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# Convexity, Majorization and Time Optimal Control of Coupled Spin Dynamics 

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#### Abstract

In this chapter, we study some control problems that derive from time optimal control of coupled spin dynamics in NMR spectroscopy and quantum information and computation. Time optimal control helps to minimize relaxation losses. In a two qubit system, the ability to synthesize, local unitaries, much more rapidly than evolution of couplings, gives a natural time scale separation in these problems. The generators of unitary evolution, $\mathfrak{g}$, are decomposed into fast generators $\mathfrak{k}$ (local Hamiltonians) and slow generators $\mathfrak{p}$ (couplings) as a Cartan decomposition $\mathfrak{g}=\mathfrak{p} \oplus \mathfrak{k}$. Using this decomposition, we exploit some convexity ideas to completely characterize the reachable set and time optimal control for these problems. The main contribution of the chapter is, we carry out a global analysis of time optimality.


Keywords: Kostant convexity, spin dynamics, Cartan decomposition, Cartan subalgebra, Weyl group, time optimal control

## 1. Introduction

A rich class of model control problems arise when one considers dynamics of two coupled spin $\frac{1}{2}$. The dynamics of two coupled spins, forms the basis for the field of quantum information processing and computing [1] and is fundamental in multidimensional NMR spectroscopy [2, 3]. Numerous experiments in NMR spectroscopy, involve synthesizing unitary transformations [4-6] that require interaction between the spins (evolution of the coupling Hamiltonian). These experiments involve transferring, coherence and polarization from one spin to another and involve evolution of interaction Hamiltonians [2]. Similarly, many protocols in quantum communication and information processing involve synthesizing entangled states starting from the separable states [1, 7, 8]. This again requires evolution of interaction Hamiltonians between the qubits.

A typical feature of many of these problems is that evolution of interaction Hamiltonians takes significantly longer than the time required to generate local unitary transformations (unitary transformations that effect individual spins only). In NMR spectroscopy [2, 3], local unitary transformations on spins are obtained by application of rf-pulses, whose strength may be orders of magnitude larger than the couplings between the spins. Given the Schróedinger equation for unitary evolution

$$
\begin{equation*}
\dot{U}=-i\left[H_{c}+\sum_{j=1}^{n} u_{j} H_{j}\right] U, \quad U(0)=I \tag{1}
\end{equation*}
$$

where $H_{c}$ represents a coupling Hamiltonian, and $u_{j}$ are controls that can be switched on and off. What is the minimum time required to synthesize any unitary transformation in the coupled spin system, when the control generators $H_{j}$ are local Hamiltonians and are much stronger than the coupling between the spins ( $u_{j}$ can be made large). Design of time optimal rf-pulse sequences is an important research subject in NMR spectroscopy and quantum information processing [4, 9-21], as minimizing the time to execute quantum operations can reduce relaxation losses, which are always present in an open quantum system [22, 23]. This problem has a special mathematical structure that helps to characterize all the time optimal trajectories [4]. The special mathematical structure manifested in the coupled two spin system, motivates a broader study of control systems with the same properties.

The Hamiltonian of a spin $\frac{1}{2}$ can be written in terms of the generators of rotations on a two dimensional space and these are the Pauli matrices $-i \sigma_{x},-i \sigma_{y},-i \sigma_{z}$, where,

$$
\sigma_{z}=\frac{1}{2}\left[\begin{array}{cc}
1 & 0  \tag{2}\\
0 & -1
\end{array}\right] ; \quad \sigma_{y}=\frac{1}{2}\left[\begin{array}{cc}
0 & -i \\
i & 0
\end{array}\right] ; \quad \sigma_{x}=\frac{1}{2}\left[\begin{array}{ll}
0 & 1 \\
1 & 0
\end{array}\right] .
$$

Note

$$
\begin{equation*}
\left[\sigma_{x}, \sigma_{y}\right]=i \sigma_{z}, \quad\left[\sigma_{y}, \sigma_{z}\right]=i \sigma_{x}, \quad\left[\sigma_{z}, \sigma_{x}\right]=i \sigma_{y}, \tag{3}
\end{equation*}
$$

where $[A, B]=A B-B A$ is the matrix commutator and

$$
\begin{equation*}
\sigma_{x}^{2}=\sigma_{y}^{2}=\sigma_{z}^{2}=\frac{1}{4} \tag{4}
\end{equation*}
$$

The Hamiltonian for a system of two coupled spins takes the general form

$$
\begin{equation*}
H_{0}=\sum a_{\alpha} \sigma_{\alpha} \otimes \mathbf{1}+\sum b_{\beta} \mathbf{1} \otimes \sigma_{\beta}+\sum J_{\alpha \beta} \sigma_{\alpha} \otimes \sigma_{\beta}, \tag{5}
\end{equation*}
$$

where $\alpha, \beta \in\{x, y, z\}$. The Hamiltonians $\sigma_{\alpha} \otimes \mathbf{1}$ and $\mathbf{1} \otimes \sigma_{\beta}$ are termed local Hamiltonians and operate on one of the spins. The Hamiltonian

$$
\begin{equation*}
H_{c}=\sum J_{\alpha \beta} \sigma_{\alpha} \otimes \sigma_{\beta}, \tag{6}
\end{equation*}
$$

is the coupling or interaction Hamiltonian and operates on both the spins.
The following notation is therefore common place in the NMR literature.

$$
\begin{equation*}
I_{\alpha}=\sigma_{\alpha} \otimes 1 ; \quad S_{\beta}=1 \quad \otimes \sigma_{\beta} . \tag{7}
\end{equation*}
$$

The operators $I_{\alpha}$ and $S_{\beta}$ commute and therefore $\exp \left(-i \sum_{\alpha} a_{\alpha} I_{\alpha}+\sum_{\beta} b_{\beta} S_{\beta}\right)=$ $\exp \left(-i \sum_{\alpha} a_{\alpha} I_{\alpha}\right) \exp \left(-i \sum_{\beta} b_{\beta} S_{\beta}\right)=\left(\exp \left(-i \sum_{\alpha} a_{\alpha} \sigma_{\alpha}\right) \otimes \boldsymbol{1}\right)\left(1 \otimes \exp \left(-i \sum_{\beta} b_{\beta} \sigma_{\beta}\right)\right.$,

The unitary transformations of the kind

$$
\exp \left(-i \sum_{\alpha} a_{\alpha} \sigma_{\alpha}\right) \otimes \exp \left(-i \sum_{\beta} b_{\beta} \sigma_{\beta}\right),
$$

obtained by evolution of the local Hamiltonians are called local unitary transformations.

The coupling Hamiltonian can be written as

$$
\begin{equation*}
H_{c}=\sum J_{\alpha \beta} I_{\alpha} S_{\beta} . \tag{9}
\end{equation*}
$$

Written explicitly, some of these matrices take the form

$$
I_{z}=\sigma_{z} \otimes \boldsymbol{1}=\frac{1}{2}\left[\begin{array}{cccc}
1 & 0 & 0 & 0  \tag{10}\\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & -1
\end{array}\right] .
$$

and

$$
I_{z} S_{z}=\sigma_{z} \otimes \sigma_{z}=\frac{1}{4}\left[\begin{array}{cccc}
1 & 0 & 0 & 0  \tag{11}\\
0 & -1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & 1
\end{array}\right]
$$

The 15 operators,

$$
-i\left\{I_{\alpha}, S_{\beta}, I_{\alpha} S_{\beta}\right\},
$$

for $\alpha, \beta \in\{x, y, z\}$, form the basis for the Lie algebra $\mathfrak{g}=s u(4)$, the $4 \times 4$, traceless skew-Hermitian matrices. For the coupled two spins, the generators $-i H_{c},-i H_{j} \in s u(4)$ and the evolution operator $U(t)$ in Eq. (1) is an element of $S U(4)$, the $4 \times 4$, unitary matrices of determinant 1 .

The Lie algebra $\mathfrak{g}=s u(4)$ has a direct sum decomposition $\mathfrak{g}=\mathfrak{p} \oplus \mathfrak{k}$, where

$$
\begin{equation*}
\mathfrak{k}=-i\left\{I_{\alpha}, S_{\beta}\right\}, \quad \mathfrak{p}=-i\left\{I_{\alpha} S_{\beta}\right\} . \tag{12}
\end{equation*}
$$

Here $\mathfrak{k}$ is a subalgebra of $\mathfrak{g}$ made from local Hamiltonians and $\mathfrak{p}$ nonlocal Hamiltonians. In Eq. (1), we have $-i H_{j} \in \mathfrak{k}$ and $-i H_{c} \in \mathfrak{p}$, It is easy to verify that

$$
\begin{equation*}
[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k}, \quad[\mathfrak{k}, \mathfrak{p}] \subset \mathfrak{p}, \quad[\mathfrak{p}, \mathfrak{p}] \subset \mathfrak{p} . \tag{13}
\end{equation*}
$$

This decomposition of a real semi-simple Lie algebra $\mathfrak{g}=\mathfrak{p} \oplus \mathfrak{k}$ satisfying (13) is called the Cartan decomposition of the Lie algebra $\mathfrak{g}$ [24].

This special structure of Cartan decomposition arising in dynamics of two coupled spins in Eq. (1), motivates study of a broader class of time optimal control problems.

Consider the following canonical problems. Given the evolution

$$
\begin{equation*}
\dot{U}=\left(X_{d}+\sum_{j} u_{j}(t) X_{j}\right) U, \quad U(0)=\mathbf{1}, \tag{14}
\end{equation*}
$$

where $U \in S U(n)$, the special Unitary group (determinant 1 , $n \times n$ matrices $U$ such that $U U^{\prime}=\mathbf{1}$,' is conjugate transpose). Where $X_{j} \in \mathfrak{k}=s o(n)$, skew symmetric matrices and

$$
X_{d}=-i\left[\begin{array}{cccc}
\lambda_{1} & 0 & \ldots & 0 \\
0 & \lambda_{2} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & \lambda_{n}
\end{array}\right], \quad \sum \lambda_{i}=0
$$

We assume $\left\{X_{j}\right\}_{L A}$, the Lie algebra ( $X_{j}$ and its matrix commutators) generated by generators $X_{j}$ is all of $s o(n)$. We want to find the minimum time to steer this system between points of interest, assuming no bounds on our controls $u_{j}(t)$. Here again we have a Cartan decomposition on generators. Given $\mathfrak{g}=s u(n)$, traceless skew-Hermitian matrices, generators of $S U(n)$, we have $\mathfrak{g}=\mathfrak{p} \oplus \mathfrak{k}$, where $\mathfrak{p}=-i A$, where $A$ is traceless symmetric and $\mathfrak{k}=s o(n)$. As before, $X_{d} \in \mathfrak{p}$ and $X_{j} \in \mathfrak{k}$. We want to find time optimal ways to steer this system. We call this $\frac{S U(n)}{S O(n)}$ problem. For $n=4$, this system models the dynamics of two coupled nuclear spins in NMR spectroscopy.

In general, $U$ is in a compact Lie group $G$ (such as $S U(n)$ ), with $X_{d}, X_{j}$ in its real semisimple (no abelian ideals) Lie algebra $\mathfrak{g}$ and

$$
\begin{equation*}
\dot{U}=\left(X_{d}+\sum_{j} u_{j}(t) X_{j}\right) U, \quad U(0)=\mathbf{1} . \tag{15}
\end{equation*}
$$

Given the Cartan decomposition $\mathfrak{g}=\mathfrak{p} \oplus \mathfrak{k}$, where $X_{d} \in \mathfrak{p},\left\{X_{j}\right\}_{L A}=\mathfrak{k}$ and $K=\exp (\mathfrak{k})$ (product of exponentials of $\mathfrak{k}$ ) a closed subgroup of G , We want to find the minimum time to steer this system between points of interest, assuming no bounds on our controls $u_{j}(t)$. Since $\left\{X_{j}\right\}_{L A}=\mathfrak{k}$, any rotation (evolution) in subgroup $K$ can be synthesized with evolution of $X_{j}[25,26]$. Since there are no bounds on $u_{j}(t)$, this can be done in arbitrarily small time [4]. We call this $\frac{G}{K}$ problem.

