Quantum control by decompositions of SU(2)

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Constructive procedures that make no use of optimization or iterative calculations for the control of many quantum and classical systems, via controls that are required to satisfy constraints on their power or pulse area, are presented. These procedures are based on structured decompositions of SU(2). A general technique for obtaining such structured decompositions is given. Illustrative examples are provided.

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I. INTRODUCTION

This paper is concerned with representing *constructively* and *exactly* (i.e., without approximations) any SU(2) matrix S as a product

$$S=\Pi_{k=1}^{Q} e^{a_k A + b_k B} \tag{1.1}$$

with (i) **O1**: $a_k>0$ and (ii) **O2**: $|b_k|\leqslant C$ for an *a priori* prescribed bound C. Here SU(2) is the group of 2×2 unitary matrices with determinant one, and A and B are linearly independent elements of su(2)—the set of 2×2 anti-Hermitian matrices with zero trace. Constructive methods will be used to obtain factorizations that simultaneously satisfy the constraints **O1** and **O2**. The number Q depends on the matrix S. Several problems in the control of quantum and classical systems motivate this question. Examples are

(1) Control of two-level systems with piecewise constant controls for applications to spin systems, molecular control, spectroscopy, and quantum information processing, [1–10]. In this case, a_k is the time a control pulse is applied for and b_k is the time multiplied by the amplitude of the kth pulse (i.e., the pulse area).

(2) Control of *two-level and N-level* systems via *sinusoidal* controls in conjunction with approximations such as averaging or the rotating wave approximation [11]. In these cases, the a_k, b_k are related to constants such as the average and duration or pulse area and phase of the pulse. (See Example 4 in Sec. IV.)

(3) Control of various classical mechanical systems such as satellites, switched electrical networks, underwater vehicles etc., [12–16].

Usually, Eq. (1.1) arises from controlling a quantum system, whose unitary generator obeys:

$$i\hbar\dot{U}(t)=H_0 U+H_e U u(t), \quad U(0)=I_2,$$

where H_0 and $H_e u(t)$ are the internal and external Hamiltonians, respectively. U is the unitary generator that is assumed to evolve on SU(2), and $u(t)$ is a scalar perturbing control field, treated classically, which is to be designed. Setting $\hbar=1$, $A=-iH_0$, and $B=-iH_e$ in the previous equation leads to

$$\dot{U}(t)=AU(t)+BU(t)u(t), \quad U(0)=I_2. \tag{1.2}$$

Briefly speaking, the right-hand side of the factorization (1.1) is nothing but the unitary generator of the system (1.2) after $a_1+\cdots+a_Q$ units of time. Thus, **O1** arises because $a_1,\ldots,a_k$ are the times for which a constant control is applied to Eq. (1.2) and hence, have to be positive. **O2** is motivated by theoretical and practical limitations such as an upper bound on the power/pulse area of a field. Indeed, in this setting, it holds that b_k is the product of the amplitude of the kth and the duration of the kth pulse, which justifies the appellation ''pulse area'' for the b_k. (See Example 1 in Sec. IV.) Thus the principal question being addressed in the paper is the generation of an arbitrary unitary transformation via control pulses, which are subject to constraints. A further discussion of these motivating examples is postponed to Sec. VI.

The aim is to produce a prescribed unitary generator and not merely a desired state. Furthermore, once the system (1.2) has been given (either exactly or via approximations), our results are exact and make no use of approximate arguments such as the linearization of a set of nonlinear equations or optimization techniques, as in Ref. [17]. *In fact, the results here are computationally attractive alternatives to optimization based approaches to control.*

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To achieve **O1** and **O2** for a given pair A, B, the basic idea is to map a pair $\hat{A},\hat{B}$, for which these two objectives are easier to establish, onto A,B via a Lie algebra isomorphism ψ. By varying the pairs, $\hat{A},\hat{B}$, different decompositions for achieving **O1** and **O2** can be arrived at. Therefore, calculations are first presented for two specific pairs, viz., $\hat{A}=i\sigma_y$, $\hat{B}=i\sigma_x$ and $\hat{A}=i\sigma_z$, $\hat{B}=i\sigma_y$. (See Secs. III A and III B.) Here, the σ's are the Pauli matrices. A comparison of the two cases appears in Sec. III C. The requirement that ψ be a Lie algebra isomorphism forces that A and B be orthogonal. This orthogonality can be attained by applying a preliminary control transformation. However, for many cases (such as those arising in switched electrical networks), taking $\hat{A}=i\sigma_y$, $\hat{B}=i\sigma_x$ allows us to omit this control transformation. (See Remark 3.4.)

It is assumed that there is only one external control operative at any given time and more importantly that the A matrix that represents the unperturbed Hamiltonian of the system is not multiplied by an external control term. In control theoretic language the A matrix is a drift term. The presence of a drift term significantly complicates achieving **O1** and **O2**, [12] and thus this paper represents a significant step forward in dealing with such systems. *The approach taken in this paper is to suitably modify Euler-like decompositions according to the objective.*

The balance of this paper is organized as follows. In the next section preliminary facts about control theory and the group SU(2) are presented. In particular, the distinction between driftless systems and systems with drift is further clarified. Section II A contains useful terminology. Section II B contains two preliminary decompositions, **R1** and **R2**, of SU(2), which are the *starting points* for the factorizations obtained in the present paper. Section III is devoted to the achieving **O1** and **O2**. Sections III A and III B address the $(i\sigma_y,i\sigma_x)$ pair and the $(i\sigma_z,i\sigma_y)$ pair, respectively. Section III C develops a unified approach for meeting **O1** and **O2** for arbitrary su(2) matrices A and B. Results for the group of rotations, SO(3), are presented in Sec. III D. The Sec. IV further elaborates on the motivating examples mentioned in the introduction. The Sec. V contains conclusions and suggests some future work.

II. PRELIMINARIES ON CONTROL THEORY AND SU(2)

The system introduced in the first section, system (1.2), is a system with ''drift'' evolving on SU(2). The word drift stems from the fact that the system continues to evolve even when the control term $u(t)$ is switched off. In keeping with this, the coefficients a_k will be called the drift coefficients. Such systems are in contrast to driftless systems. A relevant example of a driftless system associated with the system (1.2), is

$$\dot{U}=AUu_1(t)+BUu_2(t). \tag{2.1}$$

Here both $u_1(t)$ and $u_2(t)$ are external controls. Thus, Eq. (1.2) may be controlled via switching on and off only one ''perturbation'' whereas system (2.1) can be controlled by switching on and off two perturbations.

For both systems, Eqs. (1.2) and (2.1), existence results concerning **O1** and **O2** are known, [18–20]. *However, there is no constructive method for generating controls for Eq. (1.2).* The only general alternatives are to use optimal control techniques, which require substantial computation and intuition. There is an extensive literature on constructive generation of states for *driftless, classical* mechanical systems (see e.g., Refs. [13,21,22]). By way of illustration of the advantage of having no drift, note that for driftless systems evolving on SU(2), the objective **O1** can be met by decompositions $S=\Pi_{k=1}^{Q}e^{a_kA+b_kB}$, which do not ensure that $a_k>0$. However, for driftless systems this is not a hurdle because a nonpositive a_k can be viewed as a nonpositive control applied for a positive time.

