Sub-Riemannian geodesics in $SU(n)/S(U(n-1) \times U(1))$ and optimal control of three level quantum systems

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***Abstract*—We study the time optimal control problem for the evolution operator of an n-level quantum system. For the considered models, the control couples all the energy levels to a given one and is assumed to be bounded in Euclidean norm. The resulting problem is a sub-Riemannian $K-P$ problem, as introduced in [6], [18], whose underlying symmetric space is $SU(n)/S(U(n-1) \times U(1))$. Following the method of [4], we consider the action of $S(U(n-1) \times U(1))$ on $SU(n)$ as a conjugation $X \to KXK^{-1}$. This allows us to do a symmetry reduction and consider the problem on a quotient space. We give an explicit description of such a quotient space which has the structure of a stratified space. We prove several properties of sub-Riemannian problems with the given structure. We derive the explicit optimal control for the case of three level quantum systems where the desired operation is on the lowest two energy levels (Λ-systems). We reduce the latter problem to an integer quadratic optimization problem with linear constraints, which we solve completely for a specific set of final data.**

***Index Terms*—Geometric Optimal Control Theory, Symmetry Reduction, Sub-Riemannian Geometry, $K-P$ Problems, Optimal Control of Quantum Systems.**

I. Introduction

A. *Mathematical Model*

Many finite dimensional quantum systems of interest in applications can be modeled by the *Schrödinger operator equation* [12],

$$\dot{X} = \hat{A}X + \sum_{j=1}^{m} B_j X u_j, \qquad X(0) = \mathbf{1}, \tag{1}$$

where the controls u_j are *electromagnetic semi-classical fields* which can be decided by an experimenter. The unitary matrix X is the *evolution operator* (or *propagator*) of the quantum mechanical system and $\hat{A}$ and B_j are matrices in the Lie algebra $\mathfrak{su}(n)$, where n is the number of energy levels of the system. Typically, one works in the basis of the eigenvectors of the '*internal Hamiltonian*' $\hat{A}$, so that $\hat{A}$ is diagonal, while the B_j's model couplings between different levels, activated by the external fields u_j. Such couplings are described by the *energy level diagram* of the system (see, e.g., [23]). In (1), the matrix $\mathbf{1}$ represents the identity. For the class of systems we shall consider, the energy level diagram couples one of the energy levels to all the remaining ones. In a basis in which $\hat{A}$ in (1) is diagonal, the B_j's matrices are all zeros except in the $(1,l)$-th entry for $l = 2, 3, \ldots, n$ (and corresponding $(l,1)$-th entry) which are given by $\frac{1}{\sqrt{2}}$ (and $-\frac{1}{\sqrt{2}}$) or $\frac{i}{\sqrt{2}}$ (and $\frac{i}{\sqrt{2}}$). In particular we have $m = 2(n-1)$ in (1). With this choice, the B_j's are orthonormal with respect to the inner product on $\mathfrak{su}(n)$, $\langle C, D\rangle := Tr(CD^\dagger)$, and they are orthogonal to the diagonal matrix $\hat{A}$. Normalization of the B_j's can be obtained by re-scaling the controls in the problem. An example of this class of models, which will be treated in detail, is the class of the so-called Λ-*systems* [13] [14], [15], [16] , where the highest energy level is coupled to the lowest two levels (cf. Figure 1) but the lowest two energy levels are not coupled with each other directly. By going to the *interaction picture*

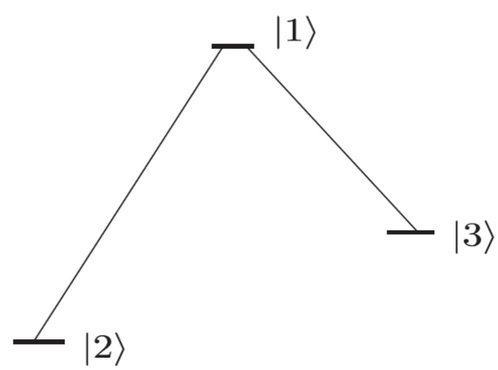

Fig. 1. Energy level diagram for a Λ-system

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[23], i.e., defining the new propagator $U := e^{-\hat{A}t}X$, we can effectively eliminate the drift in equation (1). The equation for U is

$$\dot{U} = \sum_{j=1}^{m} e^{-\hat{A}t} B_j e^{\hat{A}t} u_j U, \qquad U(0) = \mathbf{1}. \tag{2}$$

If we assume the above structure for $\hat{A}$ and B_j in (1), for each j, $e^{-\hat{A}t} B_j e^{\hat{A}t} = \sum_{k=1}^{m} a_{j,k}(t) B_k$, and replacing this into (2) and defining the new controls $v_k := \sum_{j=1}^{m} a_{j,k} u_j$ the equation becomes the *driftless* equation

$$\dot{U} = \sum_{k=1}^{m} B_k v_k U, \qquad U(0) = \mathbf{1}. \tag{3}$$

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Furthermore, this does not change the norm of the control since $\|v\| = \|u\|$.

B. Minimum Time Problem

Our main concern in this paper will be the minimum time problem for system (3). In particular, given a final condition $U_f \in SU(n)$ we wish to find the optimal control steering the state U of (3) from the identity to U_f in minimum time with the constraint that the control is bounded at any time as

$$\sum_{j=1}^{m} v_j^2 \leq \Gamma^2. \tag{4}$$

Consideration of minimum time control is natural in quantum mechanics applications to computation, in that, one would like to perform computational tasks as quickly as possible. Additionally, fast evolution is a way to counteract the negative effect of the environment (de-coherence) [10], so as to fully exploit quantum behavior.

The problem for system (3) is related to the corresponding problem for the system with a nonzero drift (1) (with $\|u\| = \|v\| \leq \Gamma$). If the task is to obtain an operation which achieves the transfer between two eigenvectors of the matrix $\hat{A}$, the minimum time obtained for the system (3) will be the same as the minimum for the system (1). This is because, if ψ_U is the state for the system (3), ($\psi_U(t) = U(t)\psi_U(0)$) the state for system (1) is $\psi(t) = X(t)\psi(0) = e^{\hat{A}t}\psi_U(t)$. This differs from $\psi_U(t)$ only by a phase factor and therefore it is still an eigenvector of $\hat{A}$. Moreover the knowledge of the optimal control for system (3) for any final condition (the *complete optimal synthesis*) gives the same information for (1). This follows from the equivalence between the knowledge of the complete optimal synthesis and knowledge of the reachable sets and from the fact that $\mathcal{R}(t) = e^{\hat{A}t}\mathcal{R}_U(t)$, where $\mathcal{R}(t)$ ($\mathcal{R}_U(t)$) is the reachable set at time t for system (1) ((3)).

The minimum time problem for system (3) with bounded norm on the control (4) is equivalent to the problem, for fixed T, to minimize the 'energy' $\int_0^T \|v(t)\|^2 dt$. The problem is also equivalent to finding the *sub-Riemannian geodesics* on $SU(n)$ where the sub-Riemannian structure is specified by the vector fields $\{B_j\}$. Sub-Riemannian geodesics are the curves minimizing length among the curves tangent to the given set of vector fields which are called *horizontal* (see, e.g., [1], [2], [4]). The optimal control with the bound (4) is the same as the one with bound

$$\|v\|^2 \leq 2 \tag{5}$$

multiplied by $\frac{\Gamma}{\sqrt{2}}$ with time scaled by $\frac{\Gamma}{\sqrt{2}}$. Therefore we shall assume w.l.g. the bound (5). Furthermore the optimal control is such that equality always holds in (4) (cf., e.g., [4]).

C. $K - P$ Systems

In the paper [18], V. Jurdjević introduced a class of problems which includes the problem on $SU(n)$ above described. Consider a semisimple Lie algebra $\mathcal{L}$ which has a (Cartan) decomposition $\mathcal{L} = \mathcal{K} \oplus \mathcal{P}$, satisfying

$$[\mathcal{K}, \mathcal{K}] \subseteq \mathcal{K}, \qquad [\mathcal{K}, \mathcal{P}] \subseteq \mathcal{P}, \qquad [\mathcal{P}, \mathcal{P}] \subseteq \mathcal{K}. \tag{6}$$

Then the minimum time problem, for the system (3), where the B_j's form an orthonormal basis in $\mathcal{P}$, and with a bound (4) is called a $K - P$ *problem* [6]. The problem for quantum systems considered in this paper is a $K - P$ problem with the Lie algebra $\mathcal{L}$ given by $\mathfrak{su}(n)$, the subalgebra $\mathcal{K}$ given by block diagonal matrices in $\mathfrak{su}(n)$ with blocks of dimension 1 and $n-1$, and the complementary subspace $\mathcal{P}$ spanned by anti-diagonal matrices with the corresponding dimensions of the blocks. Several other possibilities may occur [17]. In [18] V. Jurdjević also gave the form of the optimal control and trajectories for $K - P$ problems. By applying the Pontryagin Maximum Principle in the version for systems on Lie groups (see, e.g, [22]), he proved that there exist a matrix $P \in \mathcal{P}$ and a matrix $A \in \mathcal{K}$ such that the optimal control v in (3) satisfies

$$\sum_{k=1}^{m} B_k v_k(t) = e^{At} P e^{-At}. \tag{7}$$

From this one obtains the components v_k of the optimal control. Moreover by solving (3) with (7), the corresponding optimal trajectory is

$$U(t) = e^{At} e^{(-A+P)t}. \tag{8}$$

The problem of finding the optimal control to reach a final state U_f becomes therefore the problem of finding matrices $A \in \mathcal{K}$ and $P \in \mathcal{P}$ and real $t > 0$ such that $U_f = e^{At}e^{(-A+P)t}$ and t is the minimum positive value such that this is possible. In the $SU(n)$ case, this involves the search for $n^2 - 1$ parameters: the $n^2 - 1$ parameters in the matrices A and P, plus the parameter t, minus the normalization of P due to the fact that $\|P\| = \|v\| = \sqrt{2}$ is fixed in (5).

D. Objective and Structure of the Paper

This paper is a contribution to the theory of optimal control and sub-Riemannian geometry for systems on Lie groups. It gives tools and results to obtain the *complete optimal synthesis* for the systems (3) with bound (4). Our guiding principle is to find optimal controls to reach points in the *cut locus*, i.e., points where the optimal geodesics cease to be optimal. If one finds the optimal trajectories for all points in the cut locus, then the task to find the optimal synthesis is accomplished.

As will be detailed in the following section, $K - P$ systems admit a *group of symmetries*, i.e., a Lie group acting on the state space ($SU(n)$ in the above models), which maps optimal geodesics to optimal geodesics. This suggests that the optimal synthesis can be performed on the corresponding space of orbits of such an action, the *orbit space*. In particular, the cut locus and the reachable sets are pre-images, under the natural projection, of sets in the orbit space [4]. According to the general theory of Lie transformation groups [9], the orbit space has the structure of a *stratified space* and can be separated into an open and dense part called the *regular part* and the remaining part called the *singular part*, according to the 'size' of the isotropy group of the corresponding elements. Their pre-images under natural projection in the manifold ($SU(n)$) are also called the regular and singular part, respectively. A convexity result proved in [4] [5] says that minimizing geodesics crossing the regular part and reaching the singular part lose optimality when reaching the singular part. This suggests that points on the singular part of the manifold are good candidates as elements of the cut locus. A description of the orbit space associated with a $K-P$ problem is an important step in the determination of the optimal synthesis because 1) it describes the (lower dimensional) space where the optimal synthesis is projected so as one can recover features of the optimal synthesis on the original manifold (e.g., reachable sets) 2) it gives information on points potentially in the cut locus to be considered as final conditions. For these reasons, in Theorem 1 of section III, we give a description of the orbit space in full generality for the problem on $SU(n)$ above described.

For the rest of the paper, we shall focus on the optimal control problem on $SU(3)$ with the final condition of the form

$$X_f = \begin{pmatrix} * & 0 \\ 0 & \tilde{X}_f, \end{pmatrix} \tag{9}$$

with $\tilde{X}_f \in U(2)$. These final conditions are important because, applying Theorem 1, they can be seen to belong to the singular part of $SU(n)$, and, in fact they belong to the cut locus; the corresponding geodesics are *maximal geodesics*. From an applied point of view, it is a common scenario for $3-$level, Λ-type configurations, to manipulate states in the subspace belonging to the lowest two energy levels as in (9) [13], [14], [15]. This has led to adiabatic control algorithms such as STIRAP (see, e.g., [24]). We shall, in fact, provide a *complete solution* for a subclass of final conditions (9) but with techniques that can be extended to the general case (9).

Our results are related to the ones of [6], [8], which also deal with the optimal control of three level quantum systems. We work here at the level of the evolution operator in $SU(3)$ while [6], [8] solves minimum time/energy problem for a transfer between energy eigen-states. However in their setting, the authors of [6], [8] use a fundamental result of [7] which says that minimizers exist in resonance with the energy differences between the corresponding eigenstates. This allows them to simplify the problem to a problem on $SO(3)$ and consider more general settings, such as independent bounds on the controls and different weights on the controls (anisotropy). We shall use a different approach as compared to these papers, and, in the process, we shall prove several properties for the optimal control for system (3) on $SU(n)$, for general n.

In section II we describe the symmetry properties of the given optimal control problem and in section III we describe the associated orbit space $SU(n)/S(U(n-1)\times U(1))$. Starting from section IV we focus on the case of a *three* level quantum Λ-system and on final conditions (9). We reduce the problem of optimal control to a quadratic integer optimization problem with constraints. We solve such a problem in section V. In section VI we discuss the method in general and give an example. Concluding remarks are given in section VII.

II. Symmetry reduction for the K-P problem $SU(n)/S(U(n-1)\times U(1))$

Consider a general $K-P$ problem (cf. (3) and (6)). This optimal control problem has a solution because the set of possible values for the controls is compact and system (3) is controllable: under the assumption that the Lie algebra $\mathcal{L}$ is semisimple, it can be shown (cf., Theorem 2 in Appendix A of [6]) that equality holds in the last commutation relation in (6). Therefore the matrices B_j (which span $\mathcal{P}$) generate all of $\mathcal{L}$ and therefore the Lie algebra rank condition [19] is verified which implies controllability if the Lie group $e^{\mathcal{L}}$ is compact.[1] This is our case since $e^{\mathcal{L}} = SU(n)$. Consider the action of the Lie group associated with $\mathcal{K}$, $e^{\mathcal{K}}$, on $e^{\mathcal{L}}$, by *conjugation*, i.e., if $x \in e^{\mathcal{L}}$ and $k \in e^{\mathcal{K}}$, the action is $x \to kxk^{-1}$. For our case, $e^{\mathcal{L}} = SU(n)$ and $e^{\mathcal{K}} = S(U(n-1)\times U(1))$ is the Lie group of block diagonal matrices with blocks of dimension 1 and $n-1$ and determinant equal to 1. An element $K \in S(U(n-1)\times U(1))$ acts on an element X in $SU(n)$ by $X \to KXK^{-1} = KXK^{\dagger}$. The main observation is that, if $U_d(t)$ is a minimum time trajectory for (3) with final condition U_f, then $KU_d(t)K^{-1}$ is a minimum time trajectory (with the same time) with final condition KU_fK^{-1}. This suggests to study the time optimal control problem in the quotient space $e^{\mathcal{L}}/e^{\mathcal{K}} = SU(n)/S(U(n-1)\times U(1))$, the space of the orbits under this action. Let us denote by π the natural projection $\pi : e^{\mathcal{L}} \to e^{\mathcal{L}}/e^{\mathcal{K}}$. With the conjugation action, all geodesics on $SU(n)$, from the identity $\mathbf{1}$ to a point U_f are projected to geodesics on $SU(n)/S(U(n-1)\times U(1))$. Here, we define the distance between $\pi(\mathbf{1})$ and q in $SU(n)/S(U(n-1)\times U(1))$ as the infimum among the lengths of the horizontal curves in $SU(n)$ from $\mathbf{1}$ to the fiber $\pi^{-1}(q)$, and call geodesics the curves which realize such a distance (cf. [5]). If γ is a sub-Riemannian minimizing geodesic from the identity to U_f, then $\pi(\gamma)$ is a geodesic from $\mathbf{1}$ to $\pi(U_f)$, since the length does not depend on the element in $\pi^{-1}(\pi(U_f))$.

To simplify the notation, we shall sometimes denote by $SU(n)/_{\sim} := SU(n)/S(U(n-1)\times U(1))$ the orbit space . A matrix in $S(U(n-1)\times U(1))$ will always be considered with a 1×1 block in the upper left corner and an $(n-1)\times(n-1)$ block in the lower right corner.

For general $K-P$ problems, the action of $e^{\mathcal{K}}$ on $e^{\mathcal{L}}$ by conjugation lifts to an action (which is also conjugation) of $e^{\mathcal{K}}$ on the Lie algebra $\mathcal{L}$. The subspace $\mathcal{P} \subseteq \mathcal{L}$ is invariant under conjugation by $e^{\mathcal{K}}$ because of the second formula in (6). This symmetry reduction allows for a reduction of the number of parameters to be determined to find the optimal control law, i.e., the parameters in the matrices A and P in (7) (8). This is because we only need to consider a single representative in the equivalence class of any geodesic. By multiplying (8) on the left and right by $K \in e^{\mathcal{K}}$ and K^{-1} respectively, we see that the matrices A and P can be chosen up to a common conjugation by an element $K \in e^{\mathcal{K}}$. Therefore there is no loss of generality to consider A and P of a special form (see Proposition II.1 below). In particular, by fixing a maximal Abelian subalgebra $\mathcal{A}$ in $\mathcal{P}$ (a Cartan subalgebra), we can assume that P is an element of $\mathcal{A}$. This is because $\mathcal{P}$ may be written as $\mathcal{P} = \cup_{K\in e^{\mathcal{K}}} K\mathcal{A}K^{-1}$ (cf. Proposition 7.29 in [20]). In the case of $SU(n)$ with $\mathcal{P}$ the orthogonal complement of $\mathcal{K} = \{$block diagonal matrices with first block $1\times$

[1]We follow the convention of denoting by $e^{\mathcal{L}}$ the connected (component containing the identity of the) Lie group associated with the Lie algebra $\mathcal{L}$.

1 other block $(n-1)\times(n-1)\}$, we have that any Cartan subalgebra $\mathcal{A}$ is one dimensional. Therefore, it suffices to fix one non-zero matrix $P \in \mathcal{P}$ with $\|P\|^2 = 2$ because of (7) and (5). We will then take P to be the matrix with $(1,2)$ entry equal to i (and hence $(2,1)$ entry also equal to i) and all other entries equal to zero. We can also assume a special, tridiagonal, form for $A \in \mathcal{K}$ in (7), (8) as described in the following Proposition.

Proposition II.1. Let $A \in \mathcal{K}$ and $P \in \mathcal{P}$ with P having $(1,2)$ and $(2,1)$ entries equal to i and all others zero. Then $-A+P$ may be tridiagonalized by a special unitary matrix in $e^{\mathcal{K}} = S(U(n-1)\times U(1))$ with a 2×2 identity matrix in the upper left corner. Furthermore, the off-diagonal entries of the tridiagonalized form, starting from row 2 may also be taken purely imaginary and are nonzero if A has a nonzero nondiagonal entry in the corresponding row.

Proof. The proof proceeds by induction on the size n First, note that for 2×2 matrices, the result holds as the matrix $-A+P$ is already tridiagonal. Now, suppose that $n \geq 3$. Let $-A+P = (b_{ij})_{1\leq i,j\leq n}$ and let $\hat{v} = 0$ if $b_{32} = \ldots = b_{n2} = 0$ and $\hat{v} = i(\sum_{k=3}^{n} |b_{k2}|^2)^{-1}$ otherwise. Let $S = (s_{ij})_{1\leq i,j\leq n-2} \in SU(n-2)$ such that $s_{1j} = \frac{\bar{b}_{j+2,2}}{\hat{v}^*}$ if $\hat{v} \neq 0$ and $S \in SU(n-2)$ arbitrary otherwise. Then $S^\dagger V = B$ where V is the vector with first entry equal to $\hat{v}$ and all other entries zero and B the vector with entries $(b_{j2})_{3\leq j\leq n}$. Therefore, the following equation holds:

$$\begin{pmatrix} I_2 & 0 \\ 0 & S \end{pmatrix} \begin{pmatrix} b_{11} & b_{12} & 0 & \cdots & 0 \\ b_{21} & b_{22} & & \cdots & b_{2n} \\ 0 & \vdots & & & \vdots \\ \vdots & & & & \\ 0 & b_{n2} & & \cdots & b_{nn} \end{pmatrix} \begin{pmatrix} I_2 & 0 \\ 0 & S^\dagger \end{pmatrix} =$$

$$= \begin{pmatrix} b_{11} & b_{12} & 0 & \cdots & & 0 \\ b_{21} & b_{22} & -\hat{v}^* & 0 & \cdots & 0 \\ 0 & \hat{v} & * & \cdots & * & * \\ 0 & 0 & * & \cdots & * & * \\ \vdots & \vdots & \vdots & & & \vdots \\ 0 & 0 & * & \cdots & & * \\ 0 & 0 & * & \cdots & & * \end{pmatrix}$$

Considering now the submatrix

$$\begin{pmatrix} b_{22} & -\hat{v}^* & 0 & \cdots & 0 \\ \hat{v} & * & * & \cdots & * \\ 0 & * & * & \cdots & * \\ \vdots & \vdots & & & \vdots \\ 0 & * & \cdots & & * \\ 0 & * & \cdots & & * \end{pmatrix}$$

and recursively using the result with n replaced by $n-1$ proves the claim. The last claim of the proposition follows from the choice of $\hat{v}$ at each step. □

From the nature of $\hat{v}$ as a purely imaginary number in the above proof we have the following.

Corollary II.2. There is no loss of generality in assuming that $-A+P$ is a purely imaginary tridiagonal matrix in $\mathfrak{su}(n)$ and therefore so are $A \in \mathcal{K}$ and $P \in \mathcal{P}$.

This in particular means that we can always write $-A+P$ as i multiplied by a real symmetric tridiagonal matrix.

In sections IV and V, we shall focus on problems for final conditions in $e^{\mathcal{K}} = S(U(n-1)\times U(1))$, corresponding to operations on the lowest $n-1$ levels of the given quantum systems. In this case, in order for $e^{At}e^{(-A+P)t}$ in (8) to lie in $e^{\mathcal{K}}$, we must have $e^{(-A+P)t} \in e^{\mathcal{K}}$.

Proposition II.3. Consider the $K-P$ decomposition of $SU(n)$ as above. Suppose $A \in \mathcal{K}$ and $P \in \mathcal{P}$ such that $-A+P$ is a tridiagonal matrix with no elements of the sub-(or super-)diagonal equal to zero, and suppose $e^{(-A+P)t} \in e^{\mathcal{K}}$. Then $e^{(-A+P)t}$ is a scalar matrix.

Proof. By induction on n, first, observe that the result holds for $n=2$ by computing the matrix exponential:

$$\exp\begin{pmatrix} ait & (c+di)t \\ (-c+di)t & bit \end{pmatrix} = \frac{e^{it(a+b)/2}}{\omega}$$

$$\begin{pmatrix} \omega\cos(t\omega/2) + (a-b)i\sin(t\omega/2) & 2(c+id)\sin(t\omega/2) \\ 2(-c+id)\sin(t\omega/2) & \omega\cos(t\omega/2) - (a-b)i\sin(t\omega/2) \end{pmatrix}$$

where $\omega = \sqrt{(a-b)^2+c^2+d^2}$ and $c+di \neq 0$. If this exponential has off-diagonal entries equal to zero, then $t\omega/2 = k\pi$ for some $k \in \mathbb{Z}$, so the only possibility for the exponential is a matrix with $\pm e^{it(a+b)/2}$ on the diagonal (with the same sign) and zeros elsewhere. Now, consider $n > 2$. Let $U = e^{(-A+P)t}$. Then $-A+P$ commutes with U. Observe that $e^{\mathcal{K}}$ acting on $\mathfrak{su}(n)$ by conjugation fixes both $\mathcal{K}$ and $\mathcal{P}$ (from (6)). It also therefore fixes the natural extensions of these subspaces to subspaces of $\mathfrak{u}(n)$. Since $[U,-A+P]=0$ we have $[U,A]=[U,P]$, which is equivalent to $UAU^\dagger - A = UPU^\dagger - P$. Since the left hand side of this equality is in $\mathcal{K}$ and the right hand side is in $\mathcal{P}$, both sides are zero and $[U,A]=[U,P]=0$. Using the special form of P, $[U,P]=0$ implies $(U)_{2,2} = (U)_{1,1}$ and $(U)_{2,k} = 0$ for $k > 2$. So U is not only in $e^{\mathcal{K}}$ but it has a block diagonal form with a 2×2 (upper left) block a scalar matrix. Decompose:

$$A = A_n = \begin{pmatrix} a_{11} & 0\cdots 0 \\ 0 & \\ \vdots & \hat{A}_{n-1} \\ 0 & \end{pmatrix},$$

where $\hat{A}_{n-1} = A_{n-1} + P_{n-1}$ with

$$A_{n-1} = \begin{pmatrix} a_{22} & 0\cdots 0 \\ 0 & \\ \vdots & \hat{A}_{n-2} \\ 0 & \end{pmatrix}, P_{n-1} = \begin{pmatrix} 0 & a_{23} & 0\cdots 0 \\ -\bar{a}_{23} & & \\ 0 & & \\ \vdots & & \mathbf{0} \\ 0 & & \end{pmatrix}$$

Since U commutes with A, the lower $(n-1)\times(n-1)$ block of U, U_{n-1}, commutes with $\hat{A}_{n-1} = A_{n-1} + P_{n-1}$. Proceeding as above, by replacing U with U_{n-1} and using the fact that a_{23} is different from zero we find that $(U)_{3,3} = (U)_{2,2}$ and $(U)_{3,k} = 0$ for $k > 3$. Proceeding inductively we find that U is a scalar matrix. □

III. The orbit space $SU(n)/S(U(n-1)\times U(1))$

The Lie group $S(U(n-1)\times U(1))$ can be parametrized as:

$$\begin{pmatrix} e^{i\eta} & 0 \\ 0 & \xi V \end{pmatrix}, \tag{10}$$

$V \in SU(n-1)$, $\eta \in [0, 2\pi)$, $\xi \in \mathbb{C}$ with $\xi^{n-1} = e^{-i\eta}$.

To describe the orbit space $SU(n)/_\sim$ we also need to consider the following equivalence relation in $SU(n)$:

$$X_1 \sim_\phi X_2 \quad \Leftrightarrow \quad \exists\, U \in SU(n) \text{ such that} \tag{11}$$

$$U \begin{pmatrix} e^{i\phi} & 0 \\ 0 & I \end{pmatrix} X_1 U^\dagger = \begin{pmatrix} e^{i\phi} & 0 \\ 0 & I \end{pmatrix} X_2,$$

where I denotes the $(n-1)\times(n-1)$ identity. Equivalently for a fixed ϕ, X_1 and X_2 are $\sim_\phi$ equivalent if and only if $\begin{pmatrix} e^{i\phi} & 0 \\ 0 & I \end{pmatrix} X_1$ and $\begin{pmatrix} e^{i\phi} & 0 \\ 0 & I \end{pmatrix} X_2$ have the same spectrum. We define a topological fiber bundle on the circle S^1 as $\hat{\pi} : E_n \to S^1$ with fibers $\hat{\pi}^{-1}(e^{i\phi}) = SU(n-1)/_{\sim_\phi}$. The fibers $\hat{\pi}^{-1}(e^{i\phi}) = SU(n-1)/_{\sim_\phi}$ may not be manifolds, but are topological spaces with the coarsest topology that makes $\hat{\pi}$ a continuous map. An example is in Proposition IV.1 below.

