

# Control Theoretic Aspects of Matrix Factorizations

**U. Helmke**

University of Würzburg,  
Mathematical Institute,  
Germany

<http://www.mathematik.uni-wuerzburg.de/RM2>

Joint work with G. Dirr and M. Kleinstеuber.

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# Motivation

- Quantum Computing
- Quantum Control, Control of Spin Systems
- Control of Numerical Algorithms
- Constructive Controllability, Motion Planning in Robotics



# Time-optimal Factorization Problem

- $G$  compact connected Lie group with Lie Algebra  $\mathfrak{g}$
- $\omega := \{\Omega_1^+, \dots, \Omega_r^+, \Omega_1^-, \dots, \Omega_s^-\}$  finite set of LA generators of  $\mathfrak{g}$
- $\Omega_i^+$ : "slow, cost expensive" directions  
 $\Omega_i^-$ : "fast, cheap" directions
- Given  $X \in G$ , define

$$T_{\min}(X) = \inf \left\{ \sum_i |t_i^\pm| \mid X = \prod_{\text{finite}} e^{t_i^\pm \Omega_i^\pm} \right\}$$

## Problem:

- Is  $T_{\min} < \infty$  always? Compute  $T_{\min}$ !
- When does there exist a *finite, time-optimal* factorization?

# Example


## Optimal Condition Numbers

- $G = GL(n)$  general linear group of invertible matrices
- $\omega := \{\Omega_1^+, \dots, \Omega_r^+, \Omega_1^-, \dots, \Omega_s^-\}$  finite set of LA generators of  $\mathfrak{gl}(n)$
- $\Omega_i^+$ : "hyperbolic Jacobi rotations"  
 $\Omega_i^-$ : "standard Jacobi directions"
- Given  $X \in G$ , define ( $\kappa$  denotes the condition number)


$$T_{\min}(X) = \inf \left\{ \sum_i \kappa(e^{t_i^\pm \Omega_i^\pm}) \mid X = \prod_{\text{finite}} e^{t_i^\pm \Omega_i^\pm} \right\}$$

## Problem:

- This factorization task with minimal total condition number!
- Does there exists factorization with better condition numbers than for  $X$ ?



# Lie Groups & Lie Algebras



## Intermezzo: Lie Groups and Lie Algebras

**Example.** General linear group of invertible  $n \times n$  matrices

$$GL(n, \mathbb{R}) := \{X \in \mathbb{R}^{n \times n} \mid \det X \neq 0\}.$$

**Definition.** A matrix *Lie group* is any subgroup  $G \subset GL(n, \mathbb{R})$  that is also a (locally closed) submanifold of  $\mathbb{R}^{n \times n}$ .



# Intermezzo: Lie Groups and Lie Algebras

## Examples, cont'd:

(a) The *real orthogonal group*

$$O(n) := \{X \in \mathbb{R}^{n \times n} \mid XX^\top = I_n\}$$

(b) The *special unitary group*

$$SU(n) := \{X \in \mathbb{C}^{n \times n} \mid XX^* = I_n, \det X = 1\}$$

(c) The *Euclidean group*

$$E(n) := \left\{ \begin{bmatrix} R & p \\ 0 & 1 \end{bmatrix} \mid R \in O(n), p \in \mathbb{R}^n \right\}.$$

The first two examples are compact groups, while the third is not.



## Intermezzo: Lie Groups and Lie Algebras

**Definition.** A vector space  $V$  with a bilinear operation  $[ , ] : V \times V \rightarrow V$  satisfying

- (i)  $[x, y] = -[y, x]$
- (ii)  $[x, [y, z]] + [z, [x, y]] + [y, [z, x]] = 0$  (Jacobi Identity)

is called a *Lie Algebra*.