For systems with drift on SU(2), such as Eq. (1.2), in contrast, no constructive results are available. In the controls literature there are some extensions to classical systems with drift as in Refs. [22,12,16,23]. In Ref. [16], systems evolving on SO(3) are considered in the context of the control of satellites. Single input systems with drift are also considered but this case has not been fully resolved. In particular, the idea of using periodicity to overcome the problem of drift, which seems to be the suggestion of Ref. [16], is incorrect. Let us explain this in the context of SU(2). Suppose a decomposition of the type of Eq. (1.1), *without* ensuring positive a_k's, is available. Call the matrix being exponentiated in the typical factor, $e^{(a_kA+b_kB)}$, as C_k. As $C_k\in$ su(2), we have $e^{C_kt}=e^{C_k(t+nP_k)}$ for some period P_k and all $n\in Z,t\in R$. So, $e^{C_k}=e^{C_k(1+nP_k)}$. Thus, for some n, the coefficient of A, namely, $a_k(1+nP_k)$, will hopefully be positive. Clearly this argument is flawed on two grounds: (i) if $a_k=0$ then for no n will $a_k(1+nP_k)$ be positive and (ii) even when $a_k\neq 0$ this is not desirable, since correspondingly, $b_k(1+nP_k)$ becomes large, which will typically invalidate neglecting higher levels and processes in the basic model.

A. Some terminology

Next some terminology, used throughout this paper, will be clarified. Consider the decomposition (1.1) and, in terms of it, the following definitions:

(1) If an index k is such that $b_k=0$ then the corresponding factor is called *free evolution*. Otherwise, the corresponding factor is called a *control pulse*.

(2) a_k is called the *drift coefficient* of the kth factor.

(3) $|b_k/a_k|$ is called the *amplitude* of the kth factor.

(4) $|b_k|$ is called the *pulse area* of the kth factor. Note that the pulse area of a free evolution factor is zero.

(5) The quantity $\lambda_k=\sqrt{a_k^2+b_k^2}$ is called the *radial coordinate* of the kth factor.

B. Useful SU(2) facts

The Pauli matrices will be denoted as

$$\sigma_x=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \sigma_y=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \text{and}\quad \sigma_z=\begin{pmatrix}1&0\\0&-1\end{pmatrix}.$$

The following exponential formula is used tacitly used throughout this paper [9,24]:

$$\exp\{i[\alpha(t)\sigma_z+\beta(t)\sigma_y+\delta(t)\sigma_z]\}$$

$$=\cos[\sqrt{\lambda(t)}]I_2+i\frac{1}{\sqrt{\lambda(t)}}\sin[\sqrt{\lambda(t)}]$$

$$\times[\alpha(t)\sigma_x+\beta(t)\sigma_y+\delta(t)\sigma_z]$$

where

$$\lambda(t)=[\alpha(t)^2+\beta(t)^2+\delta(t)^2], \tag{2.2}$$

Next some representations of matrices in SU(2) are considered. The first is the Cayley-Klein parametrization:

$$S=S(\alpha,\zeta,u)=\begin{pmatrix} e^{i\zeta}\cos\alpha & e^{i\mu}\sin\alpha \\ e^{i(\pi-\mu)}\sin\alpha & e^{-i\zeta}\cos\alpha \end{pmatrix}, \tag{2.3}$$

where α, ζ, μ are the Cayley-Klein parameters of S. Since this parametrization is nothing but the entries of S written in polar form, it is clear that ζ and μ may be taken to be in $[0,2\pi)$ and α to be in $[0,\pi/2]$ (this is because $\cos\alpha$ and $\sin\alpha$, being the radial coordinates of S's entries, are non-negative.) This representation yields the following two representations of SU(2) matrices, which will be the *starting points* for the results of Sec. III.

(1) **R1**: $S=e^{id\sigma_z}e^{ie\sigma_x}e^{if\sigma_z}$. The real numbers d, e, f are related to the Cayley-Klein parameters (2.5) by

$$d=\frac{\zeta+\mu}{2}-\frac{\pi}{4};\quad e=\alpha;\quad f=\frac{\zeta-\mu}{2}+\frac{\pi}{4}.$$

(2) **R2**: $S=\Pi_{k=1}^{3}\exp[i(-\mathrm{Im}\,\gamma_k\sigma_y+\mathrm{Re}\,\gamma_k\sigma_x)]$, for appropriate $\gamma_k\in C$, $k=1,2,3$. This representation plays an important role in the generation of arbitrary unitary transformations in a N-level atom/molecule [11]. Related products involving σ_x and σ_y arise in cavity QED studies [25]. *The steps intervening in the derivation play an important role in the sequel*. So the derivation from Ref. [11] will be briefly recalled. To that end, write each factor in the decomposition as $V(\gamma_k)$, where

$$V(\gamma_k)=\exp\begin{pmatrix} 0 & i\gamma_k \\ i\tilde{\gamma}_k & 0 \end{pmatrix}.$$

It can be shown that [11]:

$$S(\alpha,\zeta,\mu)=V(\gamma_1)e^{i\zeta\sigma_a},$$

where

$$\gamma_1=\alpha e^{i(\zeta+\mu-\pi/2)}. \tag{2.4}$$

The key step is the following equation which holds for any $L\in R$:

$$e^{iL\sigma_a}=V(\hat{\gamma}_2)V(\hat{\gamma}_3),$$

where

$$\hat{\gamma}_k=\frac{\pi}{2}e^{i\hat{\theta}_k},\quad k=2,3,$$

and

$$L=\hat{\theta}_2-\hat{\theta}_3+\pi. \tag{2.5}$$

Putting Eqs. (2.4) and (2.5) together we get the desired factorization:

$$S(\alpha,\zeta,\mu)=V(\gamma_1)V(\gamma_2)V(\gamma_3) \tag{2.6}$$

with the γ_k the same as $\hat{\gamma}_k$ in Eq. (2.5), when $L=\zeta$.

Thus, both **R1** and **R2** are related to the Cayley-Klein parameters, Eq. (2.3), via simple formulas, which require no more than elementary arithmetic operations and, thereby provide a clear relationship between the parameters of the factorization (1.1) and the entries of S.

Remark 2.1: Note that in **R1** each of the three factors involves only one of the two Pauli matrices in question. On the other hand, in **R2** the typical factor will require both the Pauli matrices σ_x and, σ_y and hence, typically the complex numbers γ_k, $k=1,\ldots,3$ in **R2** cannot be taken to be either *purely real or purely imaginary*.

III. MAIN RESULTS

The main results regarding **O1** and **O2** follow. For each case, **O1** will be first addressed, and the resulting factorization will be further modified to achieve **O2** *simultaneously*. In Sec. III A, results based on an intrinsic approach to the case $A=i\sigma_y$, $B=i\sigma_x$ are provided. One advantage of this intrinsic approach is that it immediately generalizes to the case $A=ia\sigma_x+ib\sigma_y$ and $B=ic\sigma_x+id\sigma_y$, ''without''the need for a preliminary orthogonalization (which would be needed if Algorithm **V** of the unified approach of Sec. III C was applied). Next, the case $A=i\sigma_z$ and $B=i\sigma_y$ is studied. Section III C, which addresses the general A,B case, also includes a comparison of the $(i\sigma_y,i\sigma_x)$ and $(i\sigma_z,i\sigma_y)$ pairs.

The common feature of the first two sections is that it suffices, for both **O1** and **O2**, to analyze the case when the target matrix is the exponential of the remaining Pauli matrix, i.e., the exponential of (essentially) the commutator of A and B. This is in keeping with the control theoretic perspective [19].

A. The case $A=i\sigma_y$, $B=i\sigma_x$

Let $A=i\sigma_y$ and $B=i\sigma_x$. The relevant starting points are decompositions of the form $S=\Pi_{i=1}^{Q}V(\gamma_k)$, where the matrix $V(\gamma)$ is

$$V(\gamma)=\exp\begin{pmatrix} 0 & i\gamma \\ i\overline{\gamma} & 0 \end{pmatrix}=\exp[(-\mathrm{Im}\,\gamma)i\sigma_y+(\mathrm{Re}\,\gamma)i\sigma_x].$$

Thus the drift coefficients are $-\mathrm{Im}(\gamma_k)$. Thus, if for the target S each of the a_k's are positive, *equivalently if each of the complex numbers γ_k lie in the open lower half-plane*, then **R2** [specifically Eq. (2.6)] of Sec. II C provides **O1**. However, if even one of the γ_k's does not belong to the

lower half-plane then more work is needed and our starting points will be Eqs. (2.4) and (2.5) of **R2**, Sec. II C. These equations will be analyzed further to achieve **O1**. For this analysis the following observation is very crucial:

Claim: To achieve **O1** *it suffices to consider the case when the target is of the form* $S=e^{iL\sigma_z}$ *for any real* L. Indeed, the following fact is true:

$$S(\alpha,\zeta,\mu)=e^{ip\sigma_x}S(\alpha,\zeta-p,\mu-p) \tag{3.1}$$

for any $p\in R$. Equation (3.1) is proved by using Eq. (2.2).

Now, Eq. (2.4) applied to the matrix $S(\alpha,\zeta-p,\mu-p)$ yields

$$S(\alpha,\zeta-p,\mu-p)=V(\tilde{\gamma}_1)e^{i(\zeta-p)\sigma_x},$$

where

$$\tilde{\gamma}_1=\alpha e^{i(\zeta+\mu-2p-\pi/2)}, \tag{3.2}$$

This in turn gives

$$S(\alpha,\zeta,\mu)=e^{ip\sigma_x}V(\tilde{\gamma}_1)e^{i(\zeta-p)\sigma_x}. \tag{3.3}$$

By choosing p appropriately the angular coordinate of $\tilde{\gamma}_1$ *can be given any desired value, and in particular,* $V(\tilde{\gamma}_1)$ *can be chosen as a free evolution factor*, by taking p such that $\zeta+\mu-2p-\pi/2=3\pi/2$. So one needs to analyze only the terms $e^{ip\sigma_z}$ and $e^{i(\zeta-p)\sigma_z}$, but these are of the form $e^{iL\sigma_x}$, hence the claim.

Remark 3.1: Equation (3.3) contains, as special cases, the standard Euler factorizations [9]. This greater generality makes it versatile in other applications as well—such as factorizations into a product of $V(\gamma)$'s, with the γ's having their phases in a desired range. Remark 3.2 below also emphasizes this issue.

1. O1 for $A=i\sigma_y$, $B=i\sigma_x$

In accordance, with the paragraph above we consider the $S=e^{iL\sigma_x}$ case first.

O1 when $S=e^{iL\sigma_x}$*:* In representing $e^{iL\sigma_x}$ as $V(\hat{\gamma}_2)V(\hat{\gamma}_3)$ according to Eq. (2.5) of Sec. II B, the complex numbers $\hat{\gamma}_2$ and $\hat{\gamma}_3$ of Eq. (2.5) *may be chosen to lie in any open half of the complex plane*. Indeed, according to Eq. (2.5) the angular coordinates of $\hat{\gamma}_2$ and $\hat{\gamma}_3$ are related by $L=\hat{\theta}_2-\hat{\theta}_3+\pi$. Now L may be taken to be in $[0, 2\pi)$ and thus, $|L-\pi|\leqslant\pi$, with equality only if $L=0$. Since the exponential of $iL\sigma_x$ for $L=0$ is I_2, we may as well assume that $L\neq 0$. In this case, it follows that $|\hat{\theta}_2-\hat{\theta}_3|<\pi$, i.e., that $\hat{\gamma}_2$ and $\hat{\gamma}_3$ can be chosen to lie in the same open half-plane.

This leads to the following algorithm for **O1** for a general target $S(\alpha,\zeta,\mu)$.

(a) Algorithm I: O1, $A=i\sigma_y$, $B=i\sigma_x$. (1) Use Eq. (3.3) with $p=(\zeta+\mu)/2-\pi$ to write $S(\alpha,\zeta,\mu)$ as $e^{ip\sigma_x}V(-i\alpha)e^{i(\zeta-p)\sigma_x}$. Rewrite the angles p and $\zeta-p$ as angles in $[0,2\pi)$ if they are not already in that range.

(2) Prepare $e^{ip\sigma_x}$ as $V((\pi/2)e^{i\theta_1})V((\pi/2)e^{i\theta_2})$ with θ_1, $\theta_2\in(\pi,2\pi)$ by using the liberty afforded by Eq. (2.5). Likewise factor $e^{i(\zeta-p)\sigma_x}$ as $V((\pi/2)e^{i\theta_3})V((\pi/2)e^{i\theta_4})$ with θ_3, $\theta_4\in(\pi,2\pi)$.

(3) Prepare the middle term via a single free evolution factor.

(4) Thus Q is at most five (it could be less than five if any of these five factors is I_2). At least one of these five factors can be taken to be free evolution factors. The corresponding values for (a_k,b_k), $k=1,\ldots,5$ are displayed in Table II in Sec. III C.

2. Achieving O2 for $A=i\sigma_y$, $B=i\sigma_x$

The factorization yielding **O1** will now be refined to meet **O2**. Note that **O2** requires factoring a given SU(2) matrix S into a product of factors, each of the form $V(\gamma_k)$, with the scalars $\gamma_k=\lambda_k e^{i\theta_k}$'s lying in the lower half-plane and satisfying $\lambda_k|\cos(\theta_k)|\leqslant C$ for a given bound C. To achieve this proceed as follows.

First use Eq. (3.1) to write $S(\alpha,\zeta,\mu)=e^{ip\sigma_x}V(\hat{\gamma}_1)e^{i(\zeta-p)\sigma_x}$, as in Eq. (3.3). Once again choose p so that the factor $V(\hat{\gamma}_1)$ is free evolution, and thus the pulse area corresponding to this factor is *zero*. So all that is required is to be able to meet **O2** when the target matrix is of the form $e^{iL\sigma_x}$, for any $L\in R$. In writing $e^{iL\sigma_x}$ as the product $V((\pi/2)e^{i\hat{\theta}_2})V((\pi/2)e^{i\hat{\theta}_3})$, as per Eq. (2.5) of Sec. II B, choose the second of these factors to be free evolution, i.e., take $\hat{\theta}_3=3\pi/2$. This ensures that the pulse area of the factor $V(\hat{\gamma}_3)$ equals 0. Given a pulse area bound C, we can obtain a bound θ_C on the deviation of $\hat{\theta}_2$ from $3\pi/2$. In view of the equation,

$$L-\pi=\hat{\theta}_2-\hat{\theta}_3$$

the inequality $|3\pi/2-\theta_2|\leqslant\theta_C$ translates into:

$$|L-\pi|\leqslant\theta_C. \tag{3.4}$$

If L is not already of that form, then further factor $e^{iL\sigma_z}$ as $\Pi_{k=1}^{r}e^{iL_k\sigma_z}$ with each L_k satisfying the required inequality. This can always be achieved by rewriting $e^{iL\sigma_z}$ as $e^{i(L+2n\pi)\sigma_z}$ for some positive integer n, if need be. As a specific illustration of how this may be done consider the following, not necessarily optimal, recipe. Pick an even number $r=2n$ such that $L/2n\leqslant\theta_C$. Letting each L_k, $k=1,\ldots,r$ equal $\pi+L/2n$ does the job. Thus, by increasing the number of factors, if needed, one can ensure that the pulse area of any individual pulse does not exceed a prescribed bound.

(b) Algorithm II: O2; $A=i\sigma_y$, $B=i\sigma_x$. (1) Translate the bound $|b_k|\leqslant C$ into a bound θ_C on the deviation from $3(\pi/2)$, of the phases of the complex numbers, γ_k, representing the factors. Specifically choose, $\cos^{-1}(2C/\pi)$ in $[3\pi/2,2\pi)$. This is always achievable by reducing C if needed. Then take $\theta_C=\cos^{-1}(2C/\pi)-3\pi/2$.