Let D_1 be the open unit disc in $\mathbb{C}$, i.e., if $x \in D_1$ then x is a complex number with absolute value strictly less than 1. The next theorem recursively describes the orbit space $SU(n)/_\sim$.

Theorem 1. *Let Ψ be the map from $E_n \cup (D_1 \times SU(n-1)/_\sim)$ to $SU(n)/_\sim$, defined by:*

- *if $[Z]_{\sim_\phi} \in E_n$ then*

$$\Psi\left([Z]_{\sim_\phi}\right) := \left[\begin{pmatrix} e^{-i\phi} & 0 & 0 & \cdots & 0 \\ 0 & e^{i\phi} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix} \begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & Z \\ 0 & \end{pmatrix}\right]_\sim \tag{12}$$

- *if $(x, [Z]_\sim) \in D_1 \times SU(n-1)/_\sim$ then*

$$\Psi\left(x, [Z]_\sim\right) := \tag{13}$$

$$= \left[\begin{pmatrix} x & \sqrt{1-|x|^2} & 0 & \cdots & 0 \\ -\sqrt{1-|x|^2} & x^* & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix} \begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & Z \\ 0 & \end{pmatrix}\right]_\sim$$

Moreover the map Ψ is a global homeomorphism.

In the statement of the theorem, we are gluing the fiber $\hat{\pi}^{-1}(e^{i\varphi})$ in E_n to the point $e^{i\varphi}$ in the boundary of D_1.

If we identify $SU(1)/_\sim$ and $SU(1)/_{\sim_\phi}$ with a single point so that $E_2 \equiv S^1 = \partial D_1$, we have that (with $\simeq$ denoting homeomorphism) $SU(2)/_\sim \simeq \partial D_1 \cup D_1 = \bar{D}_1$ is homeomorphic to the *closed* unit disc, a special case known from the treatment of two-level quantum systems [3]. Applying Theorem 1 recursively, we obtain.

Corollary III.1. With E_1 equal by definition to a single point, we have, for $n \geq 2$

$$SU(n)/_\sim \simeq \bigcup_{j=0}^{n-1} D_1^{\times j} \times E_{n-j}. \tag{14}$$

The number of parameters characterizing the orbit depends on the subset in the right hand side of (14) where the orbit is. If, up to homeomorphism, $[X]_\sim \in D_1^{\times j} \times E_{n-j}$, for some $j \in \{0, ..., n-1\}$, the parameters are $n+j-1 = (n-j-1)+2j$, with $n-j-1$ for E_{n-j} and $2j$ for $D_1^{\times j}$.

A. Proof of Theorem 1

Proof. We need to prove that Ψ is i) well-defined, ii) onto, iii) one-to-one, and iv) continuous with continuous inverse. Here we only prove that Ψ is onto, since this shows how to find Ψ and therefore how to parametrize the elements in $SU(n)/\sim$. We postpone to the Appendix the rest of the proof.

Ψ is onto: We need to show that, for any $X_f \in SU(n)$, there exists an element $Y \in E_n \cup (D_1 \times SU(n-1)/_\sim)$ such that $\Psi(Y) = [X_f]_\sim$. Write X_f using the Cartan decomposition of type **AIII** of $SU(n)$ [17] as:

$$X_f = K_1 M K_2, \tag{15}$$

where

$$M = \begin{pmatrix} \cos(\theta) & \sin(\theta) & 0 & \cdots & 0 \\ -\sin(\theta) & \cos(\theta) & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix} \tag{16}$$

and

$$K_j = \begin{pmatrix} e^{i\eta_j} & 0 \\ 0 & e^{-\frac{i\eta_j}{n-1}} V_j \end{pmatrix}, \quad j = 1, 2, \quad V_j \in SU(n-1). \tag{17}$$

Without loss of generality we can assume $\sin(\theta) \geq 0$. In fact if $\sin(\theta) < 0$, let $L := \mathtt{diag}(i, -i, 1, 1, ..., 1)$. Then $X_f = K_1 L L^\dagger M L L^\dagger K_2$. Letting $\hat{K}_1 = K_1 L$, $\hat{K}_2 = L^\dagger K_2$, and $\hat{M} = L^\dagger M L$, we have that $X_f = \hat{K}_1 \hat{M} \hat{K}_2$, $\hat{K}_j \in S(U(n-1)\times U(1))$, and $\hat{M}$ is equal to M except for the sign of the off-diagonal elements. Given $X_f = K_1 M K_2$, where M is as in (16), with $\sin(\theta) \geq 0$, and $K_i \in S(U(n-1)\times U(1))$, as in (17) we have: $[X_f]_\sim = [K_1^\dagger K_1 M K_2 K_1]_\sim = [M K_2 K_1]_\sim$. Therefore, to conclude that Ψ is onto, it is enough that for every element

$$\begin{pmatrix} \cos(\theta) & \sin(\theta) & 0 & \cdots & 0 \\ -\sin(\theta) & \cos(\theta) & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix} \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-\frac{i\phi}{n-1}} V \end{pmatrix}, \tag{18}$$

(with $\phi = \eta_1 + \eta_2$, $V = V_2 V_1$ (cf. (17)), with $\sin(\theta) \geq 0$, there exists an $\sim$-equivalent element of the form

$$\begin{pmatrix} x & \sqrt{1-|x|^2} & 0 & \cdots & 0 \\ -\sqrt{1-|x|^2} & x^* & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix} \begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & Z \\ 0 & \end{pmatrix}, \tag{19}$$

with $Z \in SU(n-1)$ and $|x| \leq 1$. Here, if $|x| < 1$ the pre-image of the equivalence class of the above matrix will be in $(D_1 \times SU(n-1)/_\sim)$, while, if $|x| = 1$, it will be in E_n.

Consider the matrix $F := \texttt{diag}(e^{i\frac{\phi}{2}}, e^{-i\frac{\phi}{2}}, 1, 1, ..., 1)$. Then the following matrix is equivalent to (18):

$$F \begin{pmatrix} \cos(\theta) & \sin(\theta) & 0 & \cdots & 0 \\ -\sin(\theta) & \cos(\theta) & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix} F F^\dagger \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-\frac{i\phi}{n-1}} V \end{pmatrix} F^\dagger$$

We have:

$$F \begin{pmatrix} \cos(\theta) & \sin(\theta) & 0 & \cdots & 0 \\ -\sin(\theta) & \cos(\theta) & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix} F = \tag{20}$$

$$\begin{pmatrix} e^{i\phi}\cos(\theta) & \sin(\theta) & 0 & \cdots & 0 \\ -\sin(\theta) & e^{-i\phi}\cos(\theta) & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix},$$

which, by setting $x = e^{i\phi}\cos(\theta)$, is of the same form as the first matrix in formula (19), since $0 \leq \sin(\theta) = \sqrt{1-|x|^2}$. Moreover, it follows:

$$F^\dagger \begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-\frac{i\phi}{n-1}} V \end{pmatrix} F^\dagger = \begin{pmatrix} 1 & 0 \cdots 0 \\ 0 & \\ \vdots & Z \\ 0 & \end{pmatrix}, \tag{21}$$

which is of the same form as the second matrix in (19).

□

Theorem 1 and Corollary III.1 suggest that we can iterate formula (19) to obtain a *canonical form* for elements in each equivalence class in $SU(n)/\sim$. In fact, by similarity transformations in the Lie group $S(U(n-1) \times U(1))$, we can write every elements in $SU(n)$ in a form $F_1 F_2 \cdots F_j \hat{D}_{n-j}$, for $j \in \{0, 1, ..., n-1\}$, where the matrices F_k, for $k = 1, ..., j$, if any, have a block $\begin{pmatrix} x & \sqrt{1-|x|^2} \\ -\sqrt{1-|x|^2} & x^* \end{pmatrix}$ with $x \in D_1$ at the intersection of rows and columns j and $j+1$, (cf. (19)), and $\hat{D}_{n-j}$ is a diagonal matrix in $SU(n)$ with the first j elements equal to 1. The value j indicates the subset of the orbit space in the right hand side of (14) for the given class. The decomposition (14) displays the *orbit type stratification* [9] of the orbit space $SU(n)/_\sim$. The strata of the stratified space $SU(n)/_\sim$ are determined by the isotropy groups of the corresponding elements. In particular, the set $D_1^{\times n-1}$ in (14) corresponds to elements whose isotropy group is the (discrete) group of scalar matrices in $S(U(n-1) \times U(1))$. This is the *smallest* possible isotropy group and therefore $D_1^{\times n-1}$ corresponds to the (open and dense) *regular part* of $SU(n)$. The sets $D_1^{\times j}$, for $0 \leq j \leq n-2$ have strictly larger isotropy groups and therefore they correspond to the *singular part* of $SU(n)$. Among these, the set $D_1^{\times 0} \times E_n \simeq E_n$ is homeomorphic to $\pi(S(U(n-1) \times U(1)))$.

B. Use of Theorem 1 in the Determination of the Optimal Synthesis

The structure of the orbit space $SU(n)/_\sim$ is important knowledge in optimal control because the reachable sets in $SU(n)$ are the pre-images under the natural projection π of the corresponding sets in $SU(n)/_\sim$ [4] and the geometric analysis of the reachable sets is a possible approach to determining the optimal control. This was, in fact, the approach used in [3] in the case $n = 2$. We shall not pursue this here. However knowing the structure of the orbit space is important for what will follow for the following reason: According to a result in [4] and [5], points in the singular part belong to the cut locus of the sub-Riemannian synthesis, as long as the optimal trajectories leading to them cross the regular part of the orbit space. In these cases the optimal trajectories are *maximal geodesics*. This motivates the study of the optimal control problem for points that are in the singular part and requires the knowledge of the singular and regular part of the orbit space. For this reason, with the ultimate goal of finding the complete optimal synthesis for the $SU(n)/S(U(n-1) \times U(1))$ problem in the following we shall focus on final conditions in $\pi^{-1}(D_1^{\times 0} \times E_n) \simeq S(U(n-1) \times U(1))$ which belong to the singular part. We will restrict ourselves to $n = 3$.

IV. Optimal synthesis for three level quantum systems as an integer optimization problem

We shall now consider the optimal control problem for three level quantum systems in the Λ configuration of Figure 2. We can visualize $SU(3)/_\sim \simeq E_3 \cup (D_1 \times SU(2)/_\sim) \simeq E_3 \cup (D_1 \times \bar{D}_1)$ as (cf. Figure 3) an open disc $\bar{D}_1$ with, at each point attached a closed unit disc representing $SU(2)/_\sim$, so at most 4 parameters. The boundary of the disc serves as the base for the topological fiber bundle E_3. Each fiber of E_3 is given by a segment $[-1, 1]$.

Proposition IV.1. The topological fiber bundle E_3 is the closure of the Möbius band.

Proof. Consider the fiber $\pi^{-1}(e^{i\phi})$ which is the set of equivalence classes of elements X in $SU(2)$ such that $\begin{pmatrix} e^{i\phi} & 0 \\ 0 & 1 \end{pmatrix} X$ has a given spectrum. Since all elements $\begin{pmatrix} e^{i\phi} & 0 \\ 0 & 1 \end{pmatrix} X$ have the same determinant $e^{i\phi}$, the equivalence class of X is uniquely determined by the trace $Tr\left(\begin{pmatrix} e^{i\phi} & 0 \\ 0 & 1 \end{pmatrix} X\right)$ or, equivalently, by $\frac{e^{-i\frac{\phi}{2}}}{2} Tr\left(\begin{pmatrix} e^{i\phi} & 0 \\ 0 & 1 \end{pmatrix} X\right)$. By writing X as $X = \begin{pmatrix} re^{i\psi} & y \\ -y^* & re^{-i\psi} \end{pmatrix}$, we have $\frac{e^{-i\frac{\phi}{2}}}{2} Tr\left(\begin{pmatrix} e^{i\phi} & 0 \\ 0 & 1 \end{pmatrix} X\right) = r\cos(\frac{\phi}{2} + \psi)$. As this value varies in $[-1, 1]$ as r and ψ change, each fiber is identified with the interval $[-1, 1]$. Therefore E_3 is parametrized by $s = r\cos(\frac{\phi}{2} + \psi) \in [-1, 1]$ and $\phi \in [0, 2\pi]$, i.e., a rectangle with $s_0 = r\cos(\psi)$ and $s_{2\pi} = r\cos(\psi + \pi) = -r\cos(\psi) = -s_0$ identified. That is,

E_3 is a Möbius strip.[2]

□

The desired final condition is of the form

$$X_f = \begin{pmatrix} * & 0 \\ 0 & \tilde{X}_f, \end{pmatrix} \tag{22}$$

with $\tilde{X}_f \in U(2)$ the desired final transformation on the subspace corresponding to the lowest two energy levels, which, as argued in the previous section, belong to the singular part of the orbit space stratification.