## Intermezzo: Lie Groups and Lie Algebras

- Lie algebras are the tangent spaces of Lie groups.
- **Theorem.** Let  $G \subset GL(n, \mathbb{R})$  be a matrix Lie group. Then the tangent space  $\mathfrak{g} := T_I G$  at the identity matrix is a Lie algebra with commutator as the Lie bracket:

$$[X, Y] = XY - YX.$$

# Intermezzo: Lie Groups and Lie Algebras

## Examples

(a) The Lie algebra of  $O(n)$  is

$$\mathfrak{o}(n) := \{\Omega \in \mathbb{R}^{n \times n} \mid \Omega^\top = -\Omega\}.$$

(b) The Lie algebra of  $SU(n)$  is

$$\mathfrak{su}(n) := \{\Omega \in \mathbb{C}^{n \times n} \mid \Omega^* = -\Omega, \text{tr} \Omega = 0\}$$

(c) The Lie algebra of  $E(n)$  is

$$\mathfrak{e}(n) := \left\{ \begin{bmatrix} \Omega & v \\ 0 & 0 \end{bmatrix} \mid \Omega^\top = -\Omega, v \in \mathbb{R}^n \right\}.$$



# Control on Lie Groups



# Control on Lie Groups

- $G$  Lie Group with Lie Algebra  $\mathfrak{g}$ .
- Bilinear control system on  $G$

$$(\Sigma) \quad \dot{X}(t) = \left( A_d + \sum_{j=1}^m u_j(t) A_j \right) X(t), \quad X(0) = I,$$

where  $A_d, A_1, \dots, A_m \in \mathfrak{g}$ .

- Reachable Set at time  $T > 0$

$$\mathcal{R}(T) = \{X_F \in G \mid \exists u_1, \dots, u_m \text{ and } s \leq T : X(s) = X_F\}$$

- Reachable Set

$$\mathcal{R} = \cup_T \mathcal{R}(T)$$

# Control on Lie Groups

## Definition

- **Accessibility:** The reachable set  $\mathcal{R}(T)$  has an interior point
- **Local Controllability:** The identity  $I \in \mathcal{R}(T)$  is an interior point
- **Controllability:** For any  $X_F \in G$  there exist controls  $u_1(\cdot), \dots, u_m(\cdot)$  and  $T > 0$  s.t. the solution of  $(\Sigma)$  satisfies  $X(0) = I, X(T) = X_F$ .

# Control on Lie Groups

## Problem 1 (Accessibility)

- Definition (*System Lie Algebra*)

$\mathcal{L} :=$  smallest Lie subalgebra of  $\mathfrak{g}$ , containing  $A_1, \dots, A_m, A_d$

*Generators:*  $([A, B] = AB - BA)$

$$A_d, A_1, \dots, A_m, [A_d, A_i], [A_i, A_j], [A_d, [A_i, A_j]], \dots$$

- Theorem.  $(\Sigma)$  is accessible if and only if the system Lie algebra is  $\mathcal{L} = \mathfrak{g}$ .

# Control on Lie Groups

● Theorem (Lian et al. 1994) Suppose

(i) For some constant controls  $u_1, \dots, u_m$

$$(\Sigma_{const}) \quad \dot{X} = (A_d + \sum_j u_j A_j) X$$

is weakly positively Poisson stable.

(ii) The system Lie algebra  $\mathcal{L}$  satisfies  $\mathcal{L} = \mathfrak{g}$ .

Then the bilinear control system is controllable.

**Accessibility + Poisson Stability  $\Rightarrow$  Controllability**



# Control on Lie Groups

## Definition (Poisson Stability)

Flow of  $(\Sigma_{const})$ :  $\Phi : G \times \mathbb{R} \rightarrow G$ ;  $(z, t) \mapsto \Phi(z, t)$

- $(\Sigma_{const})$  is **Weakly Positively Poisson Stable** if for all  $z \in G$ , any neighborhood  $B(z)$  of  $z$  and all  $T > 0$ , there exists  $t > T$  such that  $\Phi(U_z, t) \cap B(z) \neq \emptyset$ .

Examples: a swing (no damping), satellite attitude, ball rolling in a bowl.

# Control on Lie Groups

● Theorem (Jurdjevic-Sussmann) Assume:

- (i) There exist constant controls such that  $A_d + \sum_j u_j A_j$  lies in a **compact** subalgebra  $\mathfrak{k}$  of  $\mathfrak{g}$ .
- (ii) The system Lie algebra  $\mathcal{L}$  satisfies  $\mathcal{L} = \mathfrak{g}$ .

Then the system  $(\Sigma)$  is controllable.



# Control on Lie Groups

- Corollary

Let  $G$  be a **compact** connected Lie group. Then  $(\Sigma)$  is controllable if and only if

$$\mathcal{L} = \mathfrak{g}.$$





# Time-Optimal Control on Lie Groups



# Time-Optimal Control on Lie Groups

## General Notation:

- Let  $G$  be a compact Lie Group with Lie algebra  $\mathfrak{g}$ ;  $K \subset G$  a compact connected Lie subgroup with LA  $\mathfrak{k}$ . Consider the bilinear control system on  $G$

$$(\Sigma) \quad \dot{X} = \left( A_d + \sum_{j=1}^m u_j A_j \right) X, \quad X(0) = I$$

with  $A_d \in \mathfrak{g}$ ,  $A_1, \dots, A_m \in \mathfrak{k}$ .

- Assumption:
  - $\Sigma$  is controllable, i.e.  $\mathfrak{g}$  = LA generated by  $A_d, A_1, \dots, A_m$
  - $\mathfrak{k}$  = LA generated by  $A_1, \dots, A_m$

# Time-Optimal Control on Lie Groups

- Given: Initial state  $X_0 = I$ , Final state  $X_F \in G$
- Problem 1. Find controls  $u_1(\cdot), \dots, u_m(\cdot)$  s.t. the corresponding solution  $X(t)$  of  $(\Sigma)$  satisfies

$$X(0) = X_0, \quad X(T) = X_F \quad \text{for some } T > 0$$

- Problem 2. If problem 1 has at least one solution, then find a time-optimal one, i.e. one with *minimal*  $T = T_{\text{opt}}(X_F)$ .
- Problem 1 is always solvable, provided  $(\Sigma)$  is controllable!

# Time-Optimal Control on Lie Groups

## Fast versus slow directions

- $A_d$  is called the *drift term*,  $A_1, \dots, A_m$  the *fast directions*
- **Fact 1.** If  $A_d = 0$  and  $(\Sigma)$  controllable, then can control to  $X_F$  in *arbitrarily small time*:  $T_{\text{opt}}(X_F) = 0$ , always!
- **Fact 2.** The presence of drift term  $A_d \neq 0$  is responsible for  $T_{\text{opt}} > 0$ .
- **Idea:** Factor out fast directions!

# Time-Optimal Control on Lie Groups

## Quotient System and Equivalence Principle

- Consider the quotient space

$$G/K := \{Kg \mid g \in G\}$$

of left co-sets  $Kg$ ,  $K = \exp(\mathfrak{k})$  Lie Group generated by fast controls.

- $G/K$  is a smooth manifold



# Time-Optimal Control on Lie Groups

## Example: (NMR)

- For the NMR Schrödinger Equation on  $G = SU(2^N)$

$$\dot{X} = -i \left( H_d + \sum_{j=1}^{2N} u_j H_j \right) X, \quad X(0) = I$$

$\mathfrak{k} :=$  LA generated by  $iH_1, \dots, iH_{2N}$

$K := \exp(\mathfrak{k})$  compact, connected Lie subgroup of  $SU(2^N)$ ,  
generated by  $\exp(itH_j), t \in \mathbb{R}, j = 1, \dots, 2N$ .

One verifies  $K = SU(2) \otimes \dots \otimes SU(2)$

- For  $N = 1$  :  $K = SU(2) = G$
- For  $N = 2$  :  $K = SU(2) \otimes SU(2) \simeq SO(4) \subset SU(4)$

# Time-Optimal Control on Lie Groups

## Quotient System and Equivalence Principle

- The *quotient system* of

$$(\Sigma) \quad \dot{X} = \left( A_d + \sum_{j=1}^m u_j A_j \right) X, \quad X(0) = I, \quad X(T) = X_F$$

is the control system on  $G/K$

$$(\Sigma/K) \quad \dot{P} = \text{Ad}_{U(t)}(A_d)P, \quad P(0) = K, \quad P(T) = KX_F$$

$\text{Ad}_g(A_d) = gA_dg^{-1}$ ,  $g \in K$ . The control functions for  $(\Sigma/K)$  are arbitrary  $L^1_{\text{loc}}$  functions  $t \mapsto U(t) \in K$ .

# Time-Optimal Control on Lie Groups

## Quotient System and Equivalence Principle

- Theorem (Equivalence Principle).

$(\Sigma)$  is controllable on  $G$  iff  $(\Sigma/K)$  is controllable on  $G/K$ .  
Moreover, the optimal times on  $G$  and  $G/K$  coincide.

$$T_{\text{opt}}^G(X_F) = T_{\text{opt}}^{G/K}(KX_F)$$

Proof: PhD thesis by Khaneja

- The optimal time  $T_{\text{opt}}^{G/K}$  has an interpretation within Sub-Riemannian Geometry.

# Time-Optimal Control on Lie Groups

## Sub-Riemannian Geometry

- Let  $M$  be a Riemannian manifold,  $E \subset TM$  a constant dimensional subbundle that satisfies the *Hörmander Condition*

For any  $p \in M$ , the LA of the sections of  $E$  evaluated in  $p$  is equal to  $T_p M$  (controllability cond.)

- For any two points  $x, y \in M$ , the *Sub-Riemannian distance* is

$$d(x, y) := \inf \left\{ \int_0^1 \|\dot{\alpha}(t)\| dt \mid \alpha(0) = x, \alpha(1) = y, \dot{\alpha}(t) \in E_{\alpha(t)} \right\}.$$

- **Example:**  $M = G/K$ ,  $E_p := \text{span}\{kA_d k^{-1} \mid k \in K\}P$ ,  $P \in M$  satisfies the Hörmander Cond. (Equivalence principle)
- **NMR:**  $M = SU(2^N)/SU(2) \otimes \dots \otimes SU(2)$  Sub-Riemannian space

# Time-Optimal Control on Lie Groups

## Sub-Riemannian Geometry

- Theorem.

$$T_{\text{opt}}^{G/K}(KX_F) = d(K, KX_F)$$

Sub-Riemannian distance

- Remark. The Sub-Riemannian distance  $d(x, y)$  is greater than or equal the Riemannian distance on  $G/K$ :

$$d(x, y) \geq \text{geodesic distance between } x, y$$

- There is one case where these distances are equal: *Riemannian symmetric spaces*.

# Time-Optimal Control on Lie Groups

## Sub-Riemannian Geometry

- Theorem. If  $G/K$  is a Riemannian Symmetric Space, then

$$T_{\text{opt}}(X_F) = \text{length of a geodesic in } G/K \text{ that connects } K \text{ with } KX_F$$

- Main Advantage: Riemannian distances (i.e. lengths of geodesics) are much easier to compute than Sub-Riemannian distances.



# Time-Optimal Control on Lie Groups

- **Theorem.** The homogenous space  $G/K$  is a Riemannian symmetric space, provided  $(\mathfrak{g}, \mathfrak{k})$  is a Cartan-pair, i.e.  $\mathfrak{g}$  is semisimple and

$$\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}, \quad \mathfrak{p} := \mathfrak{k}^\perp$$

satisfies

$$[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k}, \quad [\mathfrak{k}, \mathfrak{p}] \subset \mathfrak{p}, \quad [\mathfrak{p}, \mathfrak{p}] \subset \mathfrak{k}$$

# Time-Optimal Control on Lie Groups

## Riemannian Symmetric Spaces

- $SU(n)/SO(n)$  is a Riemannian Symmetric Space
- $SU(4)/SU(2) \otimes SU(2)$  is a Riemannian Symmetric Space (good! 2-Spin Case)
- $SU(8)/SU(2) \otimes SU(2) \otimes SU(2)$  is *NOT* a Riemannian Symmetric Space (bad!)





# Time-Optimal Factorization



# Time-optimal Factorization

- Let  $G$  be a connected, compact Lie group with Lie algebra  $\mathfrak{g}$ .
- Let  $K \subset G$  be a connected compact subgroup with Lie algebra  $\mathfrak{k}$ .
- Let  $\Delta \in \mathfrak{g}$  be a drift term s.t.  $\langle \Delta, \mathfrak{k} \rangle_L = \mathfrak{g}$ .
- Consider the discrete control System:

$$(\Sigma_d) \quad X_{n+1} = K_n e^{t_n \Delta} L_n X_n, \quad X_0 = I \quad K_n, L_n \in K, t_n \geq 0.$$

For  $X \in G$  let  $T_{\text{opt}}^d(X) :=$

$$\inf \left\{ \sum_{n=1}^{\infty} t_n \mid \exists (K_n, L_n, t_n) : \prod_{n=1}^{\infty} K_n e^{t_n \Delta} L_n = X \right\}.$$

# Time-optimal Factorization

## Problem:

- Is  $(\Sigma_d)$  controllable, i.e. does  $T_{\text{opt}}^d(X) < \infty$  hold for all  $X \in G$ ?
- Determine the “minimal” time  $T_{\text{opt}}^d(X)$  for  $X \in G$ .



# Time-optimal Factorization

## Generalized Version (multiple drifts)

- $G$  compact connected Lie group with LA  $\mathfrak{g}$
- $\omega := \{\Omega_1^+, \dots, \Omega_r^+, \Omega_1^-, \dots, \Omega_s^-\}$  finite set of LA generators of  $\mathfrak{k}$
- $\Omega_i^+$ : "slow, cost expensive" directions  
 $\Omega_i^-$ : "fast, cheap" directions
- Given  $X \in G$ , define

$$T_{\min}(X) = \inf \left\{ \sum_i |t_i^+| \mid X = \prod_{\text{finite}} e^{t_i^\pm \Omega_i^\pm} \right\}$$

# Time-optimal Factorization

## Problem

- Is  $T_{\min} < \infty$  always? Compute  $T_{\min}$ !
- When does there exist a *finite, time-optimal* factorization?



# Time-optimal Factorization

## Example 1 (Euler Angles)

- $SO(3)$ ,  $\omega = \{\Omega_1^+, \Omega_1^-\}$ ,

$$\Omega_1^+ := \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \Omega_1^- := \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

- *Euler Angles:*

$$X = e^{\theta_1 \Omega_1^-} e^{\theta_2 \Omega_1^+} e^{\theta_3 \Omega_1^-}, \quad \theta_i \in [-\pi, \pi]$$

- We will show: Euler Angles are time-optimal and

$$T_{\min} = |\theta_2| \in [0, \pi]$$

# Time-optimal Factorization

## Example 2 (Euler Angles)

- $SO(3)$ ,  $\omega = \{\Omega_1^+, \Omega_2^+\}$ ,  $\Omega_2^+ := \Omega_1^-$
- Then Euler angles are i.g. *NOT* time-optimal:

$$T_{\min} < \theta_1 + \theta_2 + \theta_3 ! \quad (\text{Mittenhuber})$$



# Time-optimal Factorization

## Equivalence Principle

- Let  $G$  be a connected, compact Lie group with Lie algebra  $\mathfrak{g}$ .
- Let  $\mathfrak{k} := \langle A_1, \dots, A_m \rangle_L$ ,  $K := \exp \mathfrak{k}$ .
- Let  $\Delta \in \mathfrak{g}$  be a drift term such that  $\langle \Delta, \mathfrak{k} \rangle_L = \mathfrak{g}$ .
- Theorem.
  - (a) The discrete control system  $(\Sigma_d)$  on  $G$  is controllable and thus  $T_{\text{opt}}^d(X) < \infty$
  - (b) For any  $X \in G$  the minimal times  $T_{\text{opt}}^d(X) = T_{\text{opt}}(X)$  coincide, where  $T_{\text{opt}}(X)$  is the minimal time for the control problem

$$\dot{X} = \left( \Delta + \sum_{j=1}^m u_j A_j \right) X, \quad X(0) = I, X(T) = X$$



# Time-optimal Factorization

- Problem: I.g. time optimal factorizations are infinite

Under what conditions on the drift term  $\Delta$  are they *finite*?

- Definition [Haselgrove, Nielsen, Osborne]: A drift term  $\Delta$  is called *lazy*, if there exists  $\varepsilon > 0$  such that

$$T_{\text{opt}}(e^{t\Delta}) < t \quad \text{for all } t \in (0, \varepsilon). \quad (**)$$

If  $\Delta$  is not lazy, we call it *fast*.

# Time-optimal Factorization

- Theorem. If  $\Delta$  is lazy, there are no finite, time optimal factorizations for any element  $X \in G - K$ .



# Time-optimal Factorization

- Conjecture 1: There exists a finite, time optimal factorization for all  $X \in G$  iff  $\Delta$  is fast.
- Conjecture 2:  $\Delta$  fast  $\iff [\Delta, \Delta^\perp] = 0$ .
- Remark: Conjecture 2 implies Conjecture 1.

## Computation of Optimal Time

**Theorem (Khaneja).** Let  $(\mathfrak{g}, \mathfrak{k})$  be a Cartan pair. Let  $\Delta^\perp$  be the orthogonal projection of  $\Delta$  onto  $\mathfrak{p}$  and let  $\mathfrak{a}$  be a maximal abelian subalgebra of  $\mathfrak{p}$  that contains  $\Delta^\perp$ . Then:

- Each  $X \in G$  has a decomposition of the form

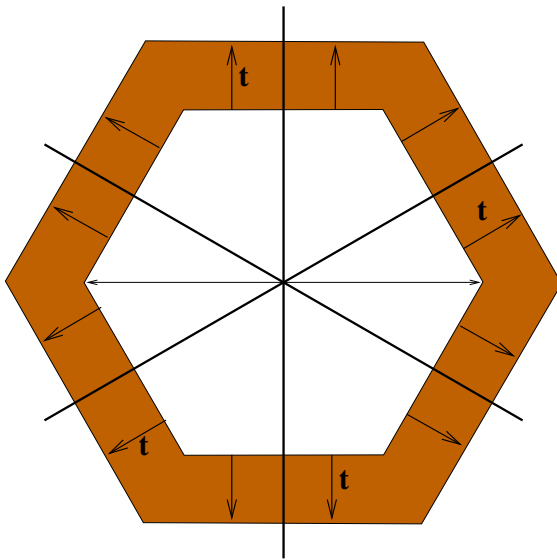
$$X = U\Sigma V \quad \text{with } U, V \in K \text{ and } \Sigma \in \exp \mathfrak{a}.$$

- The minimal time is given by

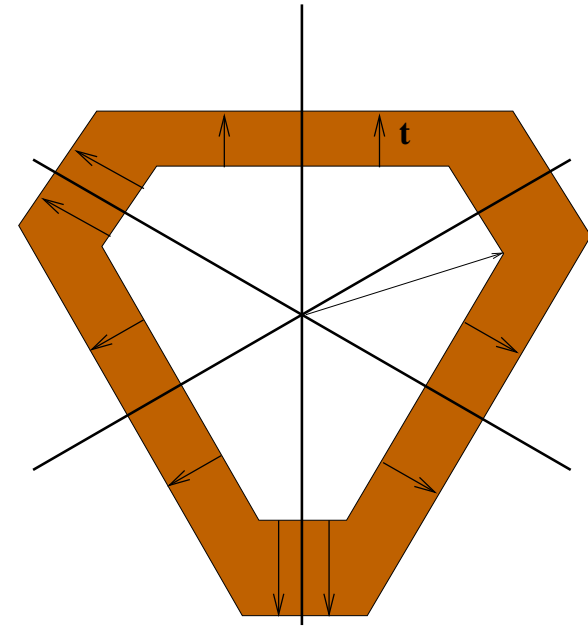
$$T_{\text{opt}}(X) = \min \left\{ t \geq 0 \mid \left( t \cdot \text{conv } \mathcal{W}(\Delta^\perp) \right) \cap \exp^{-1}(\Sigma) \neq \emptyset \right\},$$

where  $X = U\Sigma V$  is an arbitrary factorization of the above type and  $\mathcal{W}(\Delta^\perp)$  denotes the Weyl orbit of  $\Delta^\perp$ .

# Computation of Optimal Time



Convex hull of the Weyl Orbit of a "symmetric" drift term  $\Delta$



Convex hull of the Weyl Orbit of an arbitrary  $\Delta$ .

# Computation of Optimal Time

## Example 1, cont'd:

- $G := \text{SO}(3)$  and  $\mathfrak{g} := \mathfrak{so}(3)$ ,

$$\Omega_1 := \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \Omega_2 := \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

- $\Delta := \alpha\Omega_1 + \beta\Omega_2$ ,  $\mathfrak{k} := \langle \Omega_2 \rangle$

Euler Angles:  $X = e^{\theta_1\Omega_2}e^{\theta_2\Omega_1}e^{\theta_3\Omega_2}$ ,  $\theta_i \in [-\pi, \pi]$

- $T_{\text{opt}}(X) = \alpha^{-1}|\theta_2|$ ,

- $\Delta$  fast  $\iff \beta = 0$ .

# Computation of minimal time

**Example:** (NMR cont'd)

- NMR-Schrödinger equation on  $SU(4)$

$$\dot{X} = -2\pi i \left( H_d + \sum_{i=1}^4 u_i H_i \right), \quad X(0) = I,$$

where  $H_d := \sigma_z \otimes \sigma_z$ ,  $H_1 := I_2 \otimes \sigma_x$ ,  $H_2 := I_2 \otimes \sigma_y$ ,  $H_3 := \sigma_x \otimes I_2$ ,  
and  $H_4 := \sigma_y \otimes I_2$ .

- $K = SU(2) \otimes SU(2)$ .
- $\Delta = -2\pi i H_d$  and  $\mathfrak{a} := i \langle \sigma_x \otimes \sigma_x, \sigma_y \otimes \sigma_y, \sigma_z \otimes \sigma_z \rangle$ .

# Computation of minimal time

**Example:** (NMR cont'd)

**Theorem.** For all  $X = U\Sigma V \in SU(4)$  and  $U, V \in K$ , and  $\Sigma \in \exp \mathfrak{a}$  fixed it holds

$$\bullet \quad T(X) = \min \left\{ \sum_{n=1}^3 |t_n| \left| e^{t_1 2\pi i (\sigma_x \otimes \sigma_x)} e^{t_2 2\pi i (\sigma_y \otimes \sigma_y)} e^{t_3 2\pi i (\sigma_z \otimes \sigma_z)} = \Sigma \right. \right\}$$

$$\bullet \quad T(X) \leq \frac{3}{2}$$



# Computation of minimal time

## Optimization Algorithm (NMR cont'd)

Let  $X(t, u) = U(u_1, \dots, u_6) \Sigma(t_1, t_2, t_3) V(u_7, \dots, u_{12})$ ,

$$U(u_1, \dots, u_6) = e^{-i2\pi u_1 H_1} e^{-i2\pi u_2 H_2} e^{-i2\pi u_3 H_1} e^{-i2\pi u_4 H_3} e^{-i2\pi u_5 H_4} e^{-i2\pi u_6 H_3}$$

$$V(u_7, \dots, u_{12}) = e^{-i2\pi u_7 H_1} e^{-i2\pi u_8 H_2} e^{-i2\pi u_9 H_1} e^{-i2\pi u_{10} H_3} e^{-i2\pi u_{11} H_4} e^{-i2\pi u_{12} H_3}$$

$$\Sigma = e^{t_1 2\pi i (\sigma_x \otimes \sigma_x)} e^{t_2 2\pi i (\sigma_y \otimes \sigma_y)} e^{t_3 2\pi i (\sigma_z \otimes \sigma_z)}$$

To compute the minimal time  $T(X)$ , we combine simulated annealing with gradient methods to solve the nonlinear optimization problem:

$$\begin{aligned} \min \quad & f(t, u) := |t_1| + |t_2| + |t_3|, \\ \text{subject to} \quad & g(t, u) := 4 - \text{Retr}(X_F^* X(t, u)) = 0 \end{aligned}$$

where  $t = [t_1, t_2, t_3]$ ,  $u = [u_1, u_2, \dots, u_{12}] \in [-1, 1]^{12}$

# Computation of Time-optimal Pulse Sequences

Consists of two sub-problems:

- Given  $T \geq 0$ , solve

$$\begin{aligned} \min_{t,u} \quad & g(t, u), \\ \text{subject to} \quad & f(t, u) \leq T, \\ & t \geq 0. \end{aligned}$$

- Let  $V(T)$  be the global optimal value of  $g(t, u)$ , associated with a given  $T \geq 0$ .

$$\begin{aligned} \text{Minimize} \quad & T \\ \text{subject to} \quad & V(T) = 0, \\ & T \geq 0. \end{aligned}$$

# Computation of Time-optimal Pulse Sequences

## Example

$$X_F = e^{-\frac{i\pi}{4}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

$$T(X_F) = 1.499996$$

$$t = [0.499993 \mid 0.500017 \mid 0.499986]$$