(2) Use Eq. (3.3) with $p=(\zeta+\mu)/2-\pi$ to write $S(\alpha,\zeta,\mu)=e^{ip\sigma_x}V(-i\alpha)e^{i(\zeta-p)\sigma_x}$. Rewrite the angles p and $\zeta-p$ as angles in $[0, 2\pi)$ if they are not already in that range.

(3) Prepare the middle factor, $V(-i\alpha)$, via free evolution for α units of time. Recall $\alpha\in[0,\pi/2]$, and so α is always positive.

(4) Find the smallest natural number, n_1, so that $p/2n_1 \leqslant \theta_C$. Then rewrite $e^{ip\sigma_z}$ as $\Pi_{k=1}^{2n_1}\exp[i(\pi+p/2n_1)\sigma_z]$. Using Eq. (2.4) prepare each of these $2n_1$ factors as products $V(e(\pi/2)\theta_k)V(-i\pi/2)$ with $\theta_k=3\pi/2+p/2n_1$ for all k. Thus, θ_k is within θ_C of $3\pi/2$ and the pulse area corresponding to the $V(e(\pi/2)\theta_k)$ is bounded by C.

(5) Repeat Step 4 with p replaced by $\zeta-p$ and n_1 replaced by a corresponding n_2.

(6) This yields $Q\leqslant 2(2n_1+2n_2)+1$.

Remark 3.2: A,B Linear Combinations of $i\sigma_x$, $i\sigma_y$. The analysis of Sec. III A 1 showed that (i) by choosing p appropriately $\tilde{\gamma}_1$ can be allowed to have any desired angular coordinate; and that (ii) the complex numbers $\hat{\gamma}_2$ and $\hat{\gamma}_3$ can be located in any open-half plane (i.e., not necessarily the upper/lower, right/left open half-planes). Thus, this analysis can be extended verbatim to achieve **O1** when $A=i(a\sigma_x+b\sigma_y)$, $B=i(c\sigma_x+d\sigma_y)$, with (a,b) and (c,d) any linearly independent pair of vectors. Indeed, in this case **O1** would translate into an inequality of the form $\alpha(\mathrm{Re}\,\gamma)+\beta(\mathrm{Im}\,\gamma)>0$, where (α, β) is the first row of

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}^{-1}.$$

This is the same as requiring that all the γ's lie in a certain half-plane.

Similarly, **O2** can be translated into the phase of the γ's being located in a certain range. Now, virtually the same argument of Sec. III A 2 shows that any $S\in \mathrm{SU}(2)$ can be factored into a product, $\Pi_{i=1}^{Q}V(\gamma_k)$, with the γ_k's lying in a given open half-plane with their phases within θ_C of a prescribed angle ϕ in that half-plane. Indeed, the only difference is that $p\in R$ would now be chosen so that the angular coordinate of $\tilde{\gamma}_1$ in Eq. (3.3) is ϕ, and $\hat{\gamma}_2$ would likewise be chosen to have angular coordinate ϕ (cf., Remark 3.1). The balance of the argument is verbatim as in Sec. III A 2. Thus, the preliminary orthogonalization of Sec. III C can be avoided in these cases.

As an illustration, of how one (i) can do better than the conservative analysis presented for **O2**, and (ii) use a similar analysis for $A=i\sigma_x$, $B=i\sigma_y$ consider:

Example 3.1: Let $A=i\sigma_x$; $B=i\sigma_y$. Suppose the target state is the matrix $e^{i(\pi/2)\sigma_z}$ and the pulse area bound translates to a bound, $\theta_C=\pi/12$, on the deviation of the phases of the γ_k's from 0. Rewrite the target as $e^{i(13\pi)/2\sigma_z}$ and decompose the latter as $\Pi_{k=1}^{7}e^{iL_k\sigma_z}$, with $L_1=L_2=\cdots=L_5=165°$, $L_6=170°$, and $L_7=175°$. This achieves **O2**.

B. The case $A=i\sigma_z$; $B=i\sigma_y$

As in Sec. III A, the key is to show that the exponential of the remaining Pauli matrix, in this case $e^{iL\sigma_x}$, can be attained via controlled pulses. The following proposition achieves this. In this proposition the real number L is assumed to satisfy $\sin(L)\geqslant 0$, $\cos(L)\geqslant 0$, since this is the context in which it will be used to achieve **O1** for the pair at hand.

Proposition 3.1: Suppose $L\in R$ *satisfies* $\cos(L)>0$. *Then* $e^{iL\sigma_x}$ *can be written as the product of two factors* $\Pi_{k=1}^{2}e^{ia_k\sigma_z+ib_k\sigma_y}$, *where we may take* $a_k>0$, $k=1,2$ or $b_k>0$, $k=1,2$. *Furthermore, one of the factors may be taken to be free evolution if needed. If* $\cos(L)=0$, *then once again* $e^{iL\sigma_x}$ *can be written as the product of two factors* $\Pi_{k=1}^{2}e^{ia_k\sigma_z+ib_k\sigma_y}$ *with either* $a_k>0$ or $b_k>0$. *However, in this case, neither factor can be taken to be free evolution.*

Proof: Let $\lambda_k=\sqrt{a_k^2+b_k^2}$, $k=1,2$. Choose λ_k positive and satisfying $\cos(\lambda_k)=0$. Use Eq. (2.2) to evaluate $e^{ia_k\sigma_z+ib_k\sigma_y}$ and $e^{iL\sigma_x}$ and express the equation $e^{iL\sigma_x}=\Pi_{k=1}^{2}e^{ia_k\sigma_z+ib_k\sigma_y}$ in terms of equalities of the entries of the matrices in the equation. This gives a system of two equations (of the four equations that would normally result upon equating entries of the matrices on both sides, two equations are identical to the remaining two):

$$-\frac{a_1a_2+b_1b_2}{\lambda_1\lambda_2}\sin(\lambda_1)\sin(\lambda_2)=\cos(L),$$

$$-\frac{a_2b_1-a_1b_2}{\lambda_1\lambda_2}\sin(\lambda_1)\sin(\lambda_2)=\sin(L). \tag{3.5}$$

These equations may be solved as follows:

(1) $\cos(L)>0$. *Case:* Pick $\lambda_1=\pi/2$, $\lambda_2=3\pi/2$, and $b_2=0$. Then we have $a_1/\lambda_1=\cos(L)$; and $b_1/\lambda_1=\sin(L)$. So a_1 can indeed be chosen positive (thereby meeting **O1**). Also $b_1\geqslant 0$. Thus $e^{iL\sigma_x}$ can be prepared via a non-negative control since $\sin(L)\geqslant 0$.

(2) $\cos(L)=0$. *Case:* Pick $\lambda_1=\pi/2$ and $\lambda_2=\pi/2$. Since $\sin(\lambda_1)\sin(\lambda_2)=1$, the equations to solve become $(a_1a_2+b_1b_2)/\lambda_1\lambda_2=0$ and $(a_2b_1-a_1b_2)/\lambda_1\lambda_2=(-1)\sin(L)$. Note $\sin(L)=1$. Then choose $a_1=(1/\sqrt{2})/\lambda_1$ and $a_2=(1/\sqrt{2})/\lambda_2$, and $b_1=-a_1$ and $b_2=a_2$.

This finishes the proof of the proposition and leads to the following algorithm:

1. Algorithm III: O1, $A=i\sigma_x$, $B=i\sigma_y$

(1) Represent $S(\alpha,\zeta,\mu)$ as $\exp[i((\zeta+\mu)/2-\pi/4)\sigma_z]\exp[i\alpha\sigma_x]\exp[i((\zeta-\mu)/2+\pi/4)\sigma_z]$ using **R1**. Modify, by multiples of 2π, to ensure that the angles $(\zeta+\mu)/2-\pi/4$ and $(\zeta-\mu)/2+\pi/4$ are in $[0, 2\pi)$.

(2) Prepare the first and third factors in Step 1 via free evolution.