Because of the symmetry described in the previous sections, it is enough to drive the state U in (3) time optimally to a matrix $Y_f = \begin{pmatrix} * & 0 \\ 0 & \tilde{Y}_f, \end{pmatrix}$ such that $\tilde{Y}_f$ is *similar* to $\tilde{X}_f$. Therefore the problem is characterized by assigning the two eigenvalues of $\tilde{X}_f$ which we denote by $e^{i\alpha}$ and $e^{i\beta}$ with α and β in $(-\pi, \pi]$. After symmetry reduction, the problem is (cf. section II) to find real values a, b, and c and minimum $t > 0$ such that, with

$$A = \begin{pmatrix} i(a+b) & 0 & 0 \\ 0 & -ia & -ic \\ 0 & -ic & -ib \end{pmatrix}, \qquad P = \begin{pmatrix} 0 & i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \tag{23}$$

$e^{At}e^{(-A+P)t}$ is in the same equivalence class as (22). Notice that since $X_f \in e^{\mathcal{K}} = S(U(n-1) \times U(1))$ according to Proposition II.3, unless c in (23) is zero $e^{(-A+P)t}$ must be scalar. If $c = 0$, the constraints that $X_f = e^{At}e^{(-A+P)t}$ is in $e^{\mathcal{K}}$ implies that it is in the same class as $diag(e^{i\varphi}, e^{-i\varphi}, 1)$. The problem, in this case becomes a problem on the upper left 2×2 block, and therefore on $SU(2)$ which can be treated with the method of [3]. For the sake of brevity, we shall not treat this case and assume α and β both different from zero, so that we can use the fact from Proposition II.3 that $e^{(-A+P)t}$ is scalar. Furthermore, since a common phase factor is physically irrelevant in quantum mechanics, we shall consider the problem to assign eigenvalues $e^{i\alpha}$ and $e^{i\beta}$ to e^{At}, in minimum time with $e^{(-A+P)t}$ scalar.

A. A nonlinear integer optimization problem

$e^{(-A+P)t}$ scalar implies that $(-A+P)t$ has eigenvalues $\lambda_1 := i\frac{2k\pi}{3}$, $\lambda_2 := i\frac{2k\pi}{3} + i2m\pi$, $\lambda_3 := -i\frac{4k\pi}{3} - i2m\pi$, for integers k and m, where we use the fact that $0 = \lambda_1 + \lambda_2 + \lambda_3$. This is true if and only if the symmetric real matrix

$$-i(-A+P) = \begin{pmatrix} -(a+b) & 1 & 0 \\ 1 & a & c \\ 0 & c & b \end{pmatrix}, \tag{24}$$

has eigenvalues

$$-i\frac{\lambda_1}{t} = \frac{2k\pi}{3t}, \quad -i\frac{\lambda_2}{t} = \frac{2k\pi}{3t} + \frac{2m\pi}{t}, \quad -i\frac{\lambda_3}{t} = \frac{-4k\pi}{3t} - \frac{2m\pi}{t}. \tag{25}$$

The characteristic polynomial of the matrix $-i(-A+P)$ in (24) is

$$p(\lambda) = \lambda^3 - (b^2 + a^2 + c^2 + 1 + ab)\lambda + (a+b)(ab - c^2) + b.$$

By expressing the coefficients in terms of the desired eigenvalues (25) [11], we obtain the following two conditions for the real numbers a, b, c, and $t > 0$,

$$b^2 + a^2 + c^2 + 1 + ab = \left(\frac{2\pi}{t}\right)^2 \left(\frac{k^2}{3} + km + m^2\right), \tag{26}$$

$$(a+b)(ab - c^2) + b = \left(\frac{2\pi}{t}\right)^3 \left(\frac{k}{3}\left(\frac{k}{3} + m\right)\left(\frac{2k}{3} + m\right)\right). \tag{27}$$

In order to assign the eigenvalues of e^{At} to $e^{i\alpha}$ and $e^{i\beta}$ we impose that the eigenvalues of $-i\begin{pmatrix} a & c \\ c & b \end{pmatrix} t$ are $i\phi_l = i\alpha + i2\pi l$ and $i\psi_r = i\beta + i2\pi r$, for integers l and r. Therefore, the symmetric matrix

$$\tilde{C} := \begin{pmatrix} -a & -c \\ -c & -b \end{pmatrix}, \tag{28}$$

has eigenvalues $\frac{\phi_l}{t}$, $\frac{\psi_r}{t}$. The characteristic polynomial of the matrix $\tilde{C}$ in (28) is $p(\lambda) = \lambda^2 + (a+b)\lambda + (ab - c^2)$. Imposing that the eigenvalues are $\frac{\phi_l}{t}$, $\frac{\psi_r}{t}$, we obtain the two conditions to be added to (26) (27),

$$(a+b) = \frac{\phi_l + \psi_r}{t}, \tag{29}$$

$$ab - c^2 = \frac{\phi_l \psi_r}{t^2}. \tag{30}$$

Therefore the problem of optimal control becomes the following:

Problem 1 *Given α and β in $(-\pi, \pi]$, with both α and β different from zero,[3] find real numbers a, b, c, t, with $c \neq 0$, and minimum $t > 0$ such that conditions (26), (27), (29), (30) are verified for some integers k, m, l, and r.*

Using (29) and (30) in (26) and (27) we obtain

$$\frac{(\phi_l + \psi_r)^2}{t^2} - \frac{\phi_l \psi_r}{t^2} + 1 = \left(\frac{2\pi}{t}\right)^2 \left(\frac{k^2}{3} + km + m^2\right), \tag{31}$$

$$-\frac{(\phi_l + \psi_r)(\phi_l \psi_r)}{t^3} + b = \left(\frac{2\pi}{t}\right)^3 \left(\frac{k}{3}\left(\frac{k}{3} + m\right)\left(\frac{2k}{3} + m\right)\right), \tag{32}$$

which replace (26) and (27). Scale the time by replacing t with $T := \frac{t}{2\pi}$, and define $\hat{\phi}_l := \frac{\phi_l}{2\pi} = \frac{\alpha}{2\pi} + l$, $\hat{\alpha} := \frac{\alpha}{2\pi}$, $\hat{\psi}_r := \frac{\psi_r}{2\pi} = \frac{\beta}{2\pi} + r$, $\hat{\beta} := \frac{\beta}{2\pi}$, so that $\hat{\alpha}$ and $\hat{\beta}$ are both $\in (-\frac{1}{2}, \frac{1}{2}]$. Equations (31), (32), (29), (30) are therefore written as

$$(\hat{\phi}_l + \hat{\psi}_r)^2 - \hat{\phi}_l \hat{\psi}_r + T^2 = \frac{k^2}{3} + km + m^2, \tag{33}$$

$$-(\hat{\phi}_l + \hat{\psi}_r)(\hat{\phi}_l \hat{\psi}_r) + bT^3 = \frac{k}{3}\left(\frac{k}{3} + m\right)\left(\frac{2k}{3} + m\right), \tag{34}$$

[2]Notice that the curve $(\phi, s(\phi)) = (\phi, r\cos(\frac{\phi}{2} + \psi))$ for fixed $r \neq 0$ and ψ, as ϕ goes from 0 to 2π, crosses the line $s = 0$ only once. Therefore there is only one 'twist' of the rectangle $0 \leq \phi \leq 2\pi$, $-1 \leq s \leq 1$ before joining the two ends.

[3]If $(\alpha, \beta) = (0, 0)$, the target final condition becomes the identity which is obviously reached in time zero. The stronger condition that both α and β are different from zero is used to rule out final conditions in the same class as $diag(e^{i\varphi}, e^{-i\varphi}, 1)$ which are the only possibility if $c = 0$.

$$(a+b) = -\frac{\hat{\phi}_l + \hat{\psi}_r}{T}, \tag{35}$$

$$c^2 = ab - \frac{\hat{\phi}_l \hat{\psi}_r}{T^2} > 0. \tag{36}$$

Problem 1 is therefore equivalent to, given $\hat{\alpha}$ and $\hat{\beta}$ in $(-\frac{1}{2}, \frac{1}{2}]$, finding integers k, m, l, r, such that T^2 in (33) is minimized subject to the constraint (36) with b obtained from (34) and a obtained from (35). We remark that, since we have assumed $c \neq 0$, we cannot choose $\hat{\phi}_l = \hat{\psi}_r$. In fact, if this was the case, defining $\hat{\phi}_l = \hat{\psi}_r = \hat{\gamma}$, we would have, plugging (35) in (36), $-\left(b + \frac{\hat{\gamma}}{T}\right)^2 > 0$, which is a contradiction. We assume without loss of generality, that $\hat{\phi}_l > \hat{\psi}_r$. With this assumption, the constraint of the optimization problem is equivalent to the existence of a real b satisfying (34), with T^2 given in (33), and satisfying

$$-\frac{\hat{\phi}_l}{T} < b < -\frac{\hat{\psi}_r}{T}. \tag{37}$$

In order to see this, replace (35) into (36) to get

$$\left(b + \frac{\hat{\phi}_l}{T}\right)\left(b + \frac{\hat{\psi}_r}{T}\right) < 0, \tag{38}$$

which is equivalent to (37). If we multiply (37) by T^3, use (34) and (33) for T^2, we obtain the constraint

$$\hat{\phi}_l^3 - \hat{\phi}_l\left(\frac{k^2}{3} + km + m^2\right) < \frac{k}{3}\left(\frac{k}{3} + m\right)\left(\frac{2k}{3} + m\right) < \\ < \hat{\psi}_r^3 - \hat{\psi}_3\left(\frac{k^2}{3} + km + m^2\right). \tag{39}$$

The problem is therefore to find (k, m, l, r) to minimize T^2 given in (33) subject to the constraint (39). Notice that, in this formulation, the fact that T^2 in (33) has to be positive comes automatically from (39), since $\hat{\phi}_l^3 - \hat{\phi}_l\left(\frac{k^2}{3} + km + m^2\right) < \hat{\psi}_r^3 - \hat{\psi}_r\left(\frac{k^2}{3} + km + m^2\right)$, with $\hat{\phi}_l > \hat{\psi}_r$ is equivalent to $\frac{k^2}{3} + km + m^2 > \hat{\phi}_l^2 + \hat{\psi}_r^2 + \hat{\phi}_l\hat{\psi}_r$.

For a given pair l and r, (k, m) and $(k, -(k+m))$ are equivalent in that they give the same value of T^2 and they both satisfy or do not satisfy (39). Therefore we can restrict our search to values of $m \geq -\frac{k}{2}$. We define $s := m + \frac{k}{2} \geq 0$, which is an integer if k is even and a half integer if k is odd. After some algebra, we write T^2 and the constraint (39) as:

$$T^2 = \frac{k^2}{12} + s^2 - \left(\hat{\phi}_l^2 + \hat{\psi}_r^2 + \hat{\phi}_l\hat{\psi}_r\right), \tag{40}$$

$$\begin{aligned} \left(\hat{\phi}_l + \tfrac{k}{3}\right)\left(\hat{\phi}_l - \tfrac{k}{6} - s\right)\left(\hat{\phi}_l - \tfrac{k}{6} + s\right) < 0, \\ \left(\hat{\psi}_r + \tfrac{k}{3}\right)\left(\hat{\psi}_r - \tfrac{k}{6} - s\right)\left(\hat{\psi}_r - \tfrac{k}{6} + s\right) > 0. \end{aligned} \tag{41}$$

So Problem 1 becomes:

Problem 2 (**Nonlinear integer optimization problem**) *Given $\hat{\alpha}$ and $\hat{\beta}$ in $(\frac{1}{2}, \frac{1}{2}]$, both different from zero, find (l, r, k, s) with $s \geq 0$ an integer if k is even and a half-integer if k is odd, to minimize T^2 in (40) with $\hat{\phi}_l = \hat{\alpha} + l$, $\hat{\psi}_r = \hat{\beta} + r$, subject to the constraints (41).*

V. Solution to the integer optimization problem

We solve Problem 2 as a *cascade* of two minimization problems. For each (k, s), we minimize T^2 in (40) over l and r within the region specified by the constraint (41). Then we minimize the resulting function over (k, s). Minimization over (l, r) of T^2 in (40) for given (k, s) corresponds to maximization over the same region of the function

$$F = F(l, r) := \hat{\phi}_l^2 + \hat{\psi}_r^2 + \hat{\phi}_l\hat{\phi}_l = \tag{42}$$
$$= \hat{\alpha}^2 + \hat{\beta}^2 + \hat{\alpha}\hat{\beta} + (\hat{\beta} + 2\hat{\alpha})l + (\hat{\alpha} + 2\hat{\beta})r + l^2 + r^2 + lr.$$

For given (k, s), to characterize the region described in (41), we consider all possible sign combinations which give a negative sign in the first inequality and a positive sign in the second inequality. There are four cases for each inequality. Combining these cases we take into account that $\hat{\phi}_l > \hat{\psi}_r$. This reduces the possible subcases to the following three:

1) **A**
$$\frac{k}{6} - s < \hat{\psi}_r < \frac{k}{6} + s < \hat{\phi}_l < -\frac{k}{3}; \tag{43}$$
2) **B**
$$-\frac{k}{3} < \hat{\psi}_r < \frac{k}{6} - s < \hat{\phi}_l < \frac{k}{6} + s; \tag{44}$$
3) **C**
$$\frac{k}{6} - s < \hat{\psi}_r < -\frac{k}{3} < \hat{\phi}_l < \frac{k}{6} + s. \tag{45}$$

In order for the region described in **A** to be nonempty we need $-\frac{k}{2} > s > 0$. In the case **B** we need $\frac{k}{2} > s > 0$ and in the case **C** we need $\frac{|k|}{2} < s$. Therefore we can solve three optimization problems according to whether (k, s) is in the region corresponding to **A**, **B**, or **C** (cf. Figure 2) and then compare the results to find the minimum. In fact, it follows from the following two lemmas that the minimum for (k, s) in the region **A** is the same as the minimum in the region **B** and the minimum in the region **C**, and therefore only one region needs to be considered.

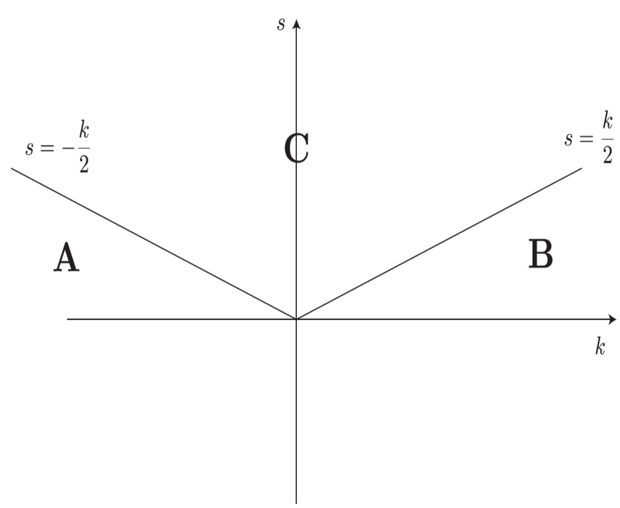

Fig. 2. Regions for the optimization Problem 2

Lemma V.1. Consider the linear transformation

$$\begin{pmatrix}\tilde{k}\\ \tilde{s}\end{pmatrix} = R\begin{pmatrix}k\\ s\end{pmatrix} \tag{46}$$

where R is the involutory matrix $R := \begin{pmatrix}-\frac{1}{2} & -3\\ -\frac{1}{4} & \frac{1}{2}\end{pmatrix}$. Then (k,s,l,r) is an admissible $4-$tuple with (k,s) in $\mathbf{A}$ if and only $(\tilde{k},\tilde{s},l,r)$ is an admissible $4-$tuple with $(\tilde{k},\tilde{s})$ in $\mathbf{C}$. Moreover (k,s,l,r) and $(\tilde{k},\tilde{s},l,r)$ give the same value of T^2.

Proof. First notice that the transformation given by the matrix R transforms (k,s) correctly into $(\tilde{k},\tilde{s})$ in the sense that if $\tilde{k}$ is even (odd) $\tilde{s}$ is an integer (half-integer).[4] Then consider (k,s,l,r) satisfying equation (43). Replacing $(k,s)^T$ with $(\tilde{k},\tilde{s})^T = R(k,s)^T$, we obtain equation (45). Finally one verifies that $\frac{\tilde{k}^2}{12}+\tilde{s}^2 = \frac{k^2}{12}+s^2$, from which it follows that the value of T^2 is the same. □

Analogously, we have:

Lemma V.2. Consider the linear transformation (46) with R the involutory matrix $R := \begin{pmatrix}-\frac{1}{2} & 3\\ \frac{1}{4} & \frac{1}{2}\end{pmatrix}$. Then (k,s,l,r) is an admissible $4-$tuple with (k,s) in $\mathbf{B}$ if and only $(\tilde{k},\tilde{s},l,r)$ is an admissible $4-$tuple with $(\tilde{k},\tilde{s})$ in $\mathbf{C}$. Moreover (k,s,l,r) and $(\tilde{k},\tilde{s},l,r)$ give the same value of T^2.

In view of these properties we shall reduce ourselves, without loss of generality, to optimization in the region $\mathbf{C}$. In the case where $\hat{\beta} = -\hat{\alpha}$, which corresponds to $\tilde{X}_f \in SU(2)$ we also have the following fact which allows us to reduce ourselves to the case $k \geq 0$.

Lemma V.3. Assume $\hat{\beta} = -\hat{\alpha}$. Let $\{k,s,l,r\}$, and $\hat{\phi}_l = \hat{\alpha}+l$, $\hat{\psi}_r = -\hat{\alpha}+r$ be admissible values, i.e., satisfying (45), giving for the time a value T. Then $\{-k,s,-r,-l\}$ and $\hat{\phi}_{-r} = \hat{\alpha}-r$, $\hat{\psi}_{-l} = -\hat{\alpha}-l$ are also admissible values and give the same value of T. In particular if (k,s) is in region $\mathbf{C}$, to the right of the s-axis, $(-k,s)$ is in region $\mathbf{C}$ to the left of the s-axis.

Proof. If (k,s) is in the region $\mathbf{C}$, taking the negative of relation (45), we obtain the same relation with k replaced by $-k$ and $\hat{\phi}_l$ replaced by $\hat{\phi}_{-r} = \alpha - r = -\hat{\psi}_r$ and $\hat{\psi}_r$ replaced by $\hat{\psi}_{-l} = -\hat{\phi}_l$. The time is the same. □

We now introduce two functions which allow us to express the constraint (45) (and (43), (44)) taking into account that l and r must be integers: The function $\mathbf{SI} = \mathbf{SI}(x)$ is the *smallest integer* strictly greater than x. The function $\mathbf{LI} = \mathbf{LI}(x)$ is the largest integer strictly smaller than x. The following properties of these functions can be easily checked and will be routinely used without further comment.

Lemma V.4. The function $\mathbf{SI}$ ($\mathbf{LI}$) is nondecreasing right (left) continuous. If p is an integer, then $\mathbf{SI}(x+p) = \mathbf{SI}(x)+p$ ($\mathbf{LI}(x+p) = \mathbf{LI}(x)+p$). If x is not an integer, $\mathbf{SI}(x) = \mathbf{LI}(x)+1$. If x is an integer, $\mathbf{SI}(x) = \mathbf{LI}(x)+2$.

[4]To verify this it is enough to check all subcases: Assume first that k is even and s is an integer. Write k as $k=-2j$. We have $\tilde{k} = j-3s$, $\tilde{s} = \frac{j}{2}+\frac{s}{2}$ from which one sees that $\tilde{k}$ even (odd) gives s is an integer (half-integer). Analogously if k is odd and s is a half-integer, we can write $k=-2j+1$ and $s=\frac{1}{2}+h$, so that $\tilde{k} = j+h-4h-2$, $\tilde{s} = \frac{j+h}{2}$, from which the claim follows directly.

A. Minimization for (k,s) in the region C ($\frac{|k|}{2} < s$)

Since $s > \frac{|k|}{2}$ and s is an (half) integer for k (odd) even, we have $s \geq \frac{|k|}{2}+1$. From equations (45), we obtain

$$\hat{c} := \mathbf{SI}\left(\frac{k}{6}-s-\hat{\beta}\right) \leq r \leq \mathbf{LI}\left(-\frac{k}{3}-\hat{\beta}\right) := \hat{d}, \tag{47}$$

$$\hat{a} := \mathbf{SI}\left(-\frac{k}{3}-\hat{\alpha}\right) \leq l \leq \mathbf{LI}\left(\frac{k}{6}+s-\hat{\alpha}\right) := \hat{b}. \tag{48}$$

We can check, using Lemma V.4, that for $\hat{\alpha}$ and $\hat{\beta} \neq \pm\frac{1}{3}, 0$ the box (47) (48) always contains at least one point. This is shown in Lemma C.1 in the Appendix. For general values of $\hat{\alpha}$ and $\hat{\beta}$ if for certain values of k and s the box (47)(48) is empty, these values have to be eliminated from the search.

From now on we shall **assume $\hat{\beta} = -\hat{\alpha}$ and $0 < |\hat{\alpha}| < \frac{1}{3}$**. In particular we assume that the desired final condition $\tilde{X}_f$ in (22) is (modulo a phase factor) a matrix in $SU(2)$. Using Lemma V.3, we can restrict ourselves, without loss of generality, to $k \geq 0$. The function $F = F(l,r)$ in (42) becomes

$$F = F(l,r) = \hat{\phi}_l^2 + \hat{\psi}_r^2 + \hat{\phi}_l\hat{\phi}_l = \hat{\alpha}^2 + \hat{\alpha}(l-r) + l^2 + r^2 + lr. \tag{49}$$

Proceeding to the maximization of $F = F(l,r)$ in (42) over the box (47) (48), the following Proposition says at which corner of the box the maximum is achieved for any given pair (k,s). The proof is given in the Appendix.

Proposition V.5. Assume $\hat{\alpha} \in (-\frac{1}{3},\frac{1}{3})$ and $\hat{\alpha} \neq 0$. Write $k = 6j+h$, with $h = 0,1,2,...,5$, and let (k,s) be in the region $\mathbf{C}$ of Figure 2. If $\hat{\alpha} > 0$ the maximum of $F(l,r)$ in (49) over the admissible values of l,r given in (47), (48) is given by $F(\hat{b},\hat{c})$ in all cases. Assume $\hat{\alpha} < 0$. If $h = 0,3$ the maximum is still given by $F(\hat{b},\hat{c})$. If $h = 2,5$, the maximum is given by $F(\hat{b},\hat{d})$. If $h = 1,4$ the maximum is at $F(\hat{a},\hat{c})$.

Proof. (See the Appendix) □

By using $T^2 = \frac{k^2}{12}+s^2-F(l,r)$ and setting, once again, $k = 6j+h$, we have

$$T^2(k,s) \geq 3j^2 + jh + \frac{h^2}{12} + s^2 - \max_{l,r} F(l,r). \tag{50}$$

We separate the case $\hat{\alpha} > 0$ and $\hat{\alpha} < 0$, which require a similar analysis and present in detail the results of the analysis for $\hat{\alpha} > 0$ and postpone to the appendix the analysis for $\hat{\alpha} < 0$.

1) Case $\hat{\alpha} > 0$: In this case, according to Proposition V.5, the maximum of $F(l,r)$ in (50) is always attained at $F(\hat{b},\hat{c})$. Therefore we compute

$$T^2(k,s) \geq 3j^2 + jh + \frac{h^2}{12} + s^2 - F(\hat{b},\hat{c}). \tag{51}$$

Use Δ_h equal to zero if h is even and equal to $\frac{1}{2}$ if h is odd. Define $\sigma_h := \mathbf{SI}\left(\frac{h}{6}+\Delta_h+\hat{\alpha}\right)$, $\lambda_h := \mathbf{LI}\left(\frac{h}{6}-\Delta_h-\hat{\alpha}\right)$. This gives, from (47) (48), $\hat{b} = j+s+\frac{1}{2}+\lambda_h$ and $\hat{c} = j-s-\Delta_h+\sigma_h$. Replacing these in (51) we obtain

$$T^2(k,s) \geq \tag{52}$$

$$(h-3(\lambda_h+\sigma_h))j - \hat{\alpha}^2 + \frac{h^2}{12} - \lambda_h^2 - \sigma_h^2 - \lambda_h\sigma_h +$$
$$(\hat{\alpha}+\Delta_h)(\sigma_h-\lambda_h) - \Delta_h^2 + (\sigma_h-\lambda_h-2\Delta_h)s - 2\Delta_h\hat{\alpha} - 2\hat{\alpha}s.$$

Calculating the values of λ_h and σ_h from the definitions:

1) $\mathbf{h = 0}$

$$T^2 \geq -\hat{\alpha}^2 + (2\hat{\alpha} - 1) + 2(1-\hat{\alpha})s \geq \\ \geq -\hat{\alpha}^2 + (2\hat{\alpha}-1) + 2(1-\hat{\alpha})(3j+1) \geq 1 - \hat{\alpha}^2. \tag{53}$$

We first used $s \geq 3j+1$ and then $j \geq 0$.

2) $\mathbf{h = 1}$

$$T^2 \geq -\hat{\alpha}^2 + j + (\hat{\alpha} - \frac{1}{6}) + (1-2\hat{\alpha})s \tag{54}$$

$$\geq -\hat{\alpha}^2 + (4 - 6\hat{\alpha})j - 2\hat{\alpha} + \frac{4}{3} \geq -\hat{\alpha}^2 - 2\hat{\alpha} + \frac{4}{3}.$$

We first used $s \geq 3j + \frac{3}{2}$ and then $j \geq 0$.

3) $\mathbf{h = 2}$

$$T^2 \geq -\hat{\alpha}^2 - j - \tfrac{2}{3} + (1-2\hat{\alpha})s + \hat{\alpha} \\ \geq (-1+3\hat{\alpha})j + \hat{\alpha} + \tfrac{1}{3} - \hat{\alpha}^2 \\ \geq -\hat{\alpha}^2 + 2j + \tfrac{4}{3} - 3\hat{\alpha} - 6\hat{\alpha}j \geq -\hat{\alpha}^2 + \tfrac{4}{3} - 3\hat{\alpha}. \tag{55}$$

We first used $s \geq 3j+2$ and then $j \geq 0$.

4) $\mathbf{h = 3}$

$$T^2 \geq -1 - \hat{\alpha}^2 + (2-2\hat{\alpha})s + 2\hat{\alpha} \tag{56}$$

$$\geq -1 - \hat{\alpha}^2 + (2-2\hat{\alpha})(3j + \frac{5}{2}) + 2\hat{\alpha} \geq 4 - \hat{\alpha}^2 - 3\hat{\alpha}.$$

We first used $s \geq 3j + \frac{5}{2}$ and then $j \geq 0$.

5) $\mathbf{h = 4}$

$$T^2 \geq 3j^2 + 4j + \tfrac{4}{3} + s^2 - F(\hat{b}, \hat{c}) = \\ j + \tfrac{1}{3} - \hat{\alpha}^2 + s - 2\hat{\alpha}s + \hat{\alpha} \geq \\ (4-6\hat{\alpha})j + \tfrac{10}{3} - \hat{\alpha}^2 - 5\hat{\alpha} \geq \tfrac{10}{3} - \hat{\alpha}^2 - 5\hat{\alpha}. \tag{57}$$

We first used $s \geq 3j+3$ and then $j \geq 0$.

6) $\mathbf{h = 5}$

$$T^2 \geq -j - \frac{7}{6} - \hat{\alpha}^2 + (1-2\hat{\alpha})s + \hat{\alpha} \tag{58}$$

$$\geq (2 - 6\hat{\alpha})j + \frac{7}{3} - \hat{\alpha}^2 - 6\hat{\alpha} \geq \frac{7}{3} - 6\hat{\alpha} - \hat{\alpha}^2.$$

We first used $s \geq 3j + \frac{7}{2}$ and then $j \geq 0$.

All the lower bounds are attained at the lowest possible values of j and s. By comparison of these lower bounds we obtain the minimum time if we assume $\hat{\alpha} > 0$.

Lemma V.6. The minimum of T^2 for values of (k, s) in the region **C** and $\hat{\alpha} \in (0, \frac{1}{3})$ is given by $\hat{T}_{+,2} := \frac{4}{3} - 3\hat{\alpha} - \hat{\alpha}^2$ if $\hat{\alpha} \in [\frac{1}{9}, \frac{1}{3})$. In this case $j = 0$ and $h = 2$ so that $k = 6j+2 = 2$, $s = 2$ and $l = \hat{b} = j + s = 2$, $r = \hat{c} = j - s + 1 = -1$. If $\hat{\alpha} \in (0, \frac{1}{9})$, the minimum is $\hat{T}^2_{+,0} := 1 - \hat{\alpha}^2$. In this case, $j = 0$ so that $k = 6j = 0$, $s = 1$, and $l = \hat{b} = j + s - 1 = 0$, $r = \hat{c} = j - s + 1 = 0$.

2) Case $\hat{\alpha} < 0$: If $\hat{\alpha} < 0$, Proposition V.5 gives different points where the maximum of $F(l, r)$ is achieved according to the value of h in $k = 6j + h$. The final result corresponding to Lemma V.6 (cf. Appendix D) is as follows.

Lemma V.7. The minimum of T^2 for values of (k, s) in the region **C** with $k \geq 0$ and $\hat{\alpha} \in (-\frac{1}{3}, 0)$ is given by $\hat{T}_{-,0} := -2\hat{\alpha} - \hat{\alpha}^2$, for all values of $\hat{\alpha}$. In this case $j = 0$ so that $k = 6j = 0$, $s = 1$, and $l = \hat{b} = j + s = 1$, $r = \hat{c} = j - s = -1$.

In the problem of reaching a certain matrix $\tilde{X}_f$ in $SU(2)$ in minimum time (cf. (22)), we can choose between positive and negative $\hat{\alpha}$. Therefore the optimal time is the minimum between the time in Lemma V.6 and the one in Lemma V.7. By comparison we obtain the following theorem which solves Problem 2 and therefore the optimal control problem for any $\tilde{X}_f \in SU(2)$ with eigenvalues $e^{i\alpha}$ and $e^{-i\alpha}$, with $0 < |\alpha| = |2\pi\hat{\alpha}| < \frac{2\pi}{3}$. We have

Theorem 2. *Assume $0 < |\hat{\alpha}| < \frac{1}{3}$. If $|\hat{\alpha}| \leq \frac{4}{15}$ the minimum time is given by $T^2 = 2|\hat{\alpha}| - \hat{\alpha}^2$, with $\hat{\alpha} < 0$, $k = 0$, $s = 1$, $l = 1$, $r = -1$. If $|\hat{\alpha}| \geq \frac{4}{15}$ the minimum is attained at $T^2 = \frac{4}{3} - 3|\hat{\alpha}| - \hat{\alpha}^2$, for $\hat{\alpha} > 0$, $k = 2$, $s = 2$, $l = 2$, $r = -1$.*

Remark V.8. We have made the assumptions $-\hat{\alpha} = \hat{\beta}$ and $0 < |\hat{\alpha}| < \frac{1}{3}$ in order to illustrate the procedure of solution and give an explicit solution for a class of problems. In practical situations one has *numerical values* for $\hat{\alpha}$ and $\hat{\beta}$ and can proceed to the maximization of (42) subject to (45). One can again follow a $\min - \min$ procedure as above, with the only difference that now Lemma V.3 may not hold and therefore the entire region **C** has to be considered.

VI. Discussion of the method and example

The result of Theorem 2, which solves the integer optimization problem, allows us to find the parameters a, b, c to be used in the matrix A in (23) and therefore the optimal control $e^{At}Pe^{-At}$ (cf. (7)). Summarizing, the procedure is as follows: Given the desired final condition (22), from the eigenvalues of $\tilde{X}_f$ (in $SU(2)$), $e^{i\alpha}$ and $e^{-i\alpha}$, we obtain α and $\hat{\alpha} = \frac{\alpha}{2\pi} \in (\frac{1}{2}, \frac{1}{2}]$. Assuming $0 < |\hat{\alpha}| < \frac{1}{3}$, Theorem 2 gives the value of $T^2 = \frac{t^2}{4\pi^2}$ (the optimal time) as well as the optimal k, $s = m + \frac{k}{2}$, l and r, and indicates whether to choose the positive or negative value for $\hat{\alpha}$. Using these values in (34) we obtain the value of b. Using this in (35) we obtain the value of a and using these in (36) we obtain c. These are the parameters for the optimal control. Such a control in general will drive optimally to a state in $\hat{X}_f \in SU(2)$ which is only *similar* to the desired $\tilde{X}_f$. The corresponding matrix in $SU(3)$ will be in the same equivalence class as the desired final condition. Therefore, in general, there will exist a $K \in SU(2)$ such that $K\hat{X}_f K^\dagger = \tilde{X}_f$. By similarity transformation of A and P with $\begin{pmatrix} 1 & 0 \\ 0 & K \end{pmatrix}$ we obtain the optimal A and P matrices to be used in the optimal control (7).

We remark that the desired final condition is indeed in the cut locus of the optimal synthesis and therefore the geodesics found this way are *maximal* geodesics. One quick way to see this is to apply Proposition 4.2 in [4]. Consider an intermediate point Y_f in the optimal geodesic. By the principle of optimality the geodesic after Y_f has to be optimal and therefore Y_f cannot belong to the cut locus. From Proposition 4.2 of [4] if $\hat{H}$ belongs to the isotropy group of Y_f, it has to satisfy $\hat{H} P \hat{H}^\dagger = P$ and $\hat{H}[A, P]\hat{H}^\dagger = [A, P]$, which implies with the form of P and A (in particular $c \neq 0$ in (23)) that $\hat{H}$ must be a scalar matrix. Therefore Y_f has to belong to the regular part of $SU(3)$ and therefore the geodesic crosses the regular part.[5]

Example VI.1. Assume we want to drive in minimum time up to a scalar matrix to the final condition

$$H = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ 0 & \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

which performs an Hadamard-like gate [21],

$$\tilde{X}_f = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}, \tag{59}$$

on the lowest two energy eigenstates. The eigenvalues of $\tilde{X}_f$ are $e^{\pm i\pi/4}$. Therefore, using the notation of the previous section, $|\hat{\alpha}| = \frac{\pi/4}{2\pi} = \frac{1}{8}$. Using Theorem 2, we find for the minimum T, $T = \frac{\sqrt{15}}{8}$, $\hat{\alpha} = -\frac{1}{8}$ and therefore negative, $k = 0$, $s = 1$, $l = 1$, $r = -1$. Notice that the eigenvalues of $(-A+P)t$ from (25) are $\lambda_1 = 0$, $\lambda_2 = 2\pi i$, $\lambda_3 = -2\pi i$ so that $e^{(-A+P)t}$ is the identity. We also get $\hat{\phi}_l = \hat{\alpha} + l = -\frac{1}{8} + 1 = \frac{7}{8}$ and $\hat{\psi}_r = -\hat{\alpha} + r = \frac{1}{8} - 1 = -\frac{7}{8}$. From (34) and (35) we obtain $b = 0$ and $a = 0$, while from (36) we obtain $c^2 = \frac{49}{15}$. Therefore, the equivalence class of H is reached in minimum time $t = 2\pi T = \frac{\sqrt{15}\pi}{4}$ (after re-scaling of time) using

$$A = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \pm\frac{7i}{\sqrt{15}} \\ 0 & \pm\frac{7i}{\sqrt{15}} & 0 \end{pmatrix}.$$

The final condition with this control is

$$e^{A\frac{\sqrt{15}\pi}{4}} = \begin{pmatrix} 1 & 0 \\ 0 & e^{\sigma_x \frac{7\pi}{4}} \end{pmatrix}, \tag{60}$$

with $\sigma_x := \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$. Explicit calculation chosing the positive value for c gives that

$$e^{\sigma_x \frac{7\pi}{4}} = \begin{pmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{pmatrix} |_{t=\frac{7\pi}{4}} = \begin{pmatrix} \frac{1}{\sqrt{2}} & -i\frac{1}{\sqrt{2}} \\ -i\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}.$$

This is not yet the desired final condition in (59) but it is similar to it using the similarity transformation $K = \mathtt{diag}(i, -i)$. Therefore to obtain the optimal control we transform by similarity transformation $\mathtt{diag}(1, i, -i)$ the matrix $e^{At}Pe^{-At}$ (7). Alternatively we could have used the negative value for c which would have given exactly the transformation in (59) without the need of an extra similarity transformation.

[5]Notice that there is a discrepancy between the terminology in [4] since there we call 'cut locus' the set of points reached by two or more geodesics and 'critical locus' what we have called cut locus here. However the argument applies since the assumption in Proposition 4.2 of [4] is weaker than what we assume here, because of Proposition 2.1 in [4].

Figure 3 represents the optimal trajectory in the orbit space which was described at the beginning of section IV. The base disk has a boundary which serves as the base of a closed Möbius strip (Proposition IV.1). Every point of the interior of the disk has attached a closed (vertical) disc and all vertical discs collapsing on segments at the border of the base disc. All the border segments form a closed Möbius strip. In our figure we have not represented the imaginary part of the coordinate on the vertical disks so as to be able to give a $3-D$ picture. For the trajectory in this example such a coordinate is identically zero. The trajectory in the quotient space for this example is represented in black. It starts from the point representing the identity and ends at the point corresponding to the final condition which is in E_2 and in the same fiber as the identity.

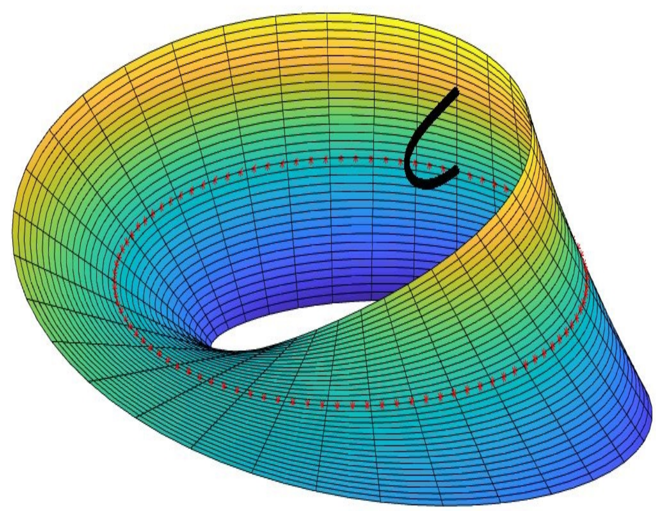

Fig. 3. Optimal trajectory in the quotient space

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VII. Conclusion

We have given tools to solve the minimum time optimal control problem for a class of systems on $SU(n)$ of interest in quantum mechanics. The presence of a symmetry group $e^{\mathcal{K}}$ in the model allows for a reduction of the unknown parameters in the optimal controls and trajectories. This was described in Proposition II.1 and Corollary II.2. The analysis of the orbit space $SU(n)/S(U(n-1) \times U(1))$ gives information on the optimal synthesis on $SU(n)$. In particular, according to the results of [4] the reachable sets in $SU(n)$ are inverse images (under the natural projection) of sets in $SU(n)/S(U(n-1) \times U(1))$ and information on the cut locus in $SU(n)$ can be obtained from the corresponding sets in $SU(n)/S(U(n-1) \times U(1))$. For these reasons, we have described the orbit space explicitly in section III. For a large part of the paper we have focused on the case of three level quantum systems. This is motivated not only to illustrate the above techniques but also by the enormous interest of three level systems in multiple applications of quantum mechanics. In fact, much interest in the quantum mechanics literature is for lambda systems of Figure 1 where one wants to perform operations on the lowest two energy levels, which is the setting we consider. The description of the orbit space of section III is used here in two ways: On one end it motivates the problem suggesting that the given final conditions are in the cut locus, since they belong to the singular part of the orbit space, and on the other hand it allows us to verify this by showing that the derived geodesics cross the regular part. We have given an explicit solution of this problem by transforming it into an integer quadratic optimization problem. Although this has been done only for a certain range of values of the final condition, we believe that the technique used in section V can be adapted for other ranges of the possible eigenvalues of the final conditions and therefore lead to optimal control laws for final conditions different from the ones considered in Theorem 2. This, together with the maximality of the geodesics discussed above, has the potential of leading to the *complete optimal synthesis* for the case of $SU(3)$, and to be extended to problems on $SU(n)$ for $n > 3$.

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APPENDIX

APPENDIX A
COMPLETION OF THE PROOF OF THEOREM 1

We are left with proving that Ψ is i) well-defined, ii) one-to-one, and iii) continuous with continuous inverse.

For $x \in D_1$, denote by $W(x)$ the first factor in (19)

i) Ψ is well-defined: Assume first that $Z, B \in SU(n)$ are such that $[Z]_{\sim_\phi} = [B]_{\sim_\phi}$ and let $U \in SU(n-1)$ be the matrix that gives the equivalence (see equation (11)), then we have:

$$\Psi\left([B]_{\sim_\phi}\right) = \left[\begin{pmatrix} e^{-i\phi} & 0 & 0 & \cdots & 0 \\ 0 & e^{i\phi} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix}\begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & B \\ 0 & \end{pmatrix}\right]_{\sim} =$$

$$\left[\begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & U \\ 0 & \end{pmatrix}\begin{pmatrix} e^{-i\phi} & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix}\right.$$
$$\left.\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & e^{i\phi} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix}\begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & B \\ 0 & \end{pmatrix}\begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & U^\dagger \\ 0 & \end{pmatrix}\right]_{\sim}$$

Since the first and the second matrices of the above expression commute, and

$$U\begin{pmatrix} e^{i\phi} & 0 \\ 0 & I \end{pmatrix} BU^\dagger = \begin{pmatrix} e^{i\phi} & 0 \\ 0 & I \end{pmatrix} Z,$$

we get that $\Psi\left([B]_{\sim_\phi}\right) = \Psi\left([Z]_{\sim_\phi}\right)$. So the result of applying Ψ does not depend on the representative in the equivalence class $\sim_\phi$. Assume now that Ψ acts on $D_1 \times SU(n-1)/_\sim$. Let $Z, B \in SU(n-1)$ with $[Z]_\sim = [B]_\sim$ and denote by $V \in SU(n-2)$ and $\eta \in [0, 2\pi]$ the matrix and the constant such that if $X = \begin{pmatrix} e^{i\eta} & 0 \\ 0 & e^{-\frac{i\eta}{n-2}}V \end{pmatrix} \in S(U(n-2)\times U(1))$, then $B = XAX^\dagger$. We have, for $x \in D_1$:

$$\Psi\left(x,[B]_\sim\right) = \left[W(x)\begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & B \\ 0 & \end{pmatrix}\right]_\sim =$$

$$\left[W(x)\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & e^{i\eta} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & e^{-\frac{i\eta}{n-2}}V & \\ 0 & 0 & & & \end{pmatrix}\right.$$

$$\left.\begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & A \\ 0 & \end{pmatrix}\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & e^{-i\eta} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & e^{\frac{i\eta}{n-2}}V^\dagger & \\ 0 & 0 & & & \end{pmatrix}\right]_\sim .$$

By writing

$$\begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ 0 & e^{i\eta} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & e^{-\frac{i\eta}{n-2}}V & \\ 0 & 0 & & & \end{pmatrix} =$$

$$\begin{pmatrix} e^{i\eta} & 0 & 0 & \cdots & 0 \\ 0 & e^{i\eta} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & e^{-\frac{i\eta}{n-2}}V & \\ 0 & 0 & & & \end{pmatrix}\begin{pmatrix} e^{-i\eta} & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix},$$

we get

$$\Psi\left(x,[B]_\sim\right) = \left[\begin{pmatrix} e^{i\eta} & 0 & 0 & \cdots & 0 \\ 0 & e^{i\eta} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & e^{-\frac{i\eta}{n-2}}V & \\ 0 & 0 & & & \end{pmatrix}\right.$$

$$\left.W(x)\begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & A \\ 0 & \end{pmatrix}\begin{pmatrix} e^{-i\eta} & 0 & 0 & \cdots & 0 \\ 0 & e^{-i\eta} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & e^{\frac{i\eta}{n-2}}V^\dagger & \\ 0 & 0 & & & \end{pmatrix}\right]_\sim$$

and multiplying inside by $1 = e^{\frac{i\eta}{n}}e^{\frac{-i\eta}{n}}$ so that the matrices on the left and right above are in $SU(n)$ yields that the above equals:

$$\left[\begin{pmatrix} x & \sqrt{1-|x|^2} & 0 & \cdots & 0 \\ -\sqrt{1-|x|^2} & x^* & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix}\begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & A \\ 0 & \end{pmatrix}\right]_\sim$$

$$= \Psi\left(x,[A]_\sim\right)$$

ii) Ψ is one-to-one: Assume, by way of contradiction, that Ψ is not one-to-one. Then there exist $x_1,\ x_2 \in \bar{D}_1$, $A_1,\ A_2 \in SU(n-1)$ and scalar ϕ and matrix $V \in SU(n-1)$ such that:

$$W(x_1)\begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & A_1 \\ 0 & \end{pmatrix} = \tag{A.1}$$

$$\begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-\frac{i\phi}{n-1}}V \end{pmatrix} W(x_2)\begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & A_2 \\ 0 & \end{pmatrix}\begin{pmatrix} e^{-i\phi} & 0 \\ 0 & e^{\frac{i\phi}{n-1}}V^\dagger \end{pmatrix}$$

By taking $x_1,\ x_2$ in $\bar{D}_1$, we can consider both cases E_n and $D_1 \times SU(n-1)/_\sim$ at the same time. Denote by v_{jk} the (j,k) element of V. By comparing the first column of the left hand side and the right hand side above, we have:

$$\begin{pmatrix} x_1 \\ -\sqrt{1-|x_1|^2} \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \begin{pmatrix} x_2 \\ -e^{-i\frac{n\phi}{n-1}}\sqrt{1-|x_2|^2}v_{11} \\ -e^{-i\frac{n\phi}{n-1}}\sqrt{1-|x_2|^2}v_{21} \\ \vdots \\ -e^{-i\frac{n\phi}{n-1}}\sqrt{1-|x_2|^2}v_{n-1,1} \end{pmatrix} \tag{A.2}$$

Thus necessarily $x_1 = x_2 := x$. This means that the pre-images are either both in E_n or both in $D_1 \times SU(n-1)/_\sim$.

Let us first assume that they are both in E_n, i.e. $|x| = 1$, so $x = e^{i\eta}$. It is easy to see that we can rewrite the left hand side in (A.1) as:

$$\begin{pmatrix} e^{i\eta} & 0 & 0 & \cdots & 0 \\ 0 & e^{-i\eta} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix}\begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & A_1 \\ 0 & \end{pmatrix} = \begin{pmatrix} e^{i\eta} & 0\cdots 0 \\ 0 & \\ \vdots & M \\ 0 & \end{pmatrix}, \tag{A.3}$$

with, using (A.1)

$$M = V\begin{pmatrix} e^{-i\eta} & 0\cdots 0 \\ 0 & \\ \vdots & I \\ 0 & \end{pmatrix} A_2 V^\dagger.$$

So we get $[A_1]_{\sim_{-\eta}} = [A_2]_{\sim_{-\eta}}$.

Consider now the case with preimage in $D_1 \times SU(n-1)/_\sim$, so $|x| < 1$. This implies that $\sqrt{1-|x|^2} \neq 0$. Thus, by using equation (A.2), we get that $v_{j1} = 0$ for $j = 2,\cdots,n-1$. Moreover, we must have: $e^{-i\frac{n\phi}{n-1}}v_{11} = 1$. Thus the matrix $\begin{pmatrix} e^{i\phi} & 0 \\ 0 & e^{-\frac{i\phi}{n-1}}V \end{pmatrix}$ in (A.1) is of the form:

$$\begin{pmatrix} e^{i\phi} & 0 & 0 & \cdots & 0 \\ 0 & e^{-\frac{i\phi}{n-1}}v_{11} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & \tilde{V} & \\ 0 & 0 & & & \end{pmatrix} = \begin{pmatrix} e^{i\phi} & 0 & 0 & \cdots & 0 \\ 0 & e^{i\phi} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & \tilde{V} & \\ 0 & 0 & & & \end{pmatrix}.$$

Since this matrix commutes with $W(x_2)$ using equation (A.1), we get:

$$A_1 = \begin{pmatrix} e^{i\phi} & 0\cdots 0 \\ 0 & \\ \vdots & \tilde{V} \\ 0 & \end{pmatrix} A_2 \begin{pmatrix} e^{-i\phi} & 0\cdots 0 \\ 0 & \\ \vdots & \tilde{V}^\dagger \\ 0 & \end{pmatrix},$$

for $\tilde{V} \in U(n-2)\times U(1)$, so $[A_1]_\sim = [A_2]_\sim$, where the equivalence is in the space of $(n-1)\times(n-1)$ matrices.

iii) Ψ is continuous with continuous inverse: It suffices to prove that Ψ is a continuous bijection from a compact space to a Hausdorff space, as any continuous bijection from a compact space to a Hausdorff space is a homeomorphism. Parts (ii) and (iii) above take care of the bijection part. $E_n \cup (D_1 \times SU(n-1)/_\sim)$ is compact because E_n is compact as it is a fiber bundle over a compact space with compact fibers; gluing this to the boundary of D_1 means that $D_1 \cup E_n \equiv \bar{D}_1 \cup E_n$ is compact, and $SU(n-1)/_\sim$ is compact as it is the continuous image of the compact space $SU(n-1)$. $SU(n)/_\sim$ is Hausdorff, as it is a stratified space [9].

So it remains to prove that Ψ is continuous. Observe that $\Psi \circ \pi = q \circ \hat{\Psi}$, where $\pi : (U(1)\times SU(n-1)) \cup (D_1 \times SU(n-1)) \to E_n \cup D_1 \times SU(n-1)/_\sim$ is the quotient map which sends $(e^{i\phi}, A) \in U(1)\times SU(n-1)$ to $[A]_\phi \in E_n$ and $(x, A) \in D_1 \times SU(n-1)$ to $(x, [A]_\sim) \in D_1 \times SU(n-1)/_\sim$; $q : SU(n) \to SU(n)/_\sim$ is the quotient map; and $\hat{\Psi}$ is defined as follows:if $(e^{i\phi}, A) \in U(1)\times SU(n-1)$ then

$$\hat{\Psi}\left((e^{i\phi}, A)\right) = \begin{pmatrix} e^{-i\phi} & 0 & 0 & \cdots & 0 \\ 0 & e^{i\phi} & 0 & \cdots & 0 \\ 0 & 0 & & & \\ \vdots & \vdots & & I & \\ 0 & 0 & & & \end{pmatrix} \begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & A \\ 0 & \end{pmatrix};$$

if $(x, A) \in D_1 \times SU(n-1)$ then

$$\hat{\Psi}(x, A) = W(x) \begin{pmatrix} 1 & 0\cdots 0 \\ 0 & \\ \vdots & A \\ 0 & \end{pmatrix}.$$

Both q and $\hat{\Psi}$ are continuous, and since π is a quotient map, it is open and surjective. From this, continuity of Ψ follows.

APPENDIX B
PROOF OF PROPOSITION V.5

We first fix $r = \hat{c} + q$, $q = 0, 1, 2, ..., \hat{d} - \hat{c}$ and maximize the function $F = F(l, r)$ over $l \in [\hat{a}, \hat{b}]$. By comparing the values of $F(\hat{a}, r)$ and $F(\hat{b}, r)$ with F in (42), we find that the maximum is achieved at $\hat{b}$ if and only if $\hat{a} = \hat{b}$ or, by writing $k := 6j + h$, $j \geq 0$, $h = 0, 1, 2, 3, 4, 5$,

$$\begin{aligned} &\mathbf{SI}\left(-\tfrac{h}{3} - \hat{\beta}\right) + 2\mathbf{SI}\left(-\tfrac{h}{3} - \hat{\alpha}\right) + q \\ &\geq \left(-\hat{\beta} - \tfrac{h}{3}\right) + 2\left(-\tfrac{h}{3} - \hat{\alpha}\right) + 1. \end{aligned} \tag{B.1}$$

This is independent of s and j and always verified when $q \geq 1$.

Proof of (B.1): If $\hat{b} > \hat{a}$, $r = \hat{c} + q$, $F(r, \hat{b}) \geq F(r, \hat{a})$ if and only if $\hat{c} + q \geq -\hat{\beta} - 2\hat{\alpha} - (\hat{a} + \hat{b})$. With the values of $\hat{a}$, $\hat{b}$ and $\hat{c}$ in (47) (48), this latest condition becomes

$$\begin{aligned} &\mathbf{SI}\left(\tfrac{k}{6} - s - \hat{\beta}\right) + q \geq \\ &-\hat{\beta} - 2\hat{\alpha} - \left(\mathbf{SI}\left(-\tfrac{k}{3} - \hat{\alpha}\right) + \mathbf{LI}\left(\tfrac{k}{6} + s - \hat{\alpha}\right)\right). \end{aligned} \tag{B.2}$$

Define Δ_k to be equal to $\frac{1}{2}$ if k is odd and equal to zero if k is even. With this definition formula (B.2) becomes

$$\begin{aligned} &\mathbf{SI}\left(\tfrac{k}{6} + \Delta_k - \hat{\beta}\right) + q \geq \\ &-\hat{\beta} - 2\hat{\alpha} - \left(\mathbf{SI}\left(-\tfrac{k}{3} - \hat{\alpha}\right) + \mathbf{LI}\left(\tfrac{k}{6} - \Delta_k - \hat{\alpha}\right)\right), \end{aligned} \tag{B.3}$$

which is independent of s. Defining $k := 6j + h$, $h = 0, 1, ..., 5$, this becomes

$$\begin{aligned} &\mathbf{SI}\left(\tfrac{h}{6} + \Delta_k - \hat{\beta}\right) + q \geq \\ &-\hat{\beta} - 2\hat{\alpha} - \left(\mathbf{SI}\left(-\tfrac{h}{3} - \hat{\alpha}\right) + \mathbf{LI}\left(\tfrac{h}{6} - \Delta_k - \hat{\alpha}\right)\right), \end{aligned} \tag{B.4}$$

which is independent of j. To obtain (B.1), write the left hand side of (B.4) as $\Delta_k + \frac{h}{2} + \mathbf{SI}\left(-\frac{h}{3} - \hat{\beta}\right) + q$ and the right hand side as $-\hat{\beta} - 2\hat{\alpha} - \left(\mathbf{SI}\left(-\frac{h}{3} - \hat{\alpha}\right) - \Delta_k - \frac{h}{2} + \mathbf{LI}\left(\frac{2h}{3} - \hat{\alpha}\right)\right)$ so that inequality (B.4) becomes

$$\begin{aligned} &\mathbf{SI}\left(-\tfrac{h}{3} - \hat{\beta}\right) + q \geq \\ &-\hat{\beta} - 2\hat{\alpha} - \left(\mathbf{SI}\left(-\tfrac{h}{3} - \hat{\alpha}\right) + \mathbf{LI}\left(\tfrac{2h}{3} - \hat{\alpha}\right)\right) = \\ &-\hat{\beta} - 2\hat{\alpha} - \left(\mathbf{SI}\left(-\tfrac{h}{3} - \hat{\alpha}\right) + h + \mathbf{LI}\left(-\tfrac{h}{3} - \hat{\alpha}\right)\right) = \\ &-\hat{\beta} - 2\hat{\alpha} - 2\mathbf{SI}\left(-\tfrac{h}{3} - \hat{\alpha}\right) + 1 - h, \end{aligned}$$

where we used Lemma V.4. This gives (B.1). □

By verifying (B.1) for $h = 0, 1, ..., 5$, we find the following result.

Lemma B.1. *Assume $\hat{\alpha} > 0$. The maximum of $F(r, l)$ as a function of l on $[\hat{a}, \hat{b}]$ is at $\hat{b}$ independently of $r \in [\hat{c}, \hat{d}]$ and the value of k, since (B.1) is always verified. If $\hat{\alpha} < 0$, the maximum is achieved at $\hat{b}$ for each value of r and each value of $k = 6j + h$ except for the cases $h = 1$ and $h = 4$. In these cases $\hat{b} \neq \hat{a}$ since $k \neq 0$ and (B.1) is not verified and the maximum is at $l = \hat{a}$ for $r = \hat{c}$ and at $l = \hat{b}$ for $r \neq \hat{c}$.*

We now study $F = F(l, r)$ as a function of r. Assume first $\hat{\alpha} > 0$ or $\hat{\alpha} < 0$ but $h \neq 1, 4$. Then according to Lemma B.1 we first study $F(\hat{b}, r)$ for r in the interval $[\hat{c}, \hat{d}]$. The maximum is achieved at $\hat{c}$ if and only if $F(\hat{b}, \hat{c}) \geq F(\hat{b}, \hat{d})$, which, using (49), is true if and only if $\hat{c} = \hat{d}$ or $\hat{c} + \hat{d} \leq \hat{\alpha} - \hat{b}$. The latter with the expressions for $\hat{b}$, $\hat{c}$ and $\hat{d}$ in (47) (48), with $\hat{\beta} = -\hat{\alpha}$ and using $k = 6j + h$ becomes:

$$\mathbf{SI}\left(\frac{h}{6} + \Delta_k + \hat{\alpha}\right) + \mathbf{LI}\left(-\frac{h}{3} + \hat{\alpha}\right) \leq \hat{\alpha} - \mathbf{LI}\left(\frac{h}{6} - \Delta_k - \hat{\alpha}\right). \tag{B.5}$$

Direct verification shows that (B.5) is always verified if $\hat{\alpha} > 0$, and thus the maximum is at $F(\hat{b}, \hat{c})$. It is also verified for $\hat{\alpha} < 0$ unless $h = 2$ or $h = 5$, which give the maximum at $F(\hat{b}, \hat{d})$. Consider $h = 1$, $h = 4$ and $\hat{\alpha} < 0$. We have two subcases:

1) $\hat{c} = \hat{d}$ which occurs if and only if $s = \frac{k}{2} + 1$ from Lemma C.1. [6] In this case, the maximum is at $F(\hat{a}, \hat{c}) = F(\hat{a}, \hat{d})$.

[6] Recall we are assuming $k \geq 0$. Therefore the second condition of the Lemma is automatically verified.

2) $s > \frac{k}{2}+1$ and therefore $\hat{d} > \hat{c}$. Then we have to compare $F(\hat{a},\hat{c})$ and $F(\hat{b},\hat{d})$. We calculate the values of $\hat{a}$, $\hat{b}$, $\hat{c}$ and $\hat{d}$ from (47) (48) in this case for $k=6j+1$ and $k=6j+4$ (recall that $j \geq 0$), we obtain: For $h=1$, $\hat{a}=-2j$, $\hat{b}=j+s-\frac{1}{2}$, $\hat{c}=j-s+\frac{1}{2}$, $\hat{d}=-2j-1$. For $h=4$, $\hat{a}=-2j-1$, $\hat{b}=j+s$, $\hat{c}=j-s+1$, $\hat{d}=-2j-2$. We have for $h=1$, $F(\hat{a},\hat{c}) = -\hat{\alpha}^2+\hat{\alpha}(-3j+s-\frac{1}{2})+3j^2+s^2+\frac{1}{4}-s$, $F(\hat{b},\hat{d}) = -\hat{\alpha}^2++\hat{\alpha}(3j+s+\frac{1}{2})+3j^2+3j+s^2+\frac{7}{4}-2s$. By comparison we have that $F(\hat{a},\hat{c}) \geq F(\hat{b},\hat{d})$ if and only if $s \geq 3j+\frac{3}{2}+\hat{\alpha}(6j+1)$, which is indeed true since (using $s \geq \frac{k}{2}+1$) $s \geq 3j+\frac{3}{2}$ and $\hat{\alpha}<0$. For $h=4$, $F(\hat{a},\hat{c}) = -\hat{\alpha}^2+\hat{\alpha}(-3j+s-2)+3j^2+3j+1+s^2-s$, $F(\hat{b},\hat{d}) = -\hat{\alpha}^2+\hat{\alpha}(3j+s+2)+3j^2+s^2+6j+4-2s$. By comparison we have that $F(\hat{a},\hat{c}) \geq F(\hat{b},\hat{d})$ if and only if $s \geq 3j+3+\hat{\alpha}(6j+4)$, which is indeed true since (using $s \geq \frac{k}{2}+1$) $s \geq 3j+3$ and $\hat{\alpha}<0$. Therefore in this case also we have that the maximum is achieved at $F(\hat{a},\hat{c})$.

Appendix C
The box (47) (48) is not empty

Lemma C.1. Assume $\hat{\alpha}$ and $\hat{\beta} \neq 0, \pm\frac{1}{3}$. In (47) $\hat{d} > \hat{c}$ unless $s=\frac{|k|}{2}+1$ and $k \geq 0$, in which case $\hat{c}=\hat{d}$. In (48) $\hat{b} > \hat{a}$ unless $s=\frac{|k|}{2}+1$ and $k \leq 0$, in which case $\hat{a}=\hat{b}$.

Proof. We prove the first statement since the proof for the second one is similar. Using $s \geq \frac{|k|}{2}+1$, we have for $\hat{c}$ in (47) $\hat{c} = \mathbf{SI}\left(\frac{k}{6}-s-\hat{\beta}\right) \leq \mathbf{SI}\left(\frac{k}{6}-\frac{|k|}{2}-1-\hat{\beta}\right) = -1+\mathbf{SI}\left(\frac{k}{6}-\frac{|k|}{2}-\hat{\beta}\right)$, with equality if and only if $s=\frac{|k|}{2}+1$. If $k<0$ the last term is $-1+\mathbf{SI}(\frac{2}{3}k-\hat{\beta}) = -1+k+\mathbf{SI}(-\frac{k}{3}-\hat{\beta}) = k+\mathbf{LI}(-\frac{k}{3}-\hat{\beta}) < \mathbf{LI}(-\frac{k}{3}-\hat{\beta}) = \hat{d}$. However if $k \geq 0$, the last term is $-1+\mathbf{SI}(-\frac{k}{3}-\hat{\beta}) = \mathbf{LI}(-\frac{k}{3}-\hat{\beta}) = \hat{d}$. ☐

Appendix D
Case $\hat{\alpha} < 0$ (Proof of Lemma V.7)

Set $k=6j+h$, with $h=0,1,2,3,4,5$ and use (47) (48).
1) $\mathbf{h=0}$, ($\hat{b}=j+s$, $\hat{c}=j-s$, $j \geq 0$, $s \geq 3j+1$)

$$\begin{gathered} T^2 \geq 3j^2+s^2-F(\hat{b},\hat{c}) = -\hat{\alpha}^2-2\hat{\alpha} \\ \geq -\hat{\alpha}^2-2\hat{\alpha}j(3j+1) \geq -\hat{\alpha}^2-2\hat{\alpha}. \end{gathered}$$

Here we used first $s \geq 3j+1$ and then $j \geq 0$. The minimum $\hat{T}^2_{-,0} = -\hat{\alpha}^2-2\hat{\alpha}$ is achieved for $j=0$ and $s=1$.
2) $\mathbf{h=1}$, ($\hat{a}=-2j$, $\hat{c}=j-s+\frac{1}{2}$)

$$\begin{gathered} T^2 \geq 3j^2+j+\frac{1}{12}+s^2-F(\hat{a},\hat{c}) = \\ -\hat{\alpha}^2-\frac{1}{6}+(1-\hat{\alpha})s+(1+3\hat{\alpha})j+\frac{\hat{\alpha}}{2} \\ \geq -\hat{\alpha}^2-\hat{\alpha}+\frac{4}{3}+3j \geq -\hat{\alpha}^2-\hat{\alpha}+\frac{4}{3}. \end{gathered}$$

Here we used first $s \geq 3j+1$ and then $j \geq 0$. The minimum is $\hat{T}^2_{-,1} = \frac{4}{3}-\hat{\alpha}-\hat{\alpha}^2$ is achieved for $j=0$ and $s=3j+\frac{3}{2}$.
3) $\mathbf{h=2}$, ($\hat{b}=j+s$, $\hat{d}=-2j-1$)

$$\begin{gathered} T^2 \geq 3j^2+2j+\frac{1}{3}+s^2-F(\hat{b},\hat{d}) = \\ -(1+3\hat{\alpha})j-\frac{2}{3}-\hat{\alpha}-\hat{\alpha}^2+(1-\hat{\alpha})s \\ \geq (2-6\hat{\alpha})j+\frac{4}{3}-3\hat{\alpha}-\hat{\alpha}^2 \geq \frac{4}{3}-3\hat{\alpha}-\hat{\alpha}^2. \end{gathered}$$

Here we first used we used $s \geq 3j+2$ and then we used $j \geq 0$. The minimum $\hat{T}^2_{-,2} = \frac{4}{3}-3\hat{\alpha}-\hat{\alpha}^2$ is achieved for $j=0$ and $s=3j+2$.
4) $\mathbf{h=3}$, ($\hat{b}=j+s+\frac{1}{2}$, $\hat{c}=j-s+\frac{1}{2}$)

$$\begin{gathered} T^2 \geq 3j^2+3j+\frac{3}{4}+s^2-F(\hat{b},\hat{c}) = -\hat{\alpha}^2-2\hat{\alpha}s \\ \geq -\hat{\alpha}^2-6\hat{\alpha}j-5\hat{\alpha} \geq -\hat{\alpha}^2-5\hat{\alpha} \end{gathered}$$

We first used $s \geq 3j+\frac{5}{2}$ and then $j \geq 0$. The minimum $\hat{T}^2_{-,3} = -\hat{\alpha}^2-5\hat{\alpha}$ is achieved for $j=0$ and $s=\frac{5}{2}$.
5) $\mathbf{h=4}$, ($\hat{a}=-2j-1$, $\hat{c}=j-s+1$)

$$\begin{gathered} T^2 \geq 3j^2+4j+\frac{4}{3}+s^2-F(\hat{a},\hat{c}) = \\ (1+3\hat{\alpha})j+(1-\hat{\alpha})s+2\hat{\alpha}+\frac{1}{3}-\hat{\alpha}^2 \\ \geq 4j-\hat{\alpha}+\frac{10}{3}-\hat{\alpha}^2 \geq \frac{10}{3}-\hat{\alpha}-\hat{\alpha}^2. \end{gathered}$$

We first used $s \geq 3j+3$. and then $j \geq 0$. The minimum $\hat{T}^2_{-,4} = \frac{10}{3}-\hat{\alpha}-\hat{\alpha}^2$ is achieved for $j=0$ and $s=3$.
6) $\mathbf{h=5}$, ($\hat{b}=j+s+\frac{1}{2}$, $\hat{d}=-2j-2$)

$$\begin{gathered} T^2 \geq 3j^2+5j+\frac{25}{12}+s^2-F(\hat{b},\hat{d}) = \\ -\frac{7}{6}+(3-3\hat{\alpha})j-\hat{\alpha}^2+(1-\hat{\alpha})s-\frac{5}{2}\hat{\alpha}. \\ \geq (6-6\hat{\alpha})j-\hat{\alpha}^2-6\hat{\alpha}+\frac{7}{3} \geq \frac{7}{3}-\hat{\alpha}^2-6\hat{\alpha} \end{gathered}$$

We first used $s \geq 3j+\frac{7}{2}$ and then $j \geq 0$. The minimum $\hat{T}^2_{-,5} = \frac{7}{3}-6\hat{\alpha}-\hat{\alpha}^2$ is achieved for $j=0$ and $s=\frac{7}{2}$. By comparison of the functions $\hat{T}^2_{-,w} = T^2_{-,w}(\hat{\alpha})$, for $w=0,1,...,5$, we obtain Lemma V.7.

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