The special structure of this problem helps in complete description of the reachable set [27]. The elements of the reachable set at time $T$, takes the form $U(T) \in$

$$
\begin{equation*}
S=K_{1} \exp \left(T \sum_{k} \alpha_{k} \mathcal{W}_{k} X_{d} \mathcal{W}_{k}^{-1}\right) K_{2}, \tag{16}
\end{equation*}
$$

where $K_{1}, K_{2}, \mathcal{W}_{k} \in \exp (\mathfrak{k})$, and $\mathcal{W}_{k} X_{d} \mathcal{W}_{k}^{-1}$ all commute, and $\alpha_{k}>0, \sum \alpha_{k}=1$. This reachable set is formed from evolution of $K_{1}, K_{2}$ and commuting Hamiltonians $\mathcal{W}_{k} X_{d} \mathcal{W}_{k}^{-1}$. Unbounded control suggests that $K_{1}, K_{2}, \mathcal{W}_{k}$ can be synthesized in negligible time.

This reachable set can be understood as follows. The Cartan decomposition of the Lie algebra $\mathfrak{g}$, in Eq. (13) leads to a decomposition of the Lie group $G$ [24]. Inside $\mathfrak{p}$ is contained the largest abelian subalgebra, denoted as $\mathfrak{a}$. Any $X \in \mathfrak{p}$ is $A d_{K}$ conjugate to an element of $\mathfrak{a}$, i.e. $X=K a_{1} K^{-1}$ for some $a_{1} \in \mathfrak{a}$.

Then, any arbitrary element of the group $G$ can be written as

$$
\begin{equation*}
G=K_{0} \exp (X)=K_{0} \exp \left(A d_{K}\left(a_{1}\right)\right)=K_{1} \exp \left(a_{1}\right) K_{2}, \tag{17}
\end{equation*}
$$

for some $X \in \mathfrak{p}$ where $K_{i} \in K$ and $a_{1} \in \mathfrak{a}$. The first equation is a fact about geodesics in $G / K$ space [24], where $K=\exp (\mathfrak{k})$ is a closed subgroup of $G$. Eq. (17) is called the KAK decomposition [24].

The results in this chapter suggest that $K_{1}$ and $K_{2}$ can be synthesized by unbounded controls $X_{i}$ in negligible time. The time consuming part of the evolution
$\exp \left(a_{1}\right)$ is synthesized by evolution of Hamiltonian $X_{d}$. Time optimal strategy suggests evolving $X_{d}$ and its conjugates $\mathcal{W}_{k} X_{d} \mathcal{W}_{k}^{-1}$ where $\mathcal{W}_{k} X_{d} \mathcal{W}_{k}^{-1}$ all commute.

Written as evolution

$$
G=K_{1} \prod_{k} \exp \left(t_{k} \mathcal{W}_{k} X_{d} \mathcal{W}_{k}^{-1}\right) K_{2}=K_{1} \prod_{k} \mathcal{W}_{k} \exp \left(t_{k} X_{d}\right) \mathcal{W}_{k}^{-1} K_{2} .
$$

where $K_{1}, K_{2}, \mathcal{W}_{k}$ take negligible time to synthesize using unbounded controls $u_{i}$ and time-optimality is characterized by synthesis of commuting Hamiltonians $\mathcal{W}_{k} X_{d} \mathcal{W}_{k}^{-1}$. This characterization of time optimality, involving commuting Hamiltonians is derived using convexity ideas [4, 28]. The remaining chapter develops these notions.

The chapter is organized as follows. In Section 2, we study the $\frac{S U(n)}{S O(n)}$ problem. In Section 3, we study the general $\frac{G}{K}$ problem. The main contribution of the chapter is, we carry out a global analysis of time optimality.

Given Lie algebra $\mathfrak{g}$, we use killing form $\langle x, y\rangle=\operatorname{tr}\left(a d_{x} a d_{y}\right)$ as an inner product on $\mathfrak{g}$. When $\mathfrak{g}=\operatorname{su}(n)$, we also use the inner product $\langle x, y\rangle=\operatorname{tr}\left(x^{\prime} y\right)$. We call this standard inner product.

## 2. Time optimal control for $S U(n) / S O(n)$ problem

Remark 1. Birkhoff's convexity states, a real $n \times n$ matrix $A$ is doubly stochastic ( $\sum_{i} A_{i j}=\sum_{j} A_{i j}=1$, for $A_{i j} \geq 0$ ) if it can be written as convex hull of permutation matrices $P_{i}$ (only one 1 and everything else zero in every row and column). Given $\Theta \in S O(n)$ and $X=\left[\begin{array}{cccc}\lambda_{1} & 0 & \ldots & 0 \\ 0 & \lambda_{2} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \lambda_{n}\end{array}\right]$, we have $\operatorname{diag}\left(\Theta X \Theta^{T}\right)=B \operatorname{diag}(X)$ where $\operatorname{diag}(X)$ is a column vector containing diagonal entries of $X$ and $B_{i j}=\left(\Theta_{i j}\right)^{2}$ and hence $\sum_{i} B_{i j}=\sum_{j} B_{i j}=1$, making $B$ a doubly stochastic matrix, which can be written as convex sum of permutations. Therefore $B \operatorname{diag}(X)=\sum_{i} \alpha_{i} P_{i} \operatorname{diag}(X)$, i.e. diagonal of a symmetric matrix $\Theta X \Theta^{T}$, lies in convex hull of its eigenvalues and its permutations. This is called Schur convexity.

Remark 2. $G=S U(n)$ has a closed subgroup $K=S O(n)$ and a Cartan decomposition of its Lie algerbra $\mathfrak{g}=s u(n)$ as $\mathfrak{g}=\mathfrak{p} \oplus \mathfrak{k}$, for $\mathfrak{k}=s o(n)$ and $p=-i A$ where $A$ is traceless symmetric and $\mathfrak{a}$ is maximal abelian subalgebra of $\mathfrak{p}$, such that
$\mathfrak{a}=-i\left[\begin{array}{ccc}\lambda_{1} & \ldots & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_{n}\end{array}\right]$, where $\sum_{i} \lambda_{i}=0$. KAK decomposition in Eq. (17) states for $U \in S U(n), U=\Theta_{1} \exp (\Omega) \Theta_{2}$ where $\Theta_{1}, \Theta_{2} \in S O(n)$ and

$$
\Omega=-i\left[\begin{array}{ccc}
\lambda_{1} & \ldots & 0 \\
0 & \ddots & 0 \\
0 & 0 & \lambda_{n}
\end{array}\right],
$$

where $\sum_{i} \lambda_{i}=0$.
Remark 3. We now give a proof of the reachable set (16), for the $\frac{S U(n)}{S O(n)}$ problem. Let $U(t) \in S U(n)$ be a solution to the differential Eq. (14)

$$
\dot{U}=\left(X_{d}+\sum_{i} u_{i} X_{i}\right) U, \quad U(0)=I .
$$

To understand the reachable set of this system we make a change of coordinates $P(t)=K^{\prime}(t) U(t)$, where, $\dot{K}=\left(\sum_{i} u_{i} X_{i}\right) K$. Then

$$
\dot{P}(t)=A d_{K^{\prime}(t)}\left(X_{d}\right) P(t), \quad A d_{K}\left(X_{d}\right)=K X K^{-1} .
$$

If we understand reachable set of $P(t)$, then the reachable set in Eq. (14) is easily derived.

Theorem 1. Let $P(t) \in S U(n)$ be a solution to the differential equation

$$
\dot{P}=A d_{K(t)}\left(X_{d}\right) P,
$$

and $K(t) \in S O(n)$ and $X_{d}=-i\left[\begin{array}{cccc}\lambda_{1} & 0 & \ldots & 0 \\ 0 & \lambda_{2} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & & \lambda_{n}\end{array}\right]$. The elements of the reachable set at time $T$, take the form $K_{1} \exp (-i \mu T) K_{2}$, where $K_{1}, K_{2} \in S O(n)$ and $\mu<\lambda(\mu$ lies in convex hull of $\lambda$ and its permutations), where $\lambda=\left(\lambda_{1}, \ldots, \lambda_{n}\right)^{\prime}$.

Proof. As a first step, discretize the evolution of $P(t)$, as piecewise constant evolution, over steps of size $\tau$. The total evolution is then

$$
\begin{equation*}
P_{n}=\prod_{i} \exp \left(A d_{k_{i}}\left(X_{d}\right) \tau\right) \tag{18}
\end{equation*}
$$

For $t \in[(n-1) \tau, n \tau]$, choose small step $\Delta$, such that $t+\Delta<n \tau$, then $P(t+\Delta)=\exp \left(A d_{K}\left(X_{d}\right) \Delta\right) P(t)$.

By KAK, $P(t)=K_{1} \underbrace{\left[\begin{array}{cccc}\exp \left(i \phi_{1}\right) & 0 & 0 & 0 \\ 0 & \exp \left(i \phi_{2}\right) & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & \exp \left(i \phi_{n}\right)\end{array}\right]}_{A} K_{2}$,
where $K_{1}, K_{2} \in \operatorname{SO}(n)$. To begin with, assume eigenvalues $\phi_{j}-\phi_{k} \neq n \pi$, where $n$ is an integer. When we take a small step of size $\Delta, P(t)$ changes to $P(t+\Delta)$ as $K_{1}, K_{2}, A$ change to

$$
K_{1}(t+\Delta)=\exp \left(\Omega_{1} \Delta\right) K_{1}, \quad K_{2}(t+\Delta)=\exp \left(\Omega_{2} \Delta\right) K_{2}, \quad A(t+\Delta)=\exp (a \Delta) A,
$$

where, $\Omega_{1}, \Omega_{2} \in \mathfrak{k}$ and $a \in \mathfrak{a}$. Let $Q(t+\Delta)=K_{1}(t+\Delta) A(t+\Delta) K_{2}(t+\Delta)$, which can be written as

$$
\begin{gather*}
Q(t+\Delta)=\exp \left(\Omega_{1} \Delta\right) K_{1} \exp (a \Delta) A \exp \left(\Omega_{2} \Delta\right) K_{2} .  \tag{19}\\
Q(t+\Delta)=\exp \left(\Omega_{1} \Delta\right) \exp \left(K_{1} a K_{1}^{\prime} \Delta\right) \exp \left(K_{1} A \Omega_{2} A^{\prime} K_{1}^{\prime} \Delta\right) P(t) . \tag{20}
\end{gather*}
$$

Observe

$$
\begin{equation*}
P(t+\Delta)=\exp \left(A d_{K}\left(X_{d}\right) \Delta\right) P(t) . \tag{21}
\end{equation*}
$$

We equate $P(t+\Delta)$ and $Q(t+\Delta)$ to first order in $\Delta$. This gives,

$$
\begin{equation*}
A d_{K}\left(X_{d}\right)=\Omega_{1}+K_{1} a K_{1}^{\prime}+K_{1} A \Omega_{2} A^{\prime} K_{1}^{\prime} . \tag{22}
\end{equation*}
$$

Multiplying both sides with $K_{1}^{\prime}(\cdot) K_{1}$ gives

$$
\begin{equation*}
A d_{\bar{K}}\left(X_{d}\right)=\Omega_{1}^{\prime}+a+A \Omega_{2} A^{\prime} . \tag{23}
\end{equation*}
$$

where, $\bar{K}=K_{1}^{\prime} K$ and $\Omega_{1}^{\prime}=K^{\prime} \Omega K$.
We evaluate $A \Omega_{2} A^{\dagger}$, for $\Omega_{2} \in \operatorname{so}(n)$.

$$
\begin{equation*}
\left\{A \Omega_{2} A^{\dagger}\right\}_{k l}=\exp \left\{i\left(\phi_{k}-\phi_{l}\right)\right\}\left(\Omega_{2}\right)_{k l}=\underbrace{\cos \left(\phi_{k}-\phi_{l}\right)\left(\Omega_{2}\right)_{k l}}_{S_{k l}}+i \underbrace{i \sin \left(\phi_{k}-\phi_{l}\right)\left(\Omega_{2}\right)_{k l}}_{R_{k l}} . \tag{24}
\end{equation*}
$$

such that $S$ is skew symmetric and $R$ is traceless symmetric matrix with $i R \in \mathfrak{p}$. Note $i R \perp \mathfrak{a}$ and onto $\mathfrak{a}^{\perp}$, by appropriate choice of $\Omega_{2}$.

Given $A d_{\bar{K}}\left(X_{d}\right) \in \mathfrak{p}$, we decompose it as

$$
A d_{\bar{K}}\left(X_{d}\right)=P\left(A d_{\bar{K}}\left(X_{d}\right)\right)+A d_{\bar{K}}\left(X_{d}\right)^{\perp}=\Omega_{1}^{\prime}+a+A \Omega_{2} A^{\prime},
$$

with $P$ denoting the projection onto $\mathfrak{a}\left(\mathfrak{a}=-i\left[\begin{array}{ccc}\lambda_{1} & \ldots & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \lambda_{n}\end{array}\right]\right.$, where $\sum_{i} \lambda_{i}=0$.) w.r.t to standard inner product and $A d_{\bar{K}}\left(X_{d}\right)^{\perp}$ to the orthogonal component. In Eq. (24), $\phi_{k}-\phi_{l} \neq 0$, $\pi$, we can solve for $\left(\Omega_{2}\right)_{k l}$ such that $i R=A d_{\bar{K}}\left(X_{d}\right)^{\perp}$. This gives $\Omega_{2}$. Let $a=P\left(A d_{\bar{K}}\left(X_{d}\right)\right)$ and choose $\Omega_{1}^{\prime}=A d_{\bar{K}}\left(X_{d}\right)^{\perp}-A \Omega_{2} A^{\dagger}=-S \in \mathfrak{k}$.

With this choice of $\Omega_{1}, \Omega_{2}$ and $a, P(t+\Delta)$ and $Q(t+\Delta)$ are matched to first order in $\Delta$ and

$$
P(t+\Delta)-Q(t+\Delta)=o\left(\Delta^{2}\right) .
$$

Consider the case, when $A$ is degenerate. Let,

$$
A=\left[\begin{array}{cccc}
A_{1} & 0 & \ldots & 0  \tag{25}\\
0 & A_{2} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & & A_{n}
\end{array}\right]
$$

where $A_{k}$ is $n_{k}$ fold degenerate (modulo sign) described by $n_{k} \times n_{k}$ block. WLOG, we arrange

$$
A_{k}=\exp \left(i \phi_{k}\right)\left[\begin{array}{cc}
I_{r \times r} & 0  \tag{26}\\
0 & -I_{s \times s}
\end{array}\right] .
$$

Consider the decomposition

$$
A d_{\bar{K}}\left(X_{d}\right)=P\left(A d_{\bar{K}}\left(X_{d}\right)\right)+A d_{\bar{K}}\left(X_{d}\right)^{\perp},
$$

where $P$ denotes projection onto $n_{k} \times n_{k}$ blocks in Eq. (25) and $A d_{K}\left(X_{d}\right)^{\perp}$, the orthogonal complement.

$$
P\left(\left[\begin{array}{cccc}
X_{11} & X_{12} & \ldots & X_{1 n}  \tag{27}\\
X_{21} & X_{22} & \ldots & X_{2 n} \\
\vdots & \vdots & \ddots & \vdots \\
X_{n 1} & X_{n 2} & \ldots & X_{n n}
\end{array}\right]\right)=\left[\begin{array}{cccc}
X_{11} & 0 & \ldots & 0 \\
0 & X_{22} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & X_{n n}
\end{array}\right],
$$

where $X_{i j}$ are blocks.
Then we write

$$
\begin{equation*}
Q(t+\Delta)=\exp \left(\Omega_{1} \Delta\right) K_{1} \exp \left(P\left(A d_{\bar{K}}\left(X_{d}\right) \Delta\right)\right) A \exp \left(\Omega_{2} \Delta\right) K_{2} . \tag{28}
\end{equation*}
$$

where in Eq. (24) we can solve for $\left(\Omega_{2}\right)_{k l}$ such that $i R=A d \overline{\bar{K}}\left(X_{d}\right)^{\perp}$. This gives $\Omega_{2}$. Choose, $A d_{\bar{K}}\left(X_{d}\right)^{\perp}-A \Omega_{2} A^{\dagger}=\Omega_{1}^{\prime} \in \mathfrak{k}$, this gives $\Omega_{1}=K_{1} \Omega_{1}^{\prime} K_{1}^{\prime}$. Again $P(t+\Delta)-Q(t+\Delta)=o\left(\Delta^{2}\right)$. We write Eq. (28) slightly differently.

Let $H_{1}$ be a rotation formed from block diagonal matrix

$$
H_{1}=\left[\begin{array}{cccc}
\Theta_{1} & 0 & \ldots & 0  \tag{29}\\
0 & \Theta_{2} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & \Theta_{n}
\end{array}\right]
$$

where $\Theta_{k}$ is $n_{k} \times n_{k}$ sub-block in $S O\left(n_{k}\right) . H_{1}=\exp \left(h_{1}\right)$ is chosen such that

$$
H_{1}^{\prime} P\left(A d_{\bar{K}}\left(X_{d}\right)\right) H_{1}=a
$$

is a diagonal matrix. Let $H_{2}=\exp (\underbrace{A^{-1} h_{1} A}_{h_{2}})$, where $h_{2}$ is skew symmetric, such that

$$
h_{1}=\left[\begin{array}{cccc}
\theta_{1} & 0 & \ldots & 0  \tag{30}\\
0 & \theta_{2} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & \theta_{n}
\end{array}\right], h_{2}=\left[\begin{array}{cccc}
\hat{\theta}_{1} & 0 & \ldots & 0 \\
0 & \hat{\theta}_{2} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & \hat{\theta}_{n}
\end{array}\right],
$$

where
$\theta_{k}, \hat{\theta}_{k}$ is $n_{k} \times n_{k}$ sub-block in so $\left(n_{k}\right)$, related by (see 26)

$$
\hat{\theta}_{k}=A_{k} \cdot \theta_{k} A_{k}, \quad \theta_{k}=\left[\begin{array}{cc}
\overbrace{\theta_{11}}^{r \times r} & \theta_{12}  \tag{31}\\
-\theta_{12}^{\dagger} & \underbrace{\theta_{22}}_{s \times s}
\end{array}\right], \hat{\theta}_{k}=\left[\begin{array}{cc}
\theta_{11} & -\theta_{12} \\
\theta_{12}^{\dagger} & \theta_{22}
\end{array}\right]
$$

Note $H_{1}^{\prime} P\left(A d_{k}\left(X_{d}\right)\right) H_{1}=a$ lies in convex hull of eigenvalues of $X_{d}$. This is true if we look at the diagonal of $H_{1}^{\prime} A d_{K}\left(X_{d}\right) H_{1}$, it follows from Schur Convexity. The diagonal of $H_{1}^{\prime} A d_{k}\left(X_{d}\right)^{\perp} H_{1}$ is zero as its inner product

$$
\operatorname{tr}\left(a_{1} H_{1}^{\prime} A d_{k}\left(X_{d}\right)^{\perp} H_{1}\right)=\operatorname{tr}\left(H_{1} a_{1} H_{1}^{\prime} A d_{k}\left(X_{d}\right)^{\perp}\right)=0
$$

as $H_{1} a_{1} H_{1}^{\prime}$ has block diagonal form which is perpendicular to $A d_{k}\left(X_{d}\right)^{\perp}$. Therefore diagonal of $H_{1}^{\prime} P\left(A d_{k}\left(X_{d}\right)\right) H_{1}$ is same as diagonal of $H_{1}^{\prime} A d_{K}\left(X_{d}\right) H_{1}$.

Now using $H_{1} A H_{2}^{\dagger}=A$, from 28, we have

$$
\begin{gather*}
Q(t+\Delta)=\exp \left(\Omega_{1} \Delta\right) K_{1} \exp \left(P\left(A d_{\bar{K}}\left(X_{d}\right) \Delta\right)\right) H_{1} A H_{2}^{\dagger} \exp \left(\Omega_{2} \Delta\right) K_{2} .  \tag{32}\\
Q(t+\Delta)=\exp \left(\Omega_{1} \Delta\right) K_{1} H_{1} \exp (a \Delta) A H_{2}^{\dagger} \exp \left(\Omega_{2} \Delta\right) K_{2} . \tag{33}
\end{gather*}
$$

where the above expression can be written as

$$
Q(t+\Delta)=\exp \left(\Omega_{1} \Delta\right) \exp \left(K_{1} H_{1} a H_{1}^{\prime} K_{1}^{\prime} \Delta\right) \exp \left(K_{1} A \Omega_{2} A^{\prime} K_{1}^{\prime} \Delta\right) P(t) .
$$

where $\Omega_{1}, H_{1}, a, \Omega_{2}$, are chosen such that

$$
\begin{gathered}
\left(\Omega_{1}+K_{1} H_{1} a H_{1}^{\prime} K_{1}^{\prime}+K_{1} A \Omega_{2} A^{\prime} K_{1}^{\prime}\right)=A d_{K}\left(X_{d}\right) . \\
\left(\Omega_{1}^{\prime}+H_{1} a H_{1}^{\prime}+A \Omega_{2} A^{\prime}\right)=A d_{\bar{K}}\left(X_{d}\right) . \\
Q(t+\Delta)-P(t+\Delta)=o\left(\Delta^{2}\right) P(t) . \\
Q(t+\Delta)=\left(I+o\left(\Delta^{2}\right)\right) P(t+\Delta) . \\
Q(t+\Delta) Q(t+\Delta)^{T}=\left(I+o\left(\Delta^{2}\right)\right) P(t+\Delta) P^{T}(t+\Delta)\left(I+o\left(\Delta^{2}\right)\right) \\
=P(t+\Delta) P^{T}(t+\Delta)\left[I+o\left(\Delta^{2}\right)\right] . \\
P(t+\Delta) P^{T}(t+\Delta)=K_{1}\left[\begin{array}{cccc}
\exp \left(i 2 \phi_{1}\right) & 0 & \ldots & 0 \\
0 & \exp \left(i 2 \phi_{2}\right) & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \exp \left(i 2 \phi_{n}\right)
\end{array}\right]
\end{gathered}
$$

Let $F=P(t+\Delta) P^{T}(t+\Delta)$ and $G=Q(t+\Delta) Q^{T}(T+\Delta)$ we relate the eigenvalues, of $F$ and $G$. Given $F, G$, as above, with $|F-G| \leq \varepsilon$, and a ordered set of eigenvalues of $F$, denote $\lambda(F)=\left[\begin{array}{c}\exp \left(i 2 \phi_{1}\right) \\ \exp \left(i 2 \phi_{2}\right) \\ \vdots \\ \exp \left(i 2 \phi_{n}\right)\end{array}\right]$, there exists an ordering (correspondence) of eigenvalues of $G$, such that $|\lambda(F)-\lambda(G)|<\varepsilon$.

