General methods to control right-invariant systems on compact Lie groups and multilevel quantum systems

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Abstract
For a right-invariant system on a compact Lie group G, I present two methods to design a control to drive the state from the identity to any element of the group. The first method, under appropriate assumptions, achieves *exact* control to the target but requires estimation of the 'size' of a neighborhood of the identity in G and solution of a nonlinear algebraic equation. The second method does not involve any mathematical difficulty and obtains control to a desired target *with arbitrary accuracy*. A third method is then given combining the main ideas of the previous methods. This is also very simple in its formulation and turns out to be generically more efficient as illustrated by one of the examples I consider. The methods described in the paper provide arbitrary constructive control for any right-invariant system on a compact Lie group. In particular, the results can be applied to the coherent control of general multilevel quantum systems to an arbitrary target.

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1. Introduction

In the last decade, there has been significant interest in developing algorithms to control quantum-mechanical systems. The combination of control theory and quantum mechanics has started a new, fruitful, area of research. This area has a large overlap with quantum information as control methods are of interest both in the practical implementation of quantum information processing and in the design of quantum algorithms. In fact, these can be seen as sequences of unitary operations on the quantum state and the design of these sequences can be treated as a problem of control.

In dealing with quantum-mechanical systems which can be considered isolated from the external environment, the Schrödinger equation is the main mathematical model. This

equation is a linear matrix equation in cases where the system can be accurately approximated as finite dimensional. In particular, the Schrödinger equation has the form

$$i\dot{X} = HX, \qquad X(0) = \mathbf{1}, \tag{1}$$

where H is an Hermitian matrix, $\mathbf{1}$ is the identity matrix and X, which represents the evolution of the system, is therefore unitary at all time. *Coherent control* of quantum-mechanical systems refers to the situation where the *Hamiltonian H* depends explicitly on some control variables which can be chosen arbitrarily from the outside. These may be classical fields or variables which allow us to switch among various Hamiltonians.

The *geometric theory of quantum control* starts from the observation that system (1) has state X varying on a compact Lie group (the unitary group $U(n)$) and is a right-invariant system (see definitions in the following section). Therefore, a lot of knowledge from the control theory of these systems can be applied and expanded. Among the successes of this approach is the explicit characterization of the set of achievable values for X in (1) (*controllability*) and several control methods and tools for various subclasses of systems. The book [9] presents an overview of this approach as well as some relevant references. The characterization of the set of achievable states for a right-invariant system on a Lie group is based on a result proved in [14] which is referred to as *the Lie algebra rank condition*. However, since the proof of this result is not constructive, it does not provide a method for control of these systems which can be applied in every situation. The goal of this paper is to develop such a method and therefore to provide a possible control methodology for every system modeled by (1).

In section 2, I recall the Lie algebra rank condition for systems on compact Lie groups and set up the stage for the treatment of the following sections. In section 3, I present a first method for constructive control. This method requires the solution of a nonlinear algebraic equation which can be difficult in higher dimensional cases. This motivates the search for alternative methods and in section 4, I give a different method which achieves control to the desired target with arbitrary accuracy and does not present any mathematical difficulties. In section 5, I combine the main ideas of the two previous sections and present a third method which allows us to control to a desired target with arbitrary accuracy and can be easily applied. Most of the discussion in these sections refers to *general* systems on compact Lie groups. In section 6, I give some remarks on the results presented in the paper and return to their application to quantum-mechanical systems.

2. The Lie algebra rank condition of geometric control theory

Consider a control system of the form

$$\dot{x} = f(x, u), \tag{2}$$

where x is the state varying on a compact Lie group and u the control. The system is said to be *right invariant* if, denoting by $x(t, u, s)$ the solution to (2) corresponding to initial condition s and control function u, we have

$$x(t, u, s) = x(t, u, \mathbf{1}) \circ s, \tag{3}$$

where $\mathbf{1}$ denotes the identity of the group and $\circ$ is the multiplication in the group. To be concrete, we shall consider the case of a matrix group G where the group operation is the standard matrix multiplication, with particular attention to subgroups of the Lie group of $n \times n$ unitary matrices $U(n)$, given the potential application to quantum systems. In particular, we shall consider systems of the form

$$\dot{X} = A(u)X, \qquad X(0) = \mathbf{1}, \tag{4}$$

where **1** is the identity matrix and the matrix $A(u)$ is in the Lie algebra associated with the Lie group G for every value of the control u. This equation models many systems of interest. In particular (cf (1)), closed (i.e., not interacting with the environment) finite-dimensional quantum systems which are coherently controlled (i.e., through a variation of their Hamiltonian) are modeled this way. In this case, equation (4) is the Schrödinger equation. We refer to [9] and references therein for several examples and introductory notions on Lie groups and Lie algebras in the context of quantum control.

If we restrict ourselves to piecewise constant controls, the problem of control for systems (4) can be described as follows. Assume we have a set of linearly independent matrices

$$\mathcal{F} := \{A_1, \ldots, A_m\}, \tag{5}$$

each corresponding to a certain value of the control u in (4). To each of them, there corresponds a semigroup

$$\mathcal{S}_j := \{e^{A_j t} | t \geqslant 0\}, \qquad j = 1, \ldots, m. \tag{6}$$

The problem of control to a matrix X_f is to choose N elements $X_l, l = 1, \ldots, N \in \mathcal{S}_j$, for some $j = 1, \ldots, m$, such that $\prod_{l=1}^{N} X_l = X_f$. If such elements exist X_f is said to be *reachable*. The question of describing the set of reachable matrices is a standard one in geometric control theory. The result in theorem 1, known as the *Lie algebra rank condition*, is classical [14] and provides the answer for compact Lie groups.

Let $\mathcal{L}$ be the Lie algebra generated by the elements in $\mathcal{F}$ defined as the smallest Lie algebra containing $\mathcal{F}$ and denote by $e^{\mathcal{L}}$ the connected Lie group associated with $\mathcal{L}$. We shall call $\mathcal{L}$ the *dynamical Lie algebra* associated with the system.

Theorem 1. *[14] Consider the Lie group $e^{\mathcal{L}}$ and assume it is compact. Then, the set of reachable values for X in (4) is equal to $e^{\mathcal{L}}$.*

This result has been elaborated upon in several papers and applied to quantum-mechanical systems (cf [1, 9, 13]). In particular, in the case of (closed) quantum-mechanical systems $\mathcal{L}$ is a subalgebra of the unitary Lie algebra $u(n)$ (the Lie algebra of $n \times n$ skew-Hermitian matrices) and, as such, can be written as the direct sum of an Abelian subalgebra and a semisimple subalgebra to which there corresponds a compact Lie group. That is, modulo an Abelian subgroup which commutes with all of $e^{\mathcal{L}}$, $e^{\mathcal{L}}$ is compact (cf [8, 23]). In particular, $e^{\mathcal{L}}$ is compact if $\mathcal{L} = u(n)$ or $\mathcal{L} = su(n)$ ($n \times n$ skew-Hermitian matrices with trace zero) in which case, the system is called controllable and $e^{\mathcal{L}}$ is the group of unitary matrices $U(n)$ or special unitary matrices $SU(n)$, i.e., $n \times n$ unitary matrices with determinant equal to one, respectively. A classical result of Lie theory (see, e.g., [29, theorem 2.15]) says that every representation of a compact Lie group is unitary. Therefore, if we assume that we consider a Lie group of matrices (as we do) $e^{\mathcal{L}}$ will always be a subgroup of $U(n)$ and $\mathcal{L}$ a subalgebra of $u(n)$.

The original proof of theorem 1 given in [14] is not constructive, i.e., in our setting, it does not show how to alternate elements in the semigroups $\mathcal{S}_j$ in (6) to obtain a given target $X_f \in e^{\mathcal{L}}$. We show how to obtain this in two ways in the following two sections. The main ideas are then combined in a third method in section 5. The first method, described in section 3, achieves exact control if the subgroups corresponding to the semigroups in (6), i.e.,

$$\tilde{\mathcal{S}}_j := \{e^{A_j t} | t \in \mathbf{R}\}, \qquad j = 1, \ldots, m, \tag{7}$$

are closed, i.e., the function $t \to e^{A_j t}$ is periodic. Otherwise it obtains control with arbitrary accuracy as it follows from proposition 3.2 and remark 3.3 below. These proposition and remark allow us to replace an exponential of the form e^{At} with $t < 0$ with an exponential of the form e^{At} with $t > 0$ which approximates it with arbitrary accuracy. These results will be utilized for the following two methods as well.

3. Method 1: exact constructive controllability

The method I am going to describe is suggested by the proof of the Lie algebra rank condition, theorem 1, given in [9] and the result on uniform finite generation of compact Lie groups given in [6]. Let $X_f \in e^{\mathcal{L}}$ be the target state. We want to obtain X_f as a product of elements in (6), if not exactly, at least, with arbitrary accuracy. We are first going to relax the problem by allowing the use of elements in the subgroups (7) rather than only elements of the semigroups (6). We shall show later how to overcome this problem (see proposition 3.2 and remark 3.3).

Since $e^{\mathcal{L}}$ is compact the exponential map is surjective, that is, there exists a matrix $A \in \mathcal{L}$ such that $e^A = X_f$, for every X_f.[1] This also implies that, given any neighborhood K of the identity in $e^{\mathcal{L}}$, we can choose an integer M sufficiently large such that $e^{\frac{A}{M}} = X_f^{\frac{1}{M}} \in K$. Assume first that $\mathcal{F}$ in (5) is a basis of $\mathcal{L}$, that is, no Lie bracket is necessary to obtain a basis of $\mathcal{L}$. This implies that, by varying $t_1, \ldots, t_m$ in a neighborhood of the origin in $\mathbf{R}^m$, $K := \{X = e^{A_m t_m} e^{A_{m-1} t_{m-1}} \cdots e^{A_1 t_1} | t_1, \ldots, t_m \in \mathbf{R} \}$, gives a neighborhood of the identity in $e^{\mathcal{L}}$ and, in particular, it contains $e^{\frac{A}{M}}$ for sufficiently large M. That is, we can find real values $\bar{t}_1, \ldots, \bar{t}_m$ such that

$$e^{\frac{A}{M}} = e^{A_m \bar{t}_m} e^{A_{m-1} \bar{t}_{m-1}} \cdots e^{A_1 \bar{t}_1}. \tag{8}$$

Therefore, by using elements from the subgroups (7) we can obtain $e^{\frac{A}{M}}$. Now assume $\mathcal{F}$ is not a basis of $\mathcal{L}$. Since $\mathcal{F} := \{A_1, \ldots, A_m\}$ generates all of $\mathcal{L}$, there exist two indices k and l, $1 \leqslant k, l \leqslant m$, such that the commutator $[A_l, A_k]$ is linearly independent of $\{A_1, \ldots, A_m\}$. This implies that there exists a value $t \in \mathbf{R}$ such that $F := e^{A_l t} A_k e^{-A_l t}$ is also linearly independent of $\{A_1, \ldots, A_m\}$. To see this, assume it is not true and write $e^{A_l t} A_k e^{-A_l t}$ as

$$e^{A_l t} A_k e^{-A_l t} = \sum_{j=1}^{m} a_j(t) A_j, \tag{9}$$

for every t. Taking the derivative with respect to t at $t = 0$, gives $[A_l, A_k] = \sum_{j=1}^{m} \dot{a}_j(0) A_j$, which contradicts the fact that $[A_l, A_k]$ is linearly independent of $\{A_1, \ldots, A_m\}$. Let $\bar{t}$ be such that

$$F := e^{A_l \bar{t}} A_k e^{-A_l \bar{t}}. \tag{10}$$

We can add F to $\{A_1, \ldots, A_m\}$ and have a linearly independent set. Moreover, we can express every exponential e^{Ft} in terms of exponentials of A_l and A_k since $e^{Ft} = e^{A_l \bar{t}} e^{A_k t} e^{-A_l \bar{t}}$. Define $A_{m+1} := F$. If $\{A_1, \ldots, A_m, A_{m+1}\}$ is a basis of $\mathcal{L}$ then we can proceed as above and obtain a neighborhood of the identity in $e^{\mathcal{L}}$ by varying $\{t_1, \ldots, t_{m+1}\} \in \mathbf{R}^{m+1}$. Such a neighborhood is given by $K := \{\prod_{j=1}^{m+1} e^{A_j t_j} | t_1, \ldots, t_{m+1} \in : \mathbf{R} \}$. If this is not the case, then we observe that $\{A_1, \ldots, A_{m+1}\}$ is still a set of generators for $\mathcal{L}$ and, as above, there must exist two elements A_k and A_l in $\{A_1, \ldots, A_{m+1}\}$, such that $[A_k, A_l]$ is linearly independent of $\{A_1, \ldots, A_{m+1}\}$ and therefore for some $\bar{t}$, $A_{m+2} := e^{A_l \bar{t}} A_k e^{-A_l \bar{t}}$ is linearly independent of $\{A_1, \ldots, A_{m+1}\}$. The exponential $e^{A_{m+2} t}$ again can be expressed in terms of exponentials of $A_1, \ldots, A_{m+1}$ and therefore in terms of exponentials of $A_1, \ldots, A_m$. Proceeding this way, one finds $\dim(\mathcal{L}) - m$ new matrices, $\{A_{m+1}, A_{m+2}, \ldots, A_{\dim(\mathcal{L})}\}$ which together with $\{A_1, \ldots, A_m\}$ give a basis of $\mathcal{L}$. Moreover, the exponentials of $\{A_{m+1}, A_{m+2}, \ldots, A_{\dim(\mathcal{L})}\}$ can be expressed as products of exponentials of the elements in $\mathcal{F}$. By taking $\prod_{j=1}^{\dim(\mathcal{L})} e^{A_j t_j}$ with $t_j \in \mathbf{R}$, $j = 1, \ldots, \dim(\mathcal{L})$, we obtain all the elements in a neighborhood of the identity and in particular $e^{\frac{A}{M}}$. Repeating the sequence M times we obtain e^A.

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[1] See, e.g., [18, 21] for generalizations of this result. See also [12, theorem 6.4.15] for the theorem of existence of the logarithm of a matrix.

Remark 3.1. In the practical application of this method one has to solve the set of n^2 (complex) nonlinear algebraic equations (8) and find the coefficients $\bar{t}_1, \ldots, \bar{t}_m$ which exist for M sufficiently large. In practice, one begins with a low value of M and increases it until a solution can be found. For large dimensional problems the solution typically has to be found numerically and the number of unknown parameters grows with the dimension of the Lie algebra (as n^2 in the case of $\mathcal{L} = u(n)$). Several numerical methods for solutions of nonlinear algebraic equations (cf e.g., [10]) exist. For low-dimensional systems it may be possible to find the solution by hand as described in example 3.3. It is this difficulty in solving equation (8) which motivates the alternative methods described in the following two sections. It must be remarked however that there is some flexibility in the choice of the matrices $A_{m+1}, \ldots, A_{\dim(\mathcal{L})}$, because of the choice of the pair A_k, A_l and of the times $\bar{t}$ (cf (10)). We can use this flexibility to make these matrices as simple as possible (e.g., block diagonal, sparse, etc) so that calculating the exponential is easier. Another type of flexibility, which may be used in calculations, is the fact that the way exponentials are arranged in (15) is arbitrary. Any different order will give a neighborhood of the identity.

3.1. Dealing with negative times

In the expression of $e^{\frac{A}{M}}$ and therefore in the expression of e^A, there will be some exponentials with negative t, i.e., some elements in the subgroups (7) which are (possibly) not in the semigroups (6). There are ways to minimize the number of these elements in the full product, for example by placing together matrices which come from similarity transformations with the same matrix so as to have cancelations of the type $e^{A_j t_1} e^{-A_j t_2} = e^{A_j (t_1-t_2)}$. Also, in many cases, the orbits $\{e^{A_j t} | t \in \mathbf{R}\}$ are periodic (closed), which allows us to assume all the $\bar{t}_j$'s positive, without loss of generality. In other cases, we can have a situation where, for every matrix $A \in \mathcal{F}$, the exponential of the negative e^{-At} is available although $-A$ is not included in the original set $\mathcal{F}$. Moreover sometimