\ K_\lambda & \cdots & * \end{pmatrix}$$

$$J(K) = \text{Tr}\{U(\rho_0 \otimes |1\rangle\langle 1|)U^\dagger(O \otimes \mathbb{I}_\lambda)\} \triangleq J(U)$$

Landscape Lifting for $J(\{K_j\}) = \sum_j \text{Tr}(K_j \rho_0 K_j^\dagger O)$

The equity $\sum_j K_j^\dagger K_j = \mathbb{I}_N$ implies that the following K is the first N columns of some enlarged unitary matrix:

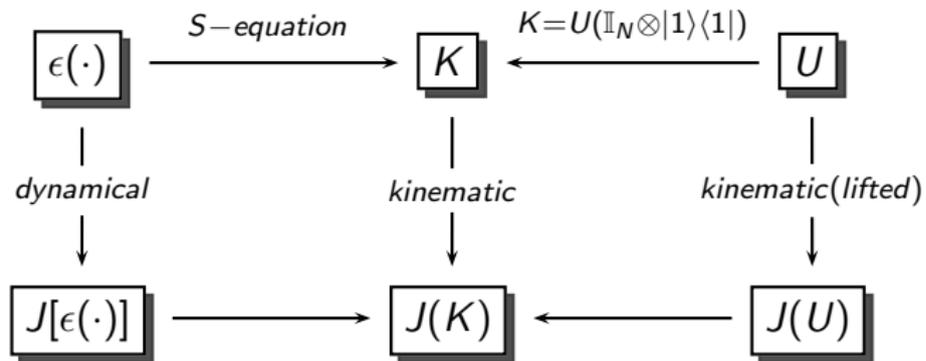
$$K = \begin{pmatrix} K_1 \\ \vdots \\ K_\lambda \end{pmatrix} = U \begin{pmatrix} I_N \\ \vdots \\ 0_N \end{pmatrix}, \quad U = \begin{pmatrix} K_1 & \cdots & * \\ \vdots & \vdots & * \\ K_\lambda & \cdots & * \end{pmatrix}$$

$$J(K) = \text{Tr}\{U(\rho_0 \otimes |1\rangle\langle 1|)U^\dagger(O \otimes \mathbb{I}_\lambda)\} \triangleq J(U)$$

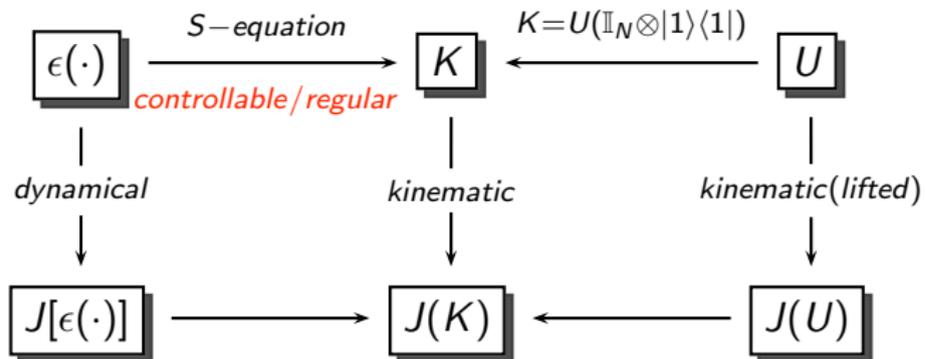
Auxiliary control landscape for “system” + “environment”.

Landscape Mapping

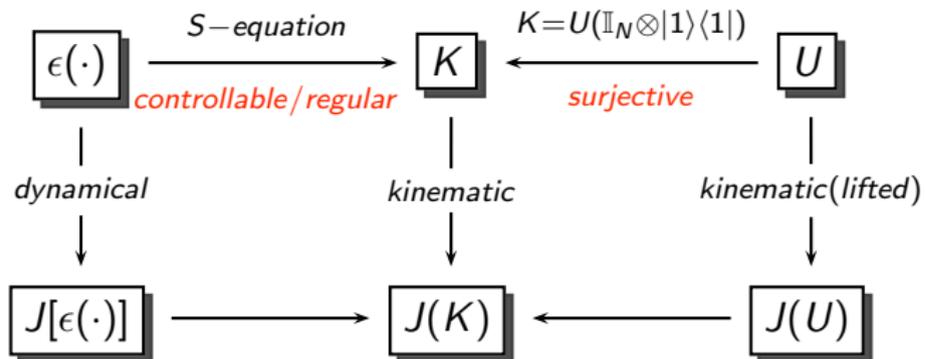
Landscape Mapping



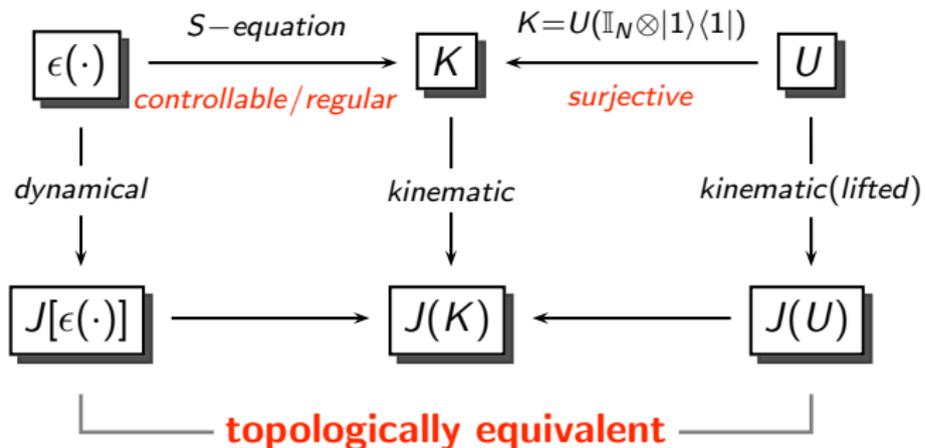
Landscape Mapping



Landscape Mapping



Landscape Mapping



Landscape Topology for open quantum systems

Landscape Topology for open quantum systems

Owing to the equivalence with a closed-system control landscape:

Landscape Topology for open quantum systems

Owing to the equivalence with a closed-system control landscape:

- Again, no false traps exist;

Landscape Topology for open quantum systems

Owing to the equivalence with a closed-system control landscape:

- Again, no false traps exist;
- Stronger controllability assumed, but not on the environment;

Landscape Topology for open quantum systems

Owing to the equivalence with a closed-system control landscape:

- Again, no false traps exist;
- Stronger controllability assumed, but not on the environment;
- Significant increase in # critical submanifolds ($\sim (\lambda N)!$);

Landscape Topology for open quantum systems

Owing to the equivalence with a closed-system control landscape:

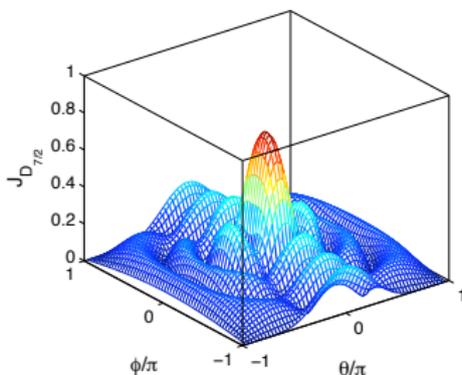
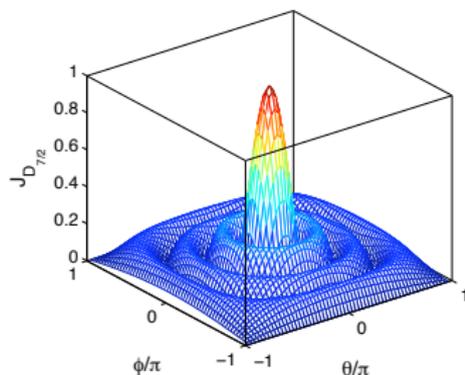
- Again, no false traps exist;
- Stronger controllability assumed, but not on the environment;
- Significant increase in # critical submanifolds ($\sim (\lambda N)!$);

R. Wu, A. Pechen et al., J. Math. Phys., 49, 022108, 2008.

A. Pechen, D. Prokhorenko, et al., J. Phys. A: Math. Theor. 41, 045205 (2008)

Open question: the role of controllability?

Almost all quantum systems are controllable (C. Altafini, J. Math. Phys. 43, 2051 (2002).) BUT...



Gate fidelity landscape $J = \|\text{Tr}(W^\dagger U)\|^2$, $U \in SU(2) \subset U(8)$.

Open question: the role of controllability?

- The loss of controllability leads to **traps** !

Open question: the role of controllability?

- The loss of controllability leads to **traps** !
- Ruggedness \nearrow when the controllability \searrow ;

Open question: the role of controllability?

- The loss of controllability leads to **traps** !
- Ruggedness \nearrow when the controllability \searrow ;
- Even worse when the target is not reachable.

Open question: the role of controllability?

- The loss of controllability leads to **traps** !
- Ruggedness \nearrow when the controllability \searrow ;
- Even worse when the target is not reachable.

Open question: the role of controllability?

- The loss of controllability leads to **traps** !
- Ruggedness \nearrow when the controllability \searrow ;
- Even worse when the target is not reachable.

The role of Controllability beyond Yes-or-No

not only the existence of “**wanted**” controls but also nonexistence of “**unwanted**” controls

R. Wu, M. Hsieh and H. Rabitz, “The role of controllability in optimizing quantum dynamics”, arXiv:0910.4702, 2010.

Open question: the role of singularity?

Open question: the role of singularity?

Look at the critical condition for $\epsilon(\cdot)$:

$$\delta J = \langle \nabla J(U(T)), \delta U(T) \rangle \equiv 0,$$

where $\delta U(T)$ is dependent on $\delta\epsilon(\cdot)$.

Open question: the role of singularity?

Look at the critical condition for $\epsilon(\cdot)$:

$$\delta J = \langle \nabla J(U(T)), \delta U(T) \rangle \equiv 0,$$

where $\delta U(T)$ is dependent on $\delta\epsilon(\cdot)$.

The mapping $\delta\epsilon(\cdot) \mapsto \delta U(T)$ can be singular.

Open question: the role of singularity?

Look at the critical condition for $\epsilon(\cdot)$:

$$\delta J = \langle \nabla J(U(T)), \delta U(T) \rangle \equiv 0,$$

where $\delta U(T)$ is dependent on $\delta\epsilon(\cdot)$.

The mapping $\delta\epsilon(\cdot) \mapsto \delta U(T)$ can be singular.

(R. Wu, J. Dominy, T.-S. Ho, H. Rabitz, arXiv:0907.2354).

Invisible critical points in the kinematic picture !

Open question: the role of singularity?

- Singular controls may become **traps**, e.g. zero field;
P. Fouquieres, S. Schirmer, arXiv:1004.3492
A. Pechen and D. Tannor, Phys. Rev. Lett. 106, 120402 (2011)

Open question: the role of singularity?

- Singular controls may become **traps**, e.g. zero field;
P. Fouquieres, S. Schirmer, arXiv:1004.3492
A. Pechen and D. Tannor, Phys. Rev. Lett. 106, 120402 (2011)
- However, never encountered in our numerical simulations. (K. Moore, *et al*, arXiv:1006.1829, arXiv:1006:3702)

Open question: the role of singularity?

- Singular controls may become **traps**, e.g. zero field;
P. Fouquieres, S. Schirmer, arXiv:1004.3492
A. Pechen and D. Tannor, Phys. Rev. Lett. 106, 120402 (2011)
- However, never encountered in our numerical simulations. (K. Moore, *et al*, arXiv:1006.1829, arXiv:1006:3702)

Important in time optimal control (Lapert et al, PRL 2010) !

Open Question: complexity?

Search efforts scaling with the system dimension and objectives, e.g., N , ρ , O or W ?

Open Question: complexity?

Search efforts scaling with the system dimension and objectives,
e.g., N , ρ , O or W ?

Katharine Moore, *et al*, J. Chem. Phys. 128, 154117 (2008);

Katharine Moore, *et al*, arXiv:1006.1829, arXiv:1006:3702;

Raj Chakrabarti, *et al*, arXiv:0708.3513

Open Question: complexity?

Search efforts scaling with the system dimension and objectives, e.g., N , ρ , O or W ?

Katharine Moore, *et al*, J. Chem. Phys. 128, 154117 (2008);

Katharine Moore, *et al*, arXiv:1006.1829, arXiv:1006:3702;

Raj Chakrabarti, *et al*, arXiv:0708.3513

Concluding Remarks

Concluding Remarks

- Trap-free landscape features can be obtained from the kinematic picture;

Concluding Remarks

- Trap-free landscape features can be obtained from the kinematic picture;
- Singularity may generate traps, but they are not likely to be encountered in practice;

Concluding Remarks

- Trap-free landscape features can be obtained from the kinematic picture;
- Singularity may generate traps, but they are not likely to be encountered in practice;
- A strong support for evident laboratory successes;

Concluding Remarks

- Trap-free landscape features can be obtained from the kinematic picture;
- Singularity may generate traps, but they are not likely to be encountered in practice;
- A strong support for evident laboratory successes;
- Open up perspectives in developing more efficient algorithms (e.g., gradient and evolutionary-strategy algorithms are going on in Princeton laboratory).

THANK YOU !