(3) Prepare the middle term via two factors by using Proposition 3.1 with $L=\alpha$. Since $\alpha\in[0,\pi/2]$, the hypothesis $\cos L\geqslant 0$, $\sin L\geqslant 0$ of Proposition 3.1 automatically hold. Of these two factors, the second can be taken to be free evolution if $\alpha\neq\pi/2$.

(4) This yields $Q\leqslant 4$. At least two of these factors (at least 3 if $\alpha\neq\pi/2$) are free evolution factors. The corresponding values of (a_k,b_k) are displayed in Table II in Sec. III C.

Remark 3.3: In the proof of Proposition 3.1 when $\cos(L) \neq 0$, the values of λ_k were chosen with the aim of rendering the control pulse to be applied for a shorter time than the free evolution factor. Note **O1** can also be achieved, in the $\cos(L) \neq 0$ case, by taking $\lambda_k = \pi/2$, $k = 1,2$. However, in this case neither pulse can be taken to be free evolution. On the other hand, this has the advantage of reducing the radial coordinates and thus the time of the factors involved.

2. O2 for the $A = i\sigma_z$; $B = i\sigma_y$ case

Next the factorization satisfying **O1** will be refined to meet **O2**. Following Proposition 3.1 and **R1**, all that is required is to prepare $e^{i\alpha\sigma_x}$, for any $\alpha \in [0, \pi/2]$ via pulses with bounded pulse area. The key to this is to note, from the proof of Proposition 3.1, that this term can be prepared by two factors, the first with pulse area $(\pi/2)\sin(\alpha)$ and the second a free evolution term. So α should be such that $(\pi/2)\sin(\alpha) \leqslant C$. This leads to the following algorithm.

(a) Algorithm IV: O2, $A = i\sigma_z$, $B = i\sigma_y$. (1) Represent $S(\alpha, \zeta, \mu)$ as $\exp[i((\zeta+\mu)/2 - \pi/4)\sigma_z]\exp[i\alpha\sigma_x]\exp[i((\zeta-\mu)/2 + \pi/4)\sigma_z]$ using **R1**. Modify, by multiples of 2π, to ensure that the angles $(\zeta+\mu)/2 - \pi/4$ and $(\zeta-\mu)/2 + \pi/4$ are in $[0, 2\pi)$.

(2) Prepare the first and third factors in Step 1 as free evolution terms.

(3) To prepare the middle term, $e^{i\alpha\sigma_x}$, first translate the bound C on the pulse area into a bound θ_C on the deviation of α from 0. Specifically, define $\theta_C \in [0, \pi/2]$, as $\sin^{-1}(C/(\pi/2))$. This can always be ensured by reducing C, if needed.

(4) If $\alpha \neq \pi/2$, factor $e^{i\alpha\sigma_x}$ as a product $\Pi_{k=1}^{r} e^{i\alpha_k\sigma_x}$, with $r = \lceil \alpha/\theta_C \rceil$ and $\alpha_k = \alpha/r$. Thus, $0 \leqslant \alpha_k \leqslant \theta_C$. Here, $\lceil \cdot \rceil$ is the ceiling function.

(5) Prepare each factor $e^{i\alpha_k\sigma_x}$ of Step 4 via two pulses as in Proposition 3.1 with α_k playing the role of L. The second pulse corresponds to a free evolution term. The first factor has pulse area equal to $(\pi/2)\sin(\alpha_k)$. This is positive and at most C by the choice of α_k.

(6) Thus, if $\alpha \neq \pi/2$, the above steps yield $Q \leqslant 2\lceil L/\theta_C \rceil + 2$. If $\alpha = \pi/2$, then write $e^{i\alpha\sigma_x}$ as, say, $e^{i(4/\pi)\sigma_x}\, e^{i(4/\pi)\sigma_x}$ and prepare each of these factors via the above steps.

C. A unified approach

In this section, A and B are allowed to be any 2×2 su(2) matrices as described. The basic idea is the following. Given a pair $A, B \in \mathrm{su}(2)$ and a target $S \in \mathrm{SU}(2)$, the problem of obtaining the factorization (1.1) is resolved by solving the same problem for one particular choice of su(2) matrices, $\hat{A}, \hat{B}$. Given the pair A,B, let ψ:su(2)$\rightarrow$su(2) be defined as:

$$\psi(a\hat{A} + b\hat{B} + c[\hat{A}, \hat{B}]) = aA + bB + c[A, B] \tag{3.6}$$

for any $a, b, c \in R$. The notation $[,]$ represents the commutator.

1. Preliminary orthonormalization

The aim is to render ψ, of Eq. (3.6), a Lie algebra isomorphism, in other words to have it satisfy $\psi([\Lambda, \Omega]) = [\psi(\Lambda), \psi(\Omega)]$ for any $\Lambda, \Omega \in \mathrm{su}(2)$. Now ψ, as it stands, need not satisfy this property. It will however do so, by virtue of the relation between the matrix commutator and the vector cross product, if both the pairs A,B and $\hat{A}, \hat{B}$ are orthonormal pairs. Recall, a pair $A, B \in \mathrm{su}(2)$ is said to be orthonormal if the vectors in R^3, obtained by expressing them as linear combinations of $(i/2)\sigma_z, (i/2)\sigma_y, (i/2)\sigma_x$, are orthonormal. Now $\hat{A} = (i/2)\sigma_z$ and $\hat{B} = (i/2)\sigma_y$ are already orthonormal. So, the proposed unified approach will work when A and B are also orthornormal.

If A,B are not orthonormal to begin with, a preliminary control transformation can be applied to render them first orthogonal to each other. Indeed, define $u(t) = k + v(t)$, with $v(t)$ the new control. Then the system (1.2) becomes;

$$\dot{U} = (A + kB)U + BUv(t).$$

The constant k is now chosen so that the new drift $A + kB$ is orthogonal to B. Thus, if the design based on $(A + kB, B)$ produced v as a piecewise constant control, then the corresponding $u(t)$, for the original pair (A,B), would also be piecewise constant with the constant k being added to each piece of $v(t)$. Orthonormalization can be achieved by further scaling $A + kB$ and B by positive constants. Note that while the application of a preliminary control does not affect **O1**, it affects **O2**. A scaling affects neither **O1** nor **O2**. Indeed, to meet **O1** and **O2** (for a given bound C) for the pA, qB system, the factorization that works for the A,B system, with the bound C replaced by qC, can be used. This leads to the following algorithm:

(a) Algorithm V: General A,B (1) Render A,B orthonormal (if needed) via the procedure described just above. Note that this step may *often* be omitted even in those cases where A and B are not orthogonal (see Remark 3.4 below).

(2) Calculate the logarithm of S and express it as a linear combination of A,B and $[A,B]$, i.e.,

$$\ln(S) = c_1 A + c_2 B + c_3 [A, B], \tag{3.7}$$

This is a linear algebraic calculation.

(3) Associate to S the matrix T defined by

$$T = \exp(c_1\hat{A} + c_2\hat{B} + c_3[\hat{A}, \hat{B}]). \tag{3.8}$$

Thus, $\phi(T) = S$. Here ϕ:SU(2)$\rightarrow$SU(2) is defined by the condition $\phi(e^K) = e^{\psi(K)}$. As ψ is a Lie algebra isomorphism, the Campbell-Baker-Hausdorff formula ensures that ϕ is a group homomorphism [26].

(4) Achieve **O1** and **O2** for $\hat{A} = (i/2)\sigma_z$, $\hat{B} = (i/2)\sigma_y$ when the target is T, via the results of Sec. III B. The only difference would be that the (a_k, b_k), $k = 1, \ldots, Q$ would now be given by be replaced by $(2a_k, 2b_k)$, $k = 1, \ldots, q$ of Sec. III B. Alternatively, choose $\hat{A} = (i/2)\sigma_y$, $\hat{B} = (i/2)\sigma_x$ and use the results of Sec. III A. This provides an explicit

TABLE I. Q for **O1**, the number of free evolution factors and cumulative radial coordinates for the two pairs.

Pair	Maximal Q for **O1**	Minimal no. of free evolution	Maximal cumulative radial coordinates
$(i\sigma_y, i\sigma_z)$	5	1	$5\frac{\pi}{2}$
$(i\sigma_x, i\sigma_y)$	4	2	4π

factorization $T=\Pi_{k=1}^{Q}\exp(a_k\hat{A}+b_k\hat{B})$ with $a_k>0$ and $|b_k|\leqslant C$, $k=1,\ldots,Q$ for the given bound C.

(5) Then, we have

$$\begin{aligned} S=\phi(T)&=\phi[\Pi_{k=1}^{Q}e^{(a_k\hat{A}+b_k\hat{B})}]\\ &=\Pi_{k=1}^{Q}\phi[e^{(a_k\hat{A}+b_k\hat{B})}] \quad (\text{as } \phi \text{ a homomorphism})\\ &=\Pi_{k=1}^{Q}e^{(a_kA+b_kB)}[\text{as } \phi(e^{L})=e^{\psi(L)}], \end{aligned} \tag{3.9}$$

Thus the *same* choice of a_k, b_k, $k=1,\ldots,Q$ that worked for the matrix T, also works for S and thereby *explicitly* provides **O1** and **O2** for the target SU(2) matrix S and the given pair of su(2) matrices.

While Algorithm **V** works for general A,B it has the following disadvantages: (i) For the case when A,B are i times Pauli matrices (which are already orthogonal), the second step of Algorithm **V** is substantially more complicated, computationally, than representing S via Cayley-Klein parameters and using a factorization like **R2**. (ii) If A,B were not orthogonal to begin with, then this method requires the application of a preliminary constant control. In certain situations where A,B are not orthogonal, this preliminary step may be undesirable. On the other hand, intrinsic approaches may be able to address nonorthogonal pairs without preliminary controls (see Remarks 3.2 and 3.4, for instance). (iii) The problem of meeting **O1** and **O2** has been ''transferred'' to the pairs of Sec. III A or III B. Thus, the resultant choice of a_k, b_k has peculiarities related to this latter pair. The only point in the algorithm where information about the given pair A,B is encoded, is in the choice of the matrix T.

2. Comparison of the σ_y,σ_x and σ_z,σ_y pairs

Depending on which pair is used in Step 4 of Algorithm **V**, different decompositions meeting **O1, O2** are obtained, and thus a comparison is in order. Two tables are presented below. In Table I, these pairs are compared with respect to significant criteria. Table II gives values for (a_k,b_k), $k=1,\ldots,Q$ for **O1** for these two pairs in terms of the Cayley-Klein coordinates of the target $S(\alpha,\zeta,\mu)$. Comparisons for **O2** have been omitted as they cannot be cast into a compact form within the confines of a table.

In the tables below, the factor of 1/2 in the pairs $\hat{A},\hat{B}$ of Step 4 of Algorithm **V** has been dropped, because (i) that factor is present in both pairs and thus does not affect the comparison, and (ii) the formulas presented in Table II are then easier to extrapolate for examples with $\hat{A},\hat{B}$ replaced by pA and qB for $p,q>0$.

(1) Cumulative radial coordinates are, by definition, $\Sigma_{k=1}^{Q}\lambda_k=\Sigma_{k=1}^{Q}\sqrt{a_k^2+b_k^2}$.

(2) The number of free evolution factors for the $i\sigma_z, i\sigma_y$ pair is 3 if $\alpha\neq\pi/2$.

(3) The $(i\sigma_z, i\sigma_y)$ pair, typically has lower cumulative pulse area, i.e., $\Sigma_{k=1}^{Q}|b_k|$. Comparisons for this criteria have been omitted, since the formulas for $|b_k|$ for $(i\sigma_y, i\sigma_x)$ have considerable liberty, thereby rendering upper bounds quite conservative.

(4) The angles θ_k, $k=1,\ldots,4$ in the second column are chosen to satisfy the stated constraints and also to be in the range $(\pi, 2\pi)$. See the Algorithm **I** in Sec. III A.

According to the first table, the $(i\sigma_z, i\sigma_y)$ performs better than the $(i\sigma_y, i\sigma_x)$ pair in all categories except for cumulative radial coordinates. Having a lower value for the cumulative radial coordinate is useful because it indicates the ability to prepare the target in a better fashion with respect to simultaneously minimizing total time and total pulse area.

TABLE II. (a_k,b_k) for **O1**.

(a_k,b_k)	$(i\sigma_y, i\sigma_x)$	$(i\sigma_z, i\sigma_y)$, $\alpha\neq\frac{\pi}{2}$	$(i\sigma_z, i\sigma_y)$, $\alpha=\frac{\pi}{2}$
(a_1,b_1)	$\left(-\frac{\pi}{2}\sin\theta_1, \frac{\pi}{2}\cos\theta_1\right)$, $\frac{\zeta+\mu}{2}-\pi=\theta_1-\theta_2+\pi$	$\left(\frac{\zeta+\mu}{2}-\frac{\pi}{4},0\right)$	$\left(\frac{\zeta+\mu}{2}-\frac{\pi}{4},0\right)$
(a_2,b_2)	$\left(-\frac{\pi}{2}\sin\theta_2, \frac{\pi}{2}\cos\theta_2\right)$, $\frac{\zeta+\mu}{2}-\pi=\theta_1-\theta_2+\pi$	$\left(\frac{\pi}{2}\cos\alpha, \frac{\pi}{2}\sin\alpha\right)$	$\left(\frac{\pi}{2\sqrt{2}}, -\frac{\pi}{2\sqrt{2}}\right)$
(a_3,b_3)	$(\alpha,0)$	$\left(\frac{3\pi}{2},0\right)$	$\left(\frac{\pi}{2\sqrt{2}}, \frac{\pi}{2\sqrt{2}}\right)$
(a_4,b_4)	$\left(-\frac{\pi}{2}\sin\theta_3, \frac{\pi}{2}\cos\theta_3\right)$, $\frac{\zeta-\mu}{2}-\pi=\theta_3-\theta_4+\pi$	$\left(\frac{\zeta-\mu}{2}+\frac{\pi}{4},0\right)$	$\left(\frac{\zeta-\mu}{2}+\frac{\pi}{4},0\right)$
(a_5,b_5)	$\left(-\frac{\pi}{2}\sin\theta_4, \frac{\pi}{2}\cos\theta_4\right)$, $\frac{\zeta-\mu}{2}-\pi=\theta_3-\theta_4+\pi$	N.A.	N.A.

The values for cumulative radii were arrived at as follows. For the $(i\sigma_y, i\sigma_x)$ pair, use is made of the fact that any S can be prepared by five factors, four of which have radial coordinates equal to $\pi/2$ and the fifth [the factor corresponding to $V(\tilde{\gamma}_1)$ in Eq. (3.11)] has radial coordinate equal to α (see the Algorithm **I** in Sec. III A or Table II). Since $\alpha \leqslant \pi/2$, the upper bound is indeed $5(\pi/2)$.

For the $(i\sigma_z, i\sigma_y)$ pair, Algorithm **III** or Table II clearly yield cumulative radial coordinates of $d+f+3(\pi/2)+\pi/2$. Now, $d=(\zeta+\mu)/2-\pi/4$, $f=(\zeta-\mu)/2+\pi/4$ (see Sec. II B). By taking ζ to be $2\pi-\epsilon(\epsilon>0)$, $\mu=0$, we see that the cumulative radial coordinates can be made arbitrarily close to 4π. Note it may be tempting to write the angle ζ as $-\epsilon$ and thus hope to get lower values of d and f. While this lowers f (if ϵ is small), it renders d negative, thus requiring the representation of d as a positive number (to meet **O1**). This rewriting gives the same value for $d+f$.

Finally, note that at the cost of reducing the number of free evolution factors, the cumulative radial coordinate for the $(i\sigma_z, i\sigma_y)$ pair can be reduced to 3π (by virtue of Remark 3.3). Likewise the cumulative radial coordinate for the other pair can be reduced to 2π by a different factorization, which however is not amenable to analyzing **O2**.

Remark 3.4, Preliminary Orthogonalization Not Always Needed: Another advantage of the pair of Sec. III A deserves attention. Suppose A and B are not orthogonal. It is often possible to handle these cases without Step 1 of Algorithm **V**. One such example is provided by A and B being two linearly independent combinations of $i\sigma_x, i\sigma_y$. (See Remark 3.2.) This example can be used to handle other cases also. For example, let $A=a(i/2)\sigma_y+b(i/2)\sigma_z$; $B=c(i/2)\sigma_y+a(i/2)\sigma_z$ with the vectors (a,b) and (c,d) linearly independent, but not orthogonal. We now use Algorithm **V** with the following changes. Step 1 is omitted. Define the Lie algebra isomorphism, ψ, through:

$$\psi\left(\frac{i}{2}\sigma_y\right)=\frac{i}{2}\sigma_y; \quad \psi\left(\frac{i}{2}\sigma_z\right)=\frac{i}{2}\sigma_x; \quad \psi\left(\frac{i}{2}\sigma_x\right)=-\frac{i}{2}\sigma_x.$$

Define ϕ via ψ as before, $\phi(e^K)=e^{\psi(K)}$, and use this new definition of ϕ in Steps 3 and 5 of Algorithm **V**. In Step 4, choose $\hat{A}$ and $\hat{B}$ as $a(i/2)\sigma_y+b(i/2)\sigma_x$ and $c(i/2)\sigma_y+d(i/2)\sigma_x 2$ and then use Remark (3.2) to to meet **O1** or **O2** for $\hat{A}$ and $\hat{B}$ and target T of the new Step 3. Then, just as in Step 5 of Algorithm **V**, the same a_k, b_k prepare the target S for A and B. In other words, the key difference is using $(i/2)\sigma_y$ and $(i/2)\sigma_x$ and not $\hat{A},\hat{B}$ (which are not orthogonal) to define ψ, and then using Remark 3.2 to find a_k, b_k.

Thus, the only cases that seem to require a preliminary control are $A=a_1(i/2)\sigma_z+b_1(i/2)\sigma_y+c_1(i/2)\sigma_x$, $B=a_2(i/2)\sigma_z 2+b_2(i/2)\sigma_y+c_2(i/2)\sigma_x$, with the vectors (a_1,b_1,c_1) and (a_2,b_2,c_2) nonorthogonal and such that either (i) at least one of the two vectors has all components nonzero or (ii) if certain components of one of these vectors are zero then at least one of the corresponding components of the other is nonzero. In retrospect, the main feature of the $i\sigma_y, i\sigma_x$ case which allows us to address nonorthogonal pairs, is the fact that its starting point **R2** unlike **R2**, uses both Pauli matrices in all its factors (cf. Remark 2.1 of Sec. II B).

D. Systems Evolving on SO(3)

In this section, the achievement of **O1** and **O2** on SU(2) will be used to achieve the same for systems on SO(3), the group of proper three dimensional rotations. This facilitated by the following facts:

(1) The transformation $R_U:\mathrm{su}(2)\to\mathrm{su}(2)$, $R_U(A)=UAU^{-1}$, when viewed as a transformation from R^3 to R^3 is an element of SO(3) [27]. This leads to a Lie group *homomorphism* $\phi:\mathrm{SU}(2)\to\mathrm{SO}(3)$, with $\phi(U)\in\mathrm{SO}(3)$. Furthermore, the entries of the SU(2) matrices, which map to a given SO(3) matrix, can be explicitly described.

(2) There is a Lie algebra isomorphism from $\psi:\mathrm{su}(2)\to\mathrm{so}(3)$, defined according to $\psi:\mathrm{su}(2)\to\mathrm{so}(3)$, defined according to [25]

$$\psi\left[\frac{-i}{2}(a\sigma_x+b\sigma_y+c\sigma_x)\right]=\begin{pmatrix}0 & -c & b\\ c & 0 & -a\\ -b & a & 0\end{pmatrix}.$$

(3) An explicit calculation shows that $\phi(e^K)=e^{\psi(K)}$, where $K=i(a\sigma_x+b\sigma_y+c\sigma_z)$ is a general element of su(2). This is shown by using Eq. (2.2) in conjunction with the Rodrigues' formula for the exponential of an arbitrary element V of so(3):

$$e^V=\cos(\|v\|)I_3+\frac{\sin(\|v\|)}{\|v\|}V+\frac{1-\cos(\|v\|)}{\|v\|^2}vv^T.$$

In the above formula v is the vector in R^3 associated to the element $V\in\mathrm{so}(3)$ and vv^T is the outer product of v and v^T. See [28] for Rodrigues' formula.

The above items can now be assembled to solve the problem of attaining any $O\in\mathrm{SO}(3)$ via controls with bounded pulse area as follows. Given a system evolving on the group SO(3):

$$\dot{U}=AU+BUu(t), \quad A,B\in\mathrm{so}(3) \tag{3.10}$$

and a desired final state O, we associate to it a system evolving on SU(2) and a final state, $S\in\mathrm{SU}(2)$:

$$\dot{U}=\hat{A}U+\hat{B}U, \quad \hat{A},\hat{B}\in\mathrm{su}(2), \tag{3.11}$$

Here $\hat{C}\in\mathrm{su}(2)$ is $\psi^{-1}(C)$ and $S\in\mathrm{SU}(2)$ is any element of SU(2) such that $\phi(S)=O$.

To prepare O, we find the controls that would prepare S. This means factoring S as a product $\Pi_{k=1}^{Q}e^{(a_k\hat{A}+b_h\hat{B})}$ with $a_k>0$ and $|b_k|\leqslant C$, $k=1,\ldots,Q$. Then the *same* choice of a_k, b_k, $k=1,\ldots,Q$ achieves **O1** and **O2** for O. This can be shown by a calculation analogous to that in Step 5 of Algorithm **V**.

The difference between this subsection and the previous subsection, regarding the homomorphism ϕ, is as follows. In this section ϕ is already given, and we only verified that it

satisfies the important property $\phi(e^K)=e^{\psi(K)}$, for $K \in \mathrm{su}(2)$. On the other hand, in the previous section, ϕ was defined via $\phi(e^K)=e^{\psi(K)}$ and this leads, in conjunction with Eq. (2.4), to an explicit expression for ϕ.

IV. MOTIVATING EXAMPLES

The basic problem set out in the Introduction is motivated by many examples in quantum and classical control. A few of them are briefly reviewed here. Examples 1 through 4 address *quantum*-mechanical examples, whereas Example 5 discusses *classical* systems.

Example 1: The decomposition, (1.1), amounts to producing piecewise constant controls for the control of a two level quantum system. Given such an externally controlled two level system, we can express the evolution of the corresponding unitary generator via Schrodinger's equation (after absorbing the i factor into the matrices A and B)

$$\dot{U}=AU+BUu(t), \quad (0)=I_2.$$

It is assumed that A,B belong to su(2). The assumption that A and B are anti-Hermitian with zero trace as opposed to being just anti-Hermitian is appropriate because either (i) that is already the case (as in the case of the control of electron spin) or (ii) it amounts to only neglecting an overall phase, which is physically irrelevant. As an illustration of the latter possibility, consider a two level atom with nondegenerate energy levels E_k, $k=1,2$ irradiated with an electromagnetic field (the field being treated semiclassically). Suppose that the diagonal matrix elements of the dipole operator vanish and μ is the nonzero matrix element of the dipole operator. Then after some manipulation we are lead to a system of the form of Eq. (1.2):

$$\dot{U}=i\left(\frac{E_2-E_1}{2}\right)\sigma_z U+i\mu\sigma_x Uu(t). \tag{4.1}$$

The system (4.1) differs from the actual evolution of the unitary generator only via an overall phase factor of $e^{(i(E_1+E_2)/2\,t)}$.

Thus, in this example it holds that $A=i(E_2-E_1)/2\,\sigma_x$ *and* $B=i\mu\sigma_x$. Hence, the results of Sec. III C are relevant to this application.

Now if Eq. (1.2) is probed by a sequence of controls $u_k(t)=f_k$, $k=1,\ldots,L$ each for a duration t_k, respectively, then the unitary generator after $t_1+\ldots+t_L$ units of time is given by $\Pi_{k=1}^{L}e^{a_kA+b_kB}$, with $a_k=t_k$; $b_k=f_kt_k$. Since, the t_k have to be positive (unless the corresponding $f_k=0$), it is necessary that $a_k>0$. The requirement that the b_k be bounded in absolute value is of importance both theoretically and practically. Indeed, there may be practical constraints on the power of the pulse. Such bounds are also required for neglecting other levels and physical processes of the system being studied.

Example 2: A second example is given on page 84 of Ref. [5]. Consider the control of the spin of an electron with $B_x=0$ and $B_z=1$. $B_y(t)$ is available for manipulation and thus is the control $u(t)$. Assume for simplicity that μ_B, the Bohr magneton is 1. Here B_x, B_y, and B_z are components of the magnetic field along the x, y, and z axes. So the Hamiltonian of the system is given by

$$H=\sigma_z+B_y(t)\sigma_y.$$

This is Case (c) of the example on page 84 of Ref. [5]. If the aim is to prepare a specific coherent superposition of the spin-up and spin-down states, then the same can be achieved by preparing the unique SU(2) matrix S that conveys the initial state to the desired coherent superposition [here, use is being made of the fact that given 2 vectors u, v on the three-dimensional sphere, there is a unique SU(2) matrix S such that $Su=v$]. This leads to studying a system of the form:

$$\dot{U}=-i\sigma_z U-i\sigma_y Uu(t),$$

where $u(t)=B_y(t)$. *This is of the form of Eq. (1.2) with* $A=-i\sigma_z$, $B=-i\sigma_y$. Hence the results, which are relevant to this example belong to Sec. III C. The other cases considered in this example of Ref. [5] correspond to the easier case of the control of *driftless* systems.

Example 3: Another class of problems that requires the creation of a final unitary matrix arises from quantum computation [6–8]. In these examples, it is required not only to prepare desired states, but also desired unitary generators. Most physical systems suggested for quantum computation consist of independently addressable two-level systems. Controlling such systems via a sequence of constant controls is attractive if they have long quantum lifetimes.

Example 4: **O1** and **O2** are also relevant for both systems with ''more'' than two levels and controls which are ''not'' piecewise constant. First, theoretically it may be shown that any control can be approximated by piecewise constant controls [29,10]. Second, controls such as sinusoidal controls may be reduced to the piecewise constant case via approximations such as the rotating wave approximation or averaging theory. In Ref. [11] an N ''level'' atom/molecule with well separated spectrum was considered. Under some additional assumptions, it was shown that the system can be controlled by addressing only pairs of levels via sinusoidal pulses resonant with the corresponding energy difference. Using the rotating wave approximation it was then shown that any desired unitary generator could then be factored as a product of direct sums of I_{N-2} and SU(2) matrices with special structure. Specifically, this special structure was

$$S=\Pi_{k=1}^{3}\exp[i(-\mathrm{Im}\,\gamma_k\sigma_x+\mathrm{Re}\,\gamma_k\sigma_y)].$$

The polar coordinates (λ_k,ϕ_k) of the complex numbers γ_k are related to the kth sinusoidal pulse as follows. λ_k is the pulse area of the kth pulse and ϕ_k is phase of the kth pulse. Thus, the requirement $a_k>0$ now translates into the phase of the pulse being located in certain ranges. Likewise, other approximations call for structures which involve the other Pauli matrices. Thus, under additional assumptions on the spectrum of the quantum system being studied, multilevel systems can be studied by using techniques for two-level systems.

An alternative approximation comes from averaging theory [30]. For instance, when the system (1.2) is probed by a sinusoidal pulse $u_k(t)=a_k \sin(\omega_k t+\phi_k)$, the evolution of the unitary operator is, under the averaging approximation, approximated by

$$\dot{U}=AU+BUu_{av,k}.$$

Here $u_{av,k}$ is the average of the kth sinusoidal pulse. In this case the corresponding a_k and b_k are related to the duration and average of the pulse. Thus, **O1** is once again necessary, while **O2** amounts to requiring that the dc component of the field be small.

Example 5: Many classical mechanical systems have either part or all of their evolution on the group of rotations, SO(3). Examples are satellites controlled via internal rotors and aerospace systems with zero angular momentum that are controlled via internal rotors. Thus, the methods of Sec. III D are relevant for these applications. A different example comes from energy transfers between dynamic storage elements in switched electrical networks used in power conversion applications [14,15]. Such networks play an important role in many communication devices. Such problems lead to systems that evolve on an Euclidean space. The differential equations which model these systems are bilinear, i.e., have the form:

$$\dot{x}=Ax+Bxu(t), \quad x\in R^k.$$

Here k is the number of circuit elements in the network. The state x usually represents inductor currents and capacitor voltages. When no power sources/loads are added, the associated equation for the ''unitary generator'' (i.e., the transition matrix) can be frequently modeled as a system evolving on SO(k), the group of proper k dimensional rotations [14]. This reflects the conservation of energy. The particular example considered in Ref. [15] has $k=3$, and the authors of Ref. [15] pass to the associated driftless system to achieve *approximate* energy transfer. Since the ''unitary'' generator in this example evolves on SO(3), we can use the results of Sec. III D. It turns out the corresponding system on SU(2) [i.e., Eq. (3.11) of Sec. III D] is of the form (1.2) with $A=ip\sigma_y$ and $B=i(q\sigma_x-p\sigma_y)$. Here p,q are nonzero constants related to the circuit elements. Thus this system can be handled *exactly* (not approximately, as in Ref. [15]) by using either Remark 3.2 in Sec. III A or by the methods of Sec. III C. The former is preferable since no preliminary orthogonalization is then called for.

V. CONCLUSIONS

In this paper an explicit procedure for factoring every SU(2) matrix into a decomposition of the form (1.1), respecting requirements **O1** and **O2**, was provided. This factorization is motivated by quantum and classical control studies. In particular, two-level and N-level quantum systems controlled via piecewise constant or piecewise sinusoidal external fields are addressed by these results. A unified approach, which requires the knowledge of a solution to **O1** and **O2** for one pair to constructively address the case of arbitrary A and B, was provided. Varying the former pair, leads to different factorizations that meet **O1** and **O2** for A,B. It is useful to have as many factorizations that meet **O1** and **O2** as possible. For instance, in many applications it is also useful to prepare a given target matrix S in minimal time. For instance, in nuclear magnetic resonance applications it is useful to finish the entire control action before relaxation processes become significant. In general, it is important to finish all the control action before the given quantum system decoheres [8]. This is a problem that is worth addressing. Another aspect of the results of this paper is that they could potentially generalize to N level systems. Indeed, one of the enabling factors of this paper is that products of exponentials can be explicitly described. We believe that the same is true for $N>2$. If this generalization can be achieved, then N-level systems can be studied without reducing the analysis to two-level systems. This could help in removing assumptions about the well separatedness of spectrum of the system being studied [11].

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