Choose an ordering of $\lambda(G)$ call $\mu$ that minimizes $|\lambda(F)-\lambda(G)|$.
$F=U_{1} D(\lambda) U_{1}^{\prime}$ and $G=U_{2} D(\mu) U_{2}^{\prime}$, where $D(\lambda)$ is diagonal with diagonal as $\lambda$, let $U=U_{1}^{\prime} U_{2}$,
$|F-G|^{2}=\left|D(\lambda)-U D(\mu) U^{\prime}\right|^{2}=|\lambda|^{2}+|\mu|^{2}-\operatorname{tr}\left(D(\lambda)^{\prime} U D(\mu) U^{\prime}+(U D(\mu) U)^{\prime} D(\lambda)\right)$,
By Schur convexity,

$$
\operatorname{tr}\left(D(\lambda)^{\prime} U D(\mu) U^{\prime}+\left(U D(\mu) U^{\prime}\right)^{\prime} D(\lambda)\right)=\sum_{i} \alpha_{i}\left(\lambda^{\prime} P_{i}(\mu)+P_{i}(\mu)^{\prime} \lambda\right),
$$

where $P_{i}$ are permutations. Therefore $|F-G|^{2}>|\lambda-\mu|^{2}$.
Therefore,

$$
\lambda\left(Q Q^{T}(t+\Delta)\right)=\lambda\left(P P^{T}(t+\Delta)\right)+o\left(\Delta^{2}\right)
$$

The difference

$$
\begin{aligned}
o\left(\Delta^{2}\right) & =\underbrace{\exp \left(\left(\Omega_{1}+K_{1} H_{1} a H_{1}^{\prime} K_{1}^{\prime}+K_{1} A \Omega_{2} A^{\prime} K_{1}^{\prime}\right) \Delta\right)}_{\exp \left(A d_{K}\left(X_{d}\right) \Delta\right)} \\
& -\exp \left(\Omega_{1} \Delta\right) \exp \left(K_{1} H_{1} a H_{1}^{\prime} K_{1}^{\prime} \Delta\right) \exp \left(K_{1} A \Omega_{2} A^{\prime} K_{1}^{\prime} \Delta\right),
\end{aligned}
$$

is regulated by size of $\Omega_{2}$, which is bounded by $\left|\Omega_{2}\right| \leq \frac{\left\|X_{d}\right\|}{\sin \left(\phi_{i}-\phi_{j}\right)}$, where $\sin \left(\phi_{i}-\phi_{j}\right)$ is smallest non-zero difference. $\Delta$ is chosen small enough such that $\left|o\left(\Delta^{2}\right)\right|<\varepsilon \Delta$.

For each point $t \in[0, T]$, we choose an open nghd $N(t)=\left(t-N_{t}, t+N_{t}\right)$, such that $o_{t}\left(\Delta^{2}\right)<\varepsilon \Delta$ for $\Delta \in N(t) . N(t)$ forms a cover of $[0, T]$. We can choose a finite subcover centered at $t_{1}, \ldots, t_{n}$ (see Figure 1A). Consider trajectory at points $P\left(t_{1}\right), \ldots, \ldots P\left(t_{n}\right)$. Let $t_{i, i+1}$ be the point in intersection of $N\left(t_{i}\right)$ and $N\left(t_{i+1}\right)$. Let $\Delta_{i}^{+}=t_{i, i+1}-t_{i}$ and $\Delta_{i+1}^{-}=t_{i+1}-t_{i, i+1}$. We consider points $P\left(t_{i}\right), P\left(t_{i+1}\right), P\left(t_{i, i+1}\right), \underbrace{Q\left(t_{i}+\Delta_{i}^{+}\right)}_{Q_{i+}}, \underbrace{Q\left(t_{i+1}-\Delta_{i+1}^{-}\right)}_{Q_{(i+1)-}}$ as shown in Figure 1B.

Then we get the following recursive relations.

$$
\begin{gather*}
\lambda\left(Q_{i+} Q_{i+}^{T}\right)=\exp \left(2 a_{i}^{+} \Delta_{i}^{+}\right) \lambda\left(P_{i} P_{i}^{T}\right)  \tag{34}\\
\lambda\left(P_{i, i+1} P_{i, i+1}^{T}\right)=\lambda\left(Q_{i+} Q_{i+}^{T}\right)+o\left(\left(\Delta_{i}^{+}\right)^{2}\right)  \tag{35}\\
\lambda\left(Q_{(i+1)-} Q_{(i+1)-}^{T}\right)=\lambda\left(P_{i, i+1} P_{i, i+1}^{T}\right)+o\left(\left(\Delta_{i+1}^{-}\right)^{2}\right)  \tag{36}\\
\exp \left(-2 a_{i+1}^{-} \Delta_{i+1}^{-}\right) \lambda\left(P_{i+1} P_{i+1}^{T}\right)=\lambda\left(Q_{(i+1)-} Q_{(i+1)-}^{T}\right) \tag{37}
\end{gather*}
$$

where $a_{i}^{+}$and $a_{i+1}^{-}$correspond to $a$ in Eq. (33) and lie in the convex hull of the eigenvalues $X_{d}$.

Adding the above equations,

$$
\begin{gather*}
\lambda\left(P_{i+1} P_{i+1}^{T}\right)=\exp \left(o\left(\Delta^{2}\right)\right) \exp \left(2\left(a_{i}^{+} \Delta_{i}^{+}+a_{i+1}^{-} \Delta_{i+1}^{-}\right) \lambda\left(P_{i} P_{i}^{\dagger}\right) .\right.  \tag{38}\\
\lambda\left(P_{n} P_{n}^{T}\right)=\exp (\underbrace{\sum o\left(\Delta^{2}\right)}_{\leq \varepsilon T}) \exp \left(2 \sum_{i} a_{i}^{+} \Delta_{i}^{+}+a_{i+1}^{-} \Delta_{i+1}^{-}\right) \lambda\left(P_{1} P_{1}^{T}\right) . \tag{39}
\end{gather*}
$$

where $o\left(\Delta^{2}\right)$ in Eq. (38) is diagonal.

$$
\begin{equation*}
\lambda\left(P_{n} P_{n}^{T}\right)=\exp (\underbrace{\sum_{\leq}^{o\left(\Delta^{2}\right)}}_{\leq \varepsilon T}) \exp \left(2 T \sum_{k} \alpha_{k} P_{k}(\lambda)\right) \lambda\left(P_{1} P_{1}^{T}\right)=\exp (\underbrace{\sum^{o\left(\Delta^{2}\right)}}_{\leq \varepsilon T}) \exp (2 \mu T) \lambda\left(P_{1} P_{1}^{T}\right), \tag{40}
\end{equation*}
$$

where $\mu<\lambda$ and $P_{1}=I$.

$$
\begin{equation*}
P_{n}=K_{1} \exp (\frac{1}{2} \underbrace{\sum o\left(\Delta^{2}\right)}_{\leq \varepsilon T}) \exp (\mu T) K_{2} \tag{41}
\end{equation*}
$$

Note, $\left|P_{n}-K_{1} \exp (\mu T) K_{2}\right|=o(\varepsilon)$. This implies that $P_{n}$ belongs to the compact set $K_{1} \exp (\mu T) K_{2}$, else it has minimum distance from this compact set and by
making $\Delta \rightarrow 0$ and hence $\varepsilon \rightarrow 0$, we can make this arbitrarily small. In Eq. (18), $P_{n} \rightarrow P(T)$ as $\tau \rightarrow 0$. Hence $P(T)$ belongs to compact set $K_{1} \exp (\mu T) K_{2}$. q.e.d.

Corollary 1. Let $U(t) \in S U(n)$ be a solution to the differential equation

$$
\dot{U}=\left(X_{d}+\sum_{i} u_{i} X_{i}\right) U
$$

where $\left\{X_{i}\right\}_{L A}$, the Lie algebra generated by $X_{i}$, is so( $n$ ) and
$X_{d}=-i\left[\begin{array}{cccc}\lambda_{1} & 0 & \ldots & 0 \\ 0 & \lambda_{2} & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \lambda_{n}\end{array}\right]$. The elements of reachable set at time $T$, takes the form
$U(T) \in K_{1} \exp (-i \mu T) K_{2}$, where $K_{1}, K_{2} \in S O(n)$ and $\mu<\lambda$, where $\lambda=\left(\lambda_{1}, \ldots, \lambda_{n}\right)^{\prime}$ and the set $S=K_{1} \exp (-i \mu T) K_{2}$ belongs to the closure of reachable set.

Proof. Let $V(t)=K^{\prime}(t) U(t)$, where, $\dot{K}=\left(\sum_{i} u_{i} X_{i}\right) K$. Then

$$
\dot{V}(t)=A d_{K^{\prime}(t)}\left(X_{d}\right) V(t) .
$$

From Theorem 1, we have $V(T) \in K_{1} \exp (-i \mu T) K_{2}$. Therefore $U(T) \in K_{1} \exp (-i \mu T) K_{2}$. Given

$$
\begin{aligned}
U=K_{1} \exp (-i \mu T) K_{2} & =K_{1} \exp \left(-i \sum_{j} \alpha_{j} P_{j}(\lambda) T\right) K_{2} \\
& =K_{1} \prod_{j} \exp \left(-i t_{j} X_{d}\right) K_{j}, \quad \sum t_{j}=T
\end{aligned}
$$

We can synthesize $K_{j}$ in negligible time, therefore $|U(T)-U|<\varepsilon$, for any desired $\varepsilon$. Hence $U$ is in closure of reachable set. q.e.d.

Remark 4. We now show how Remark 2 and Theorem 1 can be mapped to results on decomposition and reachable set for coupled spins/qubits. Consider the transformation

$$
W=\exp \left(-i \pi I_{y} S_{y}\right) \exp \left(-i \frac{\pi}{2} I_{z}\right)
$$



A


B
Figure 1.
A. Collection of overlapping neighborhoods forming the finite subcover. B. Depiction of $P_{i}, P_{i+1}, Q_{i+}, Q_{i-}$, $P_{i, i+1}$ as in proof of Theorem 1.

The transformation maps the algebra $\mathfrak{k}=s u(2) \times s u(2)=\left\{I_{\alpha}, S_{\alpha}\right\}$ to $\mathfrak{k}_{1}=s o(4)$, four dimensional skew symmetric matrices, i.e., $A d_{W}(\mathfrak{k})=\mathfrak{k}_{1}$. The transformation maps $\mathfrak{p}=\left\{I_{\alpha} S_{\beta}\right\}$ to $\mathfrak{p}_{1}=-i A$, where $A$ is traceless symmetric and maps $\mathfrak{a}=-i\left\{I_{x} S_{x}, I_{y} S_{y}, I_{z} S_{z}\right\}$ to $\mathfrak{a}_{1}=-i\left\{-\frac{S_{z}}{2}, \frac{I_{z}}{2}, I_{z} S_{z}\right\}$, space of diagonal matrices in $\mathfrak{p}_{1}$, such that $a_{x} I_{x} S_{x}+a_{y} I_{y} S_{y}+a_{z} I_{z} S_{z}$ gets mapped to the four vector (the diagonal) $\left(\lambda_{1}, \lambda_{2}, \lambda_{3}, \lambda_{4}\right)=\left(a_{y}+a_{z}-a_{x}, a_{x}+a_{y}-a_{z},-\left(a_{x}+a_{y}+a_{z}\right), a_{x}+a_{z}-a_{y}\right)$.

Corollary 2. Canonical decomposition. Given the decomposition of $\operatorname{SU}(4)$ from Remark 2, we can write

$$
U=\exp \left(\Omega_{1}\right) \exp \left(-i\left[\begin{array}{ccc}
\lambda_{1} & \ldots & 0 \\
0 & \ddots & 0 \\
0 & 0 & \lambda_{4}
\end{array}\right]\right) \exp \left(\Omega_{2}\right),
$$

where $\Omega_{1}, \Omega_{2} \in$ so(4). We write above as

$$
U=\exp \left(\Omega_{1}\right) \exp \left(-i\left(-\frac{a_{x}}{2} S_{z}+\frac{a_{y}}{2} I_{z}+a_{z} I_{z} S_{z}\right)\right) \exp \left(\Omega_{2}\right),
$$

Multiplying both sides with $W^{\prime}()$.$W gives$

$$
W^{\prime} U W=K_{1} \exp \left(-i a_{x} I_{x} S_{x}+a_{y} I_{y} S_{y}+a_{z} I_{z} S_{z}\right) K_{2},
$$

where $K_{1}, K_{2} \in S U(2) \times S U(2)$ local unitaries and we can rotate to $a_{x} \geq a_{y} \geq\left|a_{z}\right|$.
Corollary 3. Digonalization. Given $-i H_{c}=-i \sum_{\alpha \beta} J_{\alpha \beta} I_{\alpha} S_{\beta}$, there exists a local unitary $K$ such that

$$
K\left(-i H_{c}\right) K^{\prime}=-i\left(a_{x} I_{x} S_{x}+a_{y} I_{y} S_{y}+a_{z} I_{z} S_{z}\right), a_{x} \geq a_{y} \geq\left|a_{z}\right| .
$$

Note $W\left(-i H_{c}\right) W^{\prime} \in \mathfrak{p}_{1}$. Then choose $\Theta \in S O(n)$ such that $\Theta W\left(-i H_{c}\right) W^{\prime} \Theta^{\prime}=-i\left(-\frac{a_{x}}{2} S_{z}+\frac{a_{y}}{2} I_{z}+a_{z} I_{z} S_{z}\right)$ and hence

$$
\left(W^{\prime} \exp (\Omega) W\right)\left(-i H_{c}\right)\left(W \exp (\Omega) W^{\prime}\right)^{\prime}=-i\left(a_{x} I_{x} S_{x}+a_{y} I_{y} S_{y}+a_{z} I_{z} S_{z}\right) .
$$

where $K=W^{\prime} \exp (\Omega) W$ is a local unitary. We can rotate to ensure $a_{x} \geq a_{y} \geq\left|a_{z}\right|$.
Corollary 4. Given the evolution of coupled qubits $\dot{U}=-i\left(H_{c}+\sum_{j} u_{j} H_{j}\right) U$, we can diagonalize $H_{c}=\sum_{\alpha \beta} J_{\alpha \beta} I_{\alpha} S_{\beta}$ by local unitary $X_{d}=K^{\prime} H_{c} K=a_{x} I_{x} S_{x}+a_{y} I_{y} S_{y}+$ $a_{z} I_{z} S_{z}, a_{x} \geq a_{y} \geq\left|a_{z}\right|$, which we write as triple $\left(a_{x}, a_{y}, a_{z}\right)$. From this, there are 24 triples obtained by permuting and changing sign of any two by local unitary. Then $U(T) \in S$ where

$$
S=K_{1} \exp \left(T \sum_{i} \alpha_{i}\left(a_{i}, b_{i}, c_{i}\right)\right) K_{2}, \quad \alpha_{i}>0 \quad \sum_{i} \alpha_{i}=1 .
$$

Furthermore $S$ belongs to the closure of the reachable set. Alternate description of $S$ is

$$
U=K_{1} \exp \left(-i\left(\alpha I_{x} S_{x}+\beta I_{y} S_{y}+\gamma I_{z} S_{z}\right)\right) K_{2}, \quad \alpha \geq \beta \geq|\gamma|,
$$

$\alpha \leq a_{x} T$ and $\alpha+\beta \pm \gamma \leq\left(a_{x}+a_{y} \pm a_{z}\right) T$.
Proof. Let $V(t)=K^{\prime}(t) U(t)$, where $\dot{K}=\left(-i \sum_{j} u_{j} X_{j}\right) K$. Then

$$
\dot{V}(t)=A d_{K^{\prime}(t)}\left(-i X_{d}\right) V(t)
$$

Consider the product

$$
V=\prod_{i} \exp \left(A d_{K_{i}}\left(-i X_{d}\right) \Delta t\right)
$$

where $K_{i} \in S U(2) \otimes S U(2)$ and $X_{d}=a_{x} I_{x} S_{x}+a_{y} I_{y} S_{y}+a_{z} I_{z} S_{z}$, where $a_{x} \geq a_{y} \geq\left|a_{z}\right|$. Then,

$$
W V W^{\prime}=\prod_{i} \exp \left(A d_{W K_{i} W^{\prime}}\left(-i W X_{d} W^{\prime}\right) \Delta t\right)
$$

Observe $W K_{i} W^{\prime} \in S O(4)$ and $W X_{d} W^{\prime}=\operatorname{diag}\left(\lambda_{1}, \lambda_{2}, \ldots, \lambda_{4}\right)$. Then using results from Theorem 1, we have

$$
W V W^{\prime}=J_{1} \exp (-i \mu) J_{2}=J_{1} \exp \left(-i \sum_{j} \alpha_{j} P_{j}(\lambda)\right) J_{2}, \quad J_{1}, J_{2} \in S O(4), \quad \mu<\lambda T
$$

Multiplying both sides with $W^{\prime}(\cdot) W$, we get

$$
V=K_{1} \exp \left(T \sum_{i} \alpha_{i}\left(a_{i}, b_{i}, c_{i}\right)\right) K_{2}, \quad \alpha_{i}>0 \quad \sum_{i} \alpha_{i}=1 .
$$

which we can write as

$$
V=K_{1} \exp \left(-i\left(\alpha I_{x} S_{x}+\beta I_{y} S_{y}+\gamma I_{z} S_{z}\right)\right) K_{2}, \quad \alpha \geq \beta \geq|\gamma|,
$$

where using $\mu<\lambda T$, we get,

$$
\begin{gather*}
\alpha+\beta-\gamma \leq\left(a_{x}+a_{y}-a_{z}\right) T  \tag{42}\\
\alpha \leq a_{x} T  \tag{43}\\
\alpha+\beta+\gamma \leq\left(a_{x}+a_{y}+a_{z}\right) T . \tag{44}
\end{gather*}
$$

Furthermore $U=K V$. Hence the proof. q.e.d.

## 3. Time optimal control for $G / K$ problem

Remark 5. Stabilizer: Let $\mathfrak{g}=\mathfrak{p} \oplus \mathfrak{k}$ be Cartan decomposition of real semisimple Lie algebra $\mathfrak{g}$ and $\mathfrak{a} \in \mathfrak{p}$ be its Cartan subalgebra. Let $a \in \mathfrak{a}$. $a d_{a}^{2}: \mathfrak{p} \rightarrow \mathfrak{p}$ is symmetric in basis orthonormal wrt to the killing form. We can diagonalize $a d_{a}^{2}$. Let $Y_{i}$ be eigenvectors with nonzero (negative) eigenvalues $-\lambda_{i}^{2}$. Let $X_{i}=\frac{\left[a, Y_{i}\right]}{\lambda_{i}}, \lambda_{i}>0$.

$$
a d_{a}\left(Y_{i}\right)=\lambda_{i} X_{i}, \quad a d_{a}\left(X_{i}\right)=-\lambda_{i} Y_{i} .
$$

$X_{i}$ are independent, as $\sum \alpha_{i} X_{i}=0$ implies $-\sum \alpha_{i} \lambda_{i} Y_{i}=0$. Since $Y_{i}$ are independent, $X_{i}$ are independent. Given $X \perp X_{i}$, then $[a, X]=0$, otherwise we can decompose it in eigenvectors of $a d_{a}^{2}$, i.e., $[a, X]=\sum_{i} \alpha_{i} a_{i}+\sum_{j} \beta_{j} Y_{j}$, where $a_{i}$ are zero eigenvectors of $a d_{a}^{2}$. Since $0=\left\langle X[a[a, X]\rangle=-\|[a, X]\|^{2}\right.$, which means $[a, X]=0$. This is a contradiction. $Y_{i}$ are orthogonal, implies $X_{i}$ are orthogonal,
$\left\langle\left[a, Y_{i}\right]\left[a, Y_{j}\right]\right\rangle=\left\langle\left[a,\left[a, Y_{i}\right] Y_{j}\right\rangle=\lambda_{i}^{2}\left\langle Y_{i} Y_{j}\right\rangle=0\right.$. Let $\mathfrak{k}_{0} \in \mathfrak{k}$ satisfy $\left[a, \mathfrak{k}_{0}\right]=0$. Then $\mathfrak{k}_{0}=\left\{X_{i}\right\}^{\perp}$.
$\tilde{Y}_{i}$ denote eigenvectors that have $\lambda_{i}$ as non-zero integral multiples of $\pi . \tilde{X}_{i}$ are $a d_{a}$ related to $\tilde{Y}_{i}$. We now reserve $Y_{i}$ for non-zero eigenvectors that are not integral multiples of $\pi$.

Let

$$
\mathfrak{f}=\left\{a_{i}\right\} \oplus \tilde{Y}_{i}, \quad \mathfrak{h}=\mathfrak{k}_{0} \oplus \tilde{X}_{i},
$$

$\tilde{X}_{i}, X_{l}, k_{j}$ where $k_{j}$ forms a basis of $\mathfrak{k}$, forms a basis of $\mathfrak{k}$. Let $A=\exp (a)$.
$A k A^{-1}=A\left(\sum_{i} \alpha_{i} X_{i}+\sum_{l} \alpha_{l} \tilde{X}_{l}+\sum_{j} \alpha_{j} k_{j}\right) A^{-}$, where $k \in \mathfrak{k}$

$$
A k A^{-1}=\sum_{i} \alpha_{i}\left[\cos \left(\lambda_{i}\right) X_{i}-\sin \left(\lambda_{i}\right) Y_{i}\right]+\sum_{l} \pm \alpha_{l} \tilde{X}_{l}+\sum_{j} \alpha_{j} k_{j}
$$

The range of $A(\cdot) A^{-1}$ in $\mathfrak{p}$, is perpendicular to $\mathfrak{f}$. Given $Y \in \mathfrak{p}$ such that $Y \in \mathfrak{f}^{\perp}$. The norm $\|X\|$ of $X \in \mathfrak{k}$, such that $\mathfrak{p}$ part of $\left.A X A^{-1}\right|_{\mathfrak{p}}=Y$ satisfies

$$
\begin{equation*}
\|X\| \leq \frac{\|Y\|}{\sin \lambda_{s}} . \tag{45}
\end{equation*}
$$

where $\lambda_{s}^{2}$ is the smallest nonzero eigenvalue of $-a d_{a}^{2}$ such that $\lambda_{s}$ is not an integral multiple of $\pi$.
$A^{2} k A^{-2}$ stabilizes $\mathfrak{h} \in \mathfrak{k}$ and $\mathfrak{f} \in \mathfrak{p}$. If $k \in \mathfrak{k}$, is stabilized by $A^{2}(\cdot) A^{-2}, \lambda_{i}=n \pi$, i.e., $k \in \mathfrak{h}$. This means $\mathfrak{h}$ is an subalgebra, as the Lie bracket of $[y, z] \in \mathfrak{k}$ for $y, z \in \mathfrak{h}$ is stabilized by $A^{2}(\cdot) A^{-2}$.

Let $H=\exp (\mathfrak{h})$, be an integral manifold of $\mathfrak{h}$. Let $\tilde{H} \in K$ be the solution to $A^{2} \tilde{H} A^{-2}=\tilde{H}$ or $A^{2} \tilde{H}-\tilde{H} A^{-2}=0 . \tilde{H}$ is closed, $H \in \tilde{H}$. We show that $\tilde{H}$ is a manifold. Given element $H_{0} \in \tilde{H} \in K$, where $K$ is closed, we have a $\exp \left(B_{\delta}^{\mathfrak{k}}\right)$ nghd of $H_{0}$, in $\exp \left(B_{\delta}\right)$ ball nghd of $H_{0}$, which is one to one. For $x \in B_{\delta}^{\mathfrak{k}}$, $A^{2} \exp (x) A^{-2}=\exp (x)$, implies,

$$
\begin{array}{r}
A^{2} \exp \left(\sum_{i} \alpha_{i} X_{i}+\sum_{l} \beta_{l} \tilde{X}_{l}+\sum_{j} \gamma_{j} k_{j}\right) H_{0} A^{-2}=\exp \left(\sum_{i} \alpha_{i} \cos \left(2 \lambda_{i}\right) X_{i}-\sin \left(2 \lambda_{i}\right) Y_{i}\right. \\
\\
\left.+\sum_{l} \beta_{l} \tilde{X}_{l}+\sum_{j} \gamma_{j} k_{j}\right) H_{0}=\exp \left(\sum_{i} \alpha_{i} X_{i}+\sum_{l} \beta_{l} \tilde{X}_{l}+\sum_{j} \gamma_{j} k_{j}\right) H_{0}
\end{array}
$$

then by one to one property of $\exp \left(B_{\delta}\right)$, we get $\alpha_{i}=0$ and $x \in \mathfrak{h}$. Therefore $\exp \left(B_{\delta}^{\mathfrak{b}}\right) H_{0}$ is a nghd of $H_{0}$.

Given a sequence $H_{i} \in \exp (\mathfrak{h})$ converging to $H_{0}$, for $n$ large enough $H_{n} \in \exp \left(B_{\delta}^{\mathfrak{h}}\right) H_{0}$. Then $H_{0}$ is in invariant manifold $\exp (\mathfrak{h})$. Hence $\exp (\mathfrak{h})$ is closed and hence compact.

Let $y \in \mathfrak{f}$, then there exists a $h_{0} \in \mathfrak{h}$ such that $\exp \left(h_{0}\right) y \exp \left(-h_{0}\right) \in \mathfrak{a}$. We maximize the function $\left\langle a_{r}, \exp (h) y \exp (h)\right\rangle$, over the compact group $\exp (\mathfrak{h})$, for regular element $a_{r} \in \mathfrak{a}$ and $\langle.,$.$\rangle is the killing form. At the maxima, we have at t=0$, $\frac{d}{d t}\left\langle a_{r}, \exp \left(h_{1} t\right)\left(\exp \left(h_{0}\right) y \exp \left(-h_{0}\right)\right) \exp \left(-h_{1} t\right)\right\rangle=0$.

$$
\left\langle a_{r},\left[h_{1} \exp \left(h_{0}\right) y \exp \left(-h_{0}\right)\right]\right\rangle=-\left\langle h_{1},\left[a_{r} \exp \left(h_{0}\right) y \exp \left(-h_{0}\right)\right]\right\rangle,
$$

if $\exp \left(h_{0}\right) y \exp \left(-h_{0}\right) \neq \mathfrak{a}$, then $\left[a_{r}, \quad \exp \left(h_{0}\right) y \exp \left(-h_{0}\right)\right] \in \mathfrak{k}$. The bracket $\left[a_{r}, \quad \exp \left(h_{0}\right) y \exp \left(-h_{0}\right)\right]$ is $A d_{A^{2}}$ invariant and, hence, belongs to $\mathfrak{h}$. We can choose $h_{1}$ so that gradient is not zero. Hence $\exp \left(h_{0}\right) y \exp \left(-h_{0}\right) \in \mathfrak{a}$. For $z \in \mathfrak{p}$ such that $z \in \mathfrak{f}^{\perp}$, we have $\exp \left(h_{0}\right) z \exp \left(-h_{0}\right) \in \mathfrak{a}^{\perp}$.

$$
\left\langle\mathfrak{a}, \exp \left(h_{0}\right) z \exp \left(-h_{0}\right)\right\rangle=\left\langle\exp \left(-h_{0}\right) \mathfrak{a} \exp \left(h_{0}\right), z\right\rangle=0,
$$

as $\exp \left(-h_{0}\right) \mathfrak{a} \exp \left(h_{0}\right)$ is $A d_{A^{2}}$ invariant, hence $\exp \left(-h_{0}\right) \mathfrak{a} \exp \left(h_{0}\right) \in \mathfrak{f}$. In above, we worked with killing form. For $\mathfrak{g}=\operatorname{su}(n)$, we may use standard inner product.

Remark 6. Kostant's convexity: [28] Given the decomposition $\mathfrak{g}=\mathfrak{p} \oplus \mathfrak{k}$, let $\mathfrak{a} \subset \mathfrak{p}$ and $X \in \mathfrak{a}$. Let $\mathcal{W}_{i} \in \exp (\mathfrak{k})$ such that $\mathcal{W}_{i} X \mathcal{W}_{i} \in \mathfrak{a}$ are distinct, Weyl points. Then projection (w.r.t killing form) of $A d_{K}(X)$ on a lies in convex hull of these Weyl points. The $\mathcal{C}$ be the convex hull and let projection $P\left(A d_{K}(X)\right)$ lie outside this Hull. Then there is a separating hyperplane $a$, such that $\left\langle A d_{K}(X), a\right\rangle<\langle\mathcal{C}, a\rangle$. W.L.O.G we can take $a$ to be a regular element. We minimize $\left\langle A d_{K}(X), a\right\rangle$, with choice of $K$ and find that minimum happens when $\left[A d_{K}(X), a\right]=0$, i.e. $A d_{K}(X)$ is a Weyl point. Hence $P\left(A d_{K}(X)\right) \in \sum_{i} \alpha_{i} \mathcal{W}_{i} X \mathcal{W}_{i}^{-1}$, for $\alpha_{i}>0$ and $\sum_{i} \alpha_{i}=1$. The result is true with a projection w.r.t inner product that satisfies $\langle x,[y, z]\rangle=\langle[x, y], z]\rangle$, like standard inner product on $\mathfrak{g}=s u(n)$.

Theorem 2 Given a compact Lie group $G$ and Lie algebra $\mathfrak{g}$. Consider the Cartan decomposition of a real semisimple Lie algebra $\mathfrak{g}=\mathfrak{p} \oplus \mathfrak{k}$. Given the control system

$$
\dot{X}=A d_{K(t)}\left(X_{d}\right) X, \quad P(0)=\mathbf{1}
$$

where $X_{d} \in \mathfrak{a}$, the Cartan subalgebra $\mathfrak{a} \in \mathfrak{p}$ and $K(t) \in \exp \mathfrak{k}$, a closed subgroup of $G$. The end point

$$
P(T)=K_{1} \exp \left(T \sum_{i} \alpha_{i} \mathcal{W}_{i}\left(X_{d}\right)\right) K_{2}
$$

where $K_{1}, K_{2} \in \exp (\mathfrak{k})$ and $\mathcal{W}_{i}\left(X_{d}\right) \in \mathfrak{a}$ are Weyl points, $\alpha_{i}>0$ and $\sum_{i} \alpha_{i}=1$.
Proof. As in proof of Theorem 1, we define

$$
P(t+\Delta)=\exp \left(A d_{K}\left(X_{d}\right) \Delta\right) P(t)=\exp \left(A d_{K}\left(X_{d}\right) \Delta\right) K_{1} \exp (a) K_{2}
$$

and show that

$$
\begin{equation*}
\exp \left(A d_{K}\left(X_{d}\right) \Delta\right) K_{1} A K_{2}=K_{a} \exp \left(a_{0} \Delta+C \Delta^{2}\right) A K_{b}=K_{a} \exp \left(a+a_{0} \Delta+C \Delta^{2}\right) K_{b}, \tag{46}
\end{equation*}
$$

where for $\bar{K}=K_{1}^{-1} K$,

$$
A d_{\bar{K}}\left(X_{d}\right)=\underbrace{P\left(A d_{\bar{K}}\left(X_{d}\right)\right)}_{a_{0}}+A d_{\bar{K}}\left(X_{d}\right)^{\perp} .
$$

where $P$ is projection w.r.t killing form and $a_{0} \in \mathfrak{f}$, the centralizer in $\mathfrak{p}$ as defined in Remark $5, C \Delta^{2} \in \mathfrak{f}$ is a second order term that can be made small by choosing $\Delta$. $K_{a}, K_{b} \in \exp (\mathfrak{k})$.

To show Eq. (46), we show there exists $K_{1^{\prime}}^{\prime}, K_{2^{\prime}} \in K$ such that

$$
\begin{equation*}
\underbrace{\exp \left(k_{1}^{\prime \prime}\right)}_{K_{1}^{\prime \prime}} \exp \left(A d_{\bar{K}^{\prime}}\left(X_{d}\right) \Delta\right) \underbrace{\exp \left(A k_{2}^{\prime \prime} A^{-1}\right)}_{K_{2}^{\prime \prime}}=\exp \left(a_{0} \Delta+C \Delta^{2}\right) \tag{47}
\end{equation*}
$$

where $K_{1}^{\prime \prime}$ and $K_{2}^{\prime \prime}$ are constructed by a iterative procedure as described in the proof below.

Given $X$ and $Y$ as $N \times N$ matrices, considered elements of a matrix Lie algebra $\mathfrak{g}$, we have,

$$
\begin{equation*}
\log \left(e^{X} e^{Y}\right)-(X+Y)=\sum_{n>0} \frac{(-1)^{n-1}}{n} \sum_{1 \leq i \leq n} \frac{\left[X^{r_{1}} Y^{s_{1}} \ldots X^{r_{n}} Y^{s_{n}}\right]}{\sum_{i=1}^{n}\left(r_{i}+s_{i}\right) r_{1}!s_{1}!\ldots r_{n}!s_{n}!}, \tag{48}
\end{equation*}
$$

where $r_{i}+s_{i}>0$.
We bound the largest element (absolute value) of $\log \left(e^{X} e^{Y}\right)-(X+Y)$, denoted as $\left|\log \left(e^{X} e^{Y}\right)-(X+Y)\right|_{0}$, given $|X|_{0}<\Delta$ and $|Y|_{0}<b_{0} \Delta^{k}$, where $k \geq 1, \Delta<1, b_{0} \Delta<1$.

$$
\begin{gather*}
\left|\log \left(e^{X} e^{Y}\right)-(X+Y)\right|_{0} \leq \sum_{n=1} N b_{0} e \Delta^{k+1}+\sum_{n>1} \frac{1}{n} \frac{\left(2 N e^{2}\right)^{n} b_{0} \Delta^{n+k-1}}{n}  \tag{49}\\
\leq N b_{0} e \Delta^{k+1}+\left(N e^{2}\right)^{2} b_{0} \Delta^{k+1}\left(1+2 N e^{2} \Delta+\ldots\right)  \tag{50}\\
\leq N b_{0} e \Delta^{k+1}+\frac{\left(N e^{2}\right)^{2} b_{0} \Delta^{k+1}}{1-2 N e^{2} \Delta} \leq \tilde{M} b_{0} \Delta^{k+1} \tag{51}
\end{gather*}
$$

where $2 N \Delta<1$ and $\tilde{M} \Delta<1$.
Given decomposition of $\mathfrak{g}=\mathfrak{p} \oplus \mathfrak{k}, \mathfrak{p} \perp \mathfrak{k}$ with respect to the negative definite killing form $B(X, Y)=\operatorname{tr}\left(a d_{X} a d_{Y}\right)$. Furthermore there is decomposition of $\mathfrak{p}=\mathfrak{a} \oplus \mathfrak{a}^{\perp}$.

Given

$$
U_{0}=\exp \left(a_{0} \Delta+b_{0} \Delta+c_{0} \Delta\right),
$$

where $a_{0} \in \mathfrak{a}, b_{0} \in \mathfrak{a}^{\perp}$ and $c_{0} \in \mathfrak{k}$, such that $\left|a_{0}\right|_{0}+\left|b_{0}\right|_{0}+\left|c_{0}\right|_{0}<1$, which we just abbreviate as $a_{0}+b_{0}+c_{0}<1$ (we follow this convention below).

We describe an iterative procedure

$$
\begin{equation*}
U_{n}=\Pi_{k=1}^{n} \exp \left(-c_{k} \Delta\right) U_{0} \Pi_{k=0}^{n} \exp \left(-b_{k} \Delta\right), \tag{52}
\end{equation*}
$$

where $c_{k} \in \mathfrak{E}$ and $b_{k} \in \mathfrak{a}^{\perp}$, such that the limit

$$
\begin{equation*}
n \rightarrow \infty \quad U_{n}=\exp \left(a_{0} \Delta+C \Delta^{2}\right), \tag{53}
\end{equation*}
$$

where $a_{0}, C \in \mathfrak{a}$.

$$
\begin{aligned}
U_{1} & =\exp \left(-c_{0} \Delta\right) \exp \left(a_{0} \Delta+b_{0} \Delta+c_{0} \Delta\right) \exp \left(-b_{0} \Delta\right) \\
& =\exp \left(a_{0} \Delta+b_{0} \Delta+c_{0^{\prime}} \Delta^{2}\right) \exp \left(-b_{0} \Delta\right) \\
& =\exp \left(a_{0} \Delta+b_{0^{\prime}} \Delta^{2}+c_{0^{\prime}} \Delta^{2}\right) \\
& =\exp \left(\left(a_{1}+b_{1}+c_{1}\right) \Delta\right)
\end{aligned}
$$

Note $b_{0}^{\prime}$ and $c_{0}^{\prime}$ are elements of $\mathfrak{g}$ and need not be contained in $\mathfrak{a}^{\perp}$ and $\mathfrak{k}$.

Where, using bound in $c_{0}^{\prime} \leq \tilde{M} c_{0}$, which gives $a_{0}+b_{0}+c_{0}^{\prime} \Delta \leq a_{0}+b_{0}+c_{0}$. Using the bound again, we obtain, $b_{0}^{\prime} \leq \tilde{M} b_{0}$. We can decompose, $\left(b_{0}^{\prime}+c_{0}^{\prime}\right) \Delta$, into subspaces $a_{0}^{\prime \prime}+b_{1}+c_{1}$, where $a_{0}^{\prime \prime} \leq M\left(b_{0}^{\prime}+c_{0}^{\prime}\right) \Delta, b_{1} \leq M\left(b_{0}^{\prime}+c_{0}^{\prime}\right) \Delta$ and $c_{1} \leq M\left(b_{0}^{\prime}+c_{0}^{\prime}\right) \Delta$, where $-B(X, X) \leq \lambda_{\max }|X|^{2}$, where $|X|$ is Frobenius norm and $-B(X, X) \geq \lambda_{\text {min }}|X|^{2}$. Let $M=\frac{N \lambda_{\text {max }}}{\lambda_{\text {min }}}$.

This gives, $a_{0}^{\prime \prime} \leq M\left(b_{0}^{\prime}+c_{0}^{\prime}\right) \Delta, b_{1} \leq M\left(b_{0}^{\prime}+c_{0}^{\prime}\right) \Delta$ and $c_{1} \leq M\left(b_{0}^{\prime}+c_{0}^{\prime}\right) \Delta$. This gives

$$
a_{1} \leq a_{0}+\tilde{M} M\left(b_{0}+c_{0}\right) \Delta b_{1} \leq \tilde{M} M\left(b_{0}+c_{0}\right) \Delta c_{1} \leq \tilde{M} M\left(b_{0}+c_{0}\right) \Delta
$$

For $4 \tilde{M} M \Delta<1$, we have, $a_{1}+b_{1}+c_{1} \leq a_{0}+b_{0}+c_{0}$. Continuing and using $\left(b_{k}+c_{k}\right) \leq 2 \tilde{M} M \Delta\left(b_{k-1}+c_{k-1}\right) \leq(2 \tilde{M} M \Delta)^{k}\left(b_{0}+c_{0}\right)$.

Similarly,

$$
\left|a_{k}-a_{k-1}\right|_{0} \leq(2 \tilde{M} M \Delta)^{k}\left(b_{0}+c_{0}\right)
$$

Note, $\left(a_{k}, b_{k}, c_{k}\right)$ is a Cauchy sequences which converges to ( $a_{\infty}, 0,0$ ), where

$$
\left|a_{\infty}-a_{0}\right|_{0} \leq\left(b_{0}+c_{0}\right) \sum_{k=1}^{\infty}(2 \tilde{M} M \Delta)^{k} \leq \frac{2 M \tilde{M} \Delta\left(b_{0}+c_{0}\right)}{1-2 \tilde{M} M \Delta} \leq C \Delta
$$

where $C=4 \tilde{M} M\left(b_{0}+c_{0}\right)$.
The above exercise was illustrative. Now we use an iterative procedure as above to show Eq. (47).

Writing

$$
A d_{\bar{K}}\left(X_{d}\right)=\underbrace{P\left(A d_{\bar{K}}\left(X_{d}\right)\right)}_{a_{0}}+\underbrace{A d_{\bar{K}}\left(X_{d}\right)^{\perp}}_{b_{0}},
$$

where $a_{0} \in \mathfrak{f}$ and $b_{0} \in \mathfrak{f}^{\perp}$, consider again the iterations

$$
\begin{aligned}
U_{0} & =\exp \left(-\bar{c}_{0} \Delta\right) \exp \left(a_{0} \Delta+b_{0} \Delta\right) \exp \left(-b_{0} \Delta+\bar{c}_{0} \Delta\right) \\
& =\exp \left(-\bar{c}_{0} \Delta\right) \exp \left(a_{0} \Delta+\bar{c}_{0} \Delta+b_{0^{\prime}} \Delta^{2}\right) \\
& =\exp \left(a_{0} \Delta+b_{0^{\prime}} \Delta^{2}+c_{0^{\prime}} \Delta^{2}\right) \\
& =\exp \left(a_{1} \Delta+b_{1} \Delta+c_{1} \Delta\right)
\end{aligned}
$$

We refer to Remark 5, Eq. (45). Given $b_{0} \Delta \in \mathfrak{p}$ such that $b_{0} \Delta \in \mathfrak{f}^{\perp}$. If $A k^{\prime} A^{\prime}=-b_{0} \Delta+\bar{c}_{0} \Delta$, then $\left\|k^{\prime}\right\| \leq h\left\|b_{0} \Delta\right\|$ (killing norm).
$\bar{c}_{0} \in \mathfrak{k}$, is bounded $\bar{c}_{0} \leq M h b_{0}$, where $M$ as before converts between two different norms. Using bounds derived above $b_{0}^{\prime} \leq \tilde{M}(M h+1) b_{0}$, and $c_{0}^{\prime} \leq \tilde{M} M h b_{0}$, $2 \tilde{M}(M h+1) \Delta<1$, we obtain.
which gives $a_{0}+b_{0}^{\prime} \Delta+\bar{c}_{0} \leq a_{0}+b_{0}(\tilde{M}(M h+1) \Delta+M h) \leq 1$. For appropriate $M^{\prime}$, we have

$$
\begin{aligned}
& a_{1} \leq a_{0}+\frac{M^{\prime}}{3}\left(b_{0}+c_{0}\right) \Delta \\
& b_{1} \leq \frac{M^{\prime}}{3}\left(b_{0}+c_{0}\right) \Delta \\
& c_{1} \leq \frac{M^{\prime}}{3}\left(b_{0}+c_{0}\right) \Delta
\end{aligned}
$$

we obtain

$$
a_{1}+b_{1}+c_{1} \leq a_{0}+M^{\prime}\left(b_{0}+c_{0}\right) \Delta \leq a_{0}+b_{0}+c_{0}
$$

where $\Delta$ is chosen small.

$$
\begin{aligned}
U_{1} & =\exp \left(-\left(c_{1}+\bar{c}_{1}\right) \Delta\right) \exp \left(a_{1} \Delta+b_{1} \Delta+c_{1} \Delta\right) \exp \left(-b_{1} \Delta+\bar{c}_{1} \Delta\right) \\
& =\exp \left(-\left(c_{1}+\bar{c}_{1}\right) \Delta\right) \exp \left(a_{1} \Delta+\left(c_{1}+\bar{c}_{1}\right) \Delta+b_{1}^{\prime} \Delta^{2}\right) \\
& =\exp \left(a_{1} \Delta+b_{1}^{\prime} \Delta^{2}+c_{1}^{\prime} \Delta^{2}\right) \\
& =\exp \left(a_{2} \Delta+b_{2} \Delta+c_{2} \Delta\right)
\end{aligned}
$$

where $\bar{c}_{1} \in \mathfrak{k}$, such that $\bar{c}_{1} \leq M h b_{1}$.
where, using bounds derived above $b_{1}^{\prime} \leq \tilde{M}(M h+1) b_{1}$, and $c_{1}^{\prime} \leq \tilde{M}\left(M h b_{1}+c_{1}\right)$, where using the bound $2 \tilde{M}(M h+1) \Delta<1$, we obtain
which gives $a_{1}+b_{1}^{\prime} \Delta+\left(c_{1}+\bar{c}_{1}\right) \leq a_{1}+\left((1+M h) b_{1}+c_{1}\right) \leq a_{0}+b_{0}+c_{0}$.
We can decompose, $\left(b_{1}^{\prime}+c_{1}^{\prime}\right) \Delta^{2}$, into subspaces $\left(a_{1^{\prime}}^{\prime}+b_{2}+c_{2}\right) \Delta$, where $a_{1}^{\prime \prime} \leq M\left(b_{1}^{\prime}+c_{1}^{\prime}\right) \Delta, b_{2} \leq M\left(b_{1}^{\prime}+c_{1}^{\prime}\right) \Delta$ and $c_{2} \leq M\left(b_{1}^{\prime}+c_{1}^{\prime}\right) \Delta$, where $M$ as before converts between two different norms.

This gives

$$
a_{2} \leq a_{1}+4 \tilde{M} M^{2} h\left(b_{1}+c_{1}\right) \Delta b_{2} \leq 4 \tilde{M} M^{2} h\left(b_{1}+c_{1}\right) \Delta c_{2} \leq 4 \tilde{M} M^{2} h\left(b_{1}+c_{1}\right) \Delta
$$

For $x=8 \tilde{M} M^{2} h \Delta<\frac{2}{3}$, we have, $a_{2}+b_{2}+c_{2} \leq a_{1}+\left(b_{1}+c_{1}\right) \leq a_{0}+b_{0}+c_{0}$,
Using $\left(b_{k}+c_{k}\right) \leq x\left(b_{k-1}+c_{k-1}\right) \leq x^{k}\left(b_{0}+c_{0}\right)$.
Similarly,

$$
\left|a_{k}-a_{k-1}\right|_{0} \leq x^{k}\left(b_{0}+c_{0}\right)
$$

Note, $\left(a_{k}, b_{k}, c_{k}\right)$ is a Cauchy sequences which converges to $\left(a_{\infty}, 0,0\right)$, where

$$
\left|a_{\infty}-a_{0}\right|_{0} \leq x\left(b_{0}+c_{0}\right) \sum_{k=0}^{\infty} x^{k} \leq \frac{x\left(b_{0}+c_{0}\right)}{1-x} \leq C \Delta
$$

where $C=16 \tilde{M} M^{2} h\left(b_{0}+c_{0}\right)$.
The above iterative procedure generates $k_{1}^{\prime}$ and $k_{2}^{\prime \prime}$ in Eq. (47), such that

$$
\exp \left(\left(K_{1}^{\prime} A d_{K}\left(X_{d}\right) K_{1}\right) \Delta\right)=\exp \left(-k_{1}^{\prime \prime}\right) \exp \left(a_{0} \Delta+C \Delta^{2}\right) \exp \left(-A k_{2}^{\prime \prime} A^{\prime}\right)
$$

where $a_{0} \Delta+C \Delta^{2} \in \mathfrak{f}$. By using a stabilizer $H_{1}, H_{2}$, we can rotate them to $\mathfrak{a}$ such that

$$
\exp \left(A d_{K}\left(X_{d}\right) \Delta\right) K_{1} A K_{2}=K_{a} H_{1} \exp \left(a_{0}^{\prime} \Delta+C^{\prime} \Delta^{2}\right) A H_{2} K_{b}
$$

such that $H_{1}^{-1}\left(a_{0} \Delta+C \Delta^{2}\right) H_{1}=a_{0}^{\prime} \Delta+C^{\prime} \Delta^{2}$ is in $\mathfrak{a}$ and $a_{0}^{\prime}=P\left(H_{1}^{-1} a_{0} H_{1}\right)$ is projection onto $\mathfrak{a}$ such that

$$
P\left(H_{1}^{-1} a_{0} H_{1}\right)=\sum_{k} \alpha_{k} \mathcal{W}_{k}\left(X_{d}\right)
$$

This follows because the orthogonal part of $A d_{\bar{K}}\left(X_{d}\right)$ to $f$ written as $A d_{\bar{K}}\left(X_{d}\right)^{\perp}$ remains orthogonal of $\mathfrak{f}$

$$
\left\langle H^{-1} A d_{K}\left(X_{d}\right)^{\perp} H, \mathfrak{a}\right\rangle=\left\langle A d_{K}\left(X_{d}\right)^{\perp}, H \mathfrak{a} H^{-1}\right\rangle=\left\langle A d_{K}\left(X_{d}\right)^{\perp}, \mathfrak{a}^{\prime \prime}\right\rangle=0
$$

( $a^{\prime \prime} \in \mathfrak{f}$ ), remains orthogonal to $\mathfrak{a}$. Therefore
$P\left(H_{1}^{-1} a_{0} H_{1}\right)=P\left(H_{1}^{-1} A d_{\bar{K}}\left(X_{d}\right) H_{1}\right)=\sum_{k} \alpha_{k} \mathcal{W}_{k}\left(X_{d}\right)$.

$$
\exp \left(A d_{K}\left(X_{d}\right) \Delta\right) K_{1} A K_{2}=K_{a} \exp \left(a+a_{0} \Delta+C^{\prime} \Delta^{2}\right) K_{b}
$$

Lemma 1 Given $P=K_{1} \underbrace{\exp \left(a+a_{1} \Delta\right)}_{A_{1}} K_{2}=K_{3} \underbrace{\exp \left(b-b_{1} \Delta\right)}_{A_{2}} K_{4}$, where $a, b, a_{1}, b_{1} \in \mathfrak{a}$. We can express

$$
\exp (b)=K_{a} \exp \left(a+a_{1} \Delta+\mathcal{W}\left(b_{1}\right) \Delta\right) K_{b}
$$

where $\mathcal{W}\left(b_{1}\right)$ is Weyl element of $b_{1}$. Furthermore

$$
\exp \left(b+b_{2} \Delta\right)=K_{a^{\prime}} \exp \left(a+a_{1} \Delta+\mathcal{W}\left(b_{1}\right) \Delta+\mathcal{W}\left(b_{2}\right) \Delta\right) K_{b^{\prime}}
$$

Proof. Note, $A_{2}=K_{3}^{-1} P K_{4}^{-1}$, commutes with $b_{1}$. This implies
$A_{2}=\tilde{K} \exp \left(a+a_{1} \Delta\right) K$ commutes with $b_{1}$. This implies $A_{2} b_{1} A_{2}^{-1}=b_{1}$, i.e., $\tilde{K} \exp \left(a+a_{1} \Delta\right) A d_{K}\left(b_{1}\right) \exp \left(-\left(a+a_{1} \Delta\right)\right) \tilde{K}^{\prime}=b_{1}$, which implies that $A d_{K}\left(b_{1}\right) \in \mathfrak{f}$. Recall, from Remark 5,

$$
\exp \left(a+a_{1} \Delta\right) A d_{K}\left(b_{1}\right) \exp \left(-\left(a+a_{1} \Delta\right)\right)=\sum_{k} c_{k}\left(Y_{k} \cos \left(\lambda_{k}\right)+X_{k} \sin \left(\lambda_{k}\right)\right)
$$

This implies $\sum_{k} c_{k} \sin \left(\lambda_{k}\right) X_{k}=0$, implying $\lambda_{k}=n \pi$. Therefore,

$$
\exp \left(2\left(a+a_{1} \Delta\right)\right) A d_{K}\left(b_{1}\right) \exp \left(-2\left(a+a_{1} \Delta\right)\right)=A d_{K}\left(b_{1}\right)
$$

We have shown existence of $H_{1}$ such that $H_{1} A d_{K}\left(b_{1}\right) H_{1}^{-1} \in \mathfrak{a}$, using $H_{1}, H_{2}$ as before,

$$
\begin{array}{r}
\tilde{K} \exp \left(a+a_{1} \Delta\right) K \exp \left(b_{1} \Delta\right)=\tilde{K} H_{2} \exp \left(a+a_{1} \Delta\right) H_{1} \exp \left(A d_{K}\left(b_{1}\right) \Delta\right) K \\
=K_{a} \exp \left(a+a_{1} \Delta+\mathcal{W}\left(b_{1}\right) \Delta\right) K_{b} .
\end{array}
$$

Applying the theorem again to
$K_{a} \exp \left(a+a_{1} \Delta+\mathcal{W}\left(b_{1}\right) \Delta\right) K_{b} \exp \left(b_{2} \Delta\right)=K_{a^{\prime \prime}} \exp \left(a+a_{1} \Delta+\mathcal{W}\left(b_{1}\right) \Delta+\mathcal{W}\left(b_{2}\right) \Delta\right) K_{b^{\prime \prime}}$.
Lemma 2 Given $P_{i}=K_{1}^{i} A^{i} K_{2}^{i}=K_{1}^{i} \exp \left(a^{i}\right) K_{2}^{i}$, we have $P_{i, i+1}=\exp \left(H_{i}^{+} \Delta_{i}^{+}\right) P_{i}$, and $P_{i, i+1}=\exp \left(-H_{i+1}^{-} \Delta_{i+1}^{-}\right) P_{i+1}$, where $H_{i}^{+}=A d_{K_{i}}\left(X_{d}\right)$. From above we can express

$$
P_{i, i+1}=K_{a}^{i+} \exp \left(a^{i}+a_{1}^{i+} \Delta_{+}^{i}+a_{2}^{i+}\left(\Delta_{+}^{i}\right)^{2}\right) K_{b}^{i+} .
$$

where $a_{1}^{i+}$ and $a_{2}^{i+}$ are first and second order increments to $a_{i}$ in the positive direction. The remaining notation is self-explanatory.

$$
\begin{gathered}
P_{i, i+1}=K_{a}^{(i+1)-} \exp \left(a^{i+1}-a_{1}^{(i+1)-} \Delta_{-}^{i+1}-a_{2}^{(i+1)-}\left(\Delta_{-}^{i+1}\right)^{2}\right) K_{b}^{(i+1)-} . \\
\exp \left(a^{i+1}\right)=K_{1} \exp \left(a^{i}+a_{1}^{i+} \Delta_{+}^{i}+a_{2}^{i+}\left(\Delta_{+}^{i}\right)^{2}+\mathcal{W}\left(a_{1}^{(i+1)-} \Delta_{-}^{i+1}+a_{2}^{(i+1)-}\left(\Delta_{-}^{i+1}\right)^{2}\right)\right) K_{2} \\
\mathcal{W}\left(a_{1}^{(i+1)-} \Delta_{-}^{i+1}+a_{2}^{(i+1)-}\left(\Delta_{-}^{i+1}\right)^{2}\right)=\mathcal{P}\left(\mathcal{W}\left(a_{1}^{(i+1)-}\right)\right) \Delta_{-}^{i+1}+\mathcal{P}\left(\mathcal{W}\left(a_{2}^{(i+1)-}\right)\right)\left(\Delta_{-}^{i+1}\right)^{2} \\
=\sum_{k} \alpha_{k} \mathcal{W}_{k}\left(X_{d}\right) \Delta_{-}^{i+1}+o\left(\left(\Delta_{-}^{i+1}\right)^{2}\right)
\end{gathered}
$$

where, $a^{i}, a_{1}^{i}, a_{2}^{i} \in \mathfrak{a}$.
Using Lemma 1 and 2, we can express

$$
P_{n}(T)=K_{1} \exp \left(a_{n}\right) \exp K_{2}=K_{1} \exp \left(\sum_{i} \mathcal{W}\left(a_{i}^{+}\right) \Delta_{i}^{+}+\mathcal{W}\left(a_{i+1}^{-}\right) \Delta_{i+1}^{-}\right) \exp (\underbrace{\sum o\left(\Delta^{2}\right)}_{\leq \varepsilon T}) K_{2}
$$

Letting $\varepsilon$ go to 0 , we have

$$
P_{n}(T)=K_{1} \exp \left(T \sum_{i} \alpha_{i} \mathcal{W}_{i}\left(X_{d}\right)\right) K_{2} .
$$

Hence the proof of theorem. q.e.d.

## 4. Conclusion

In this chapter, we studied some control problems that derive from time optimal control of coupled spin dynamics in NMR spectroscopy and quantum information and computation. We saw how dynamics was decomposed into fast generators $\mathfrak{k}$ (local Hamiltonians) and slow generators $\mathfrak{p}$ (couplings) as a Cartan decomposition $\mathfrak{g}=\mathfrak{p} \oplus \mathfrak{k}$. Using this decomposition, we used some convexity ideas to completely characterize the reachable set and time optimal control for these problems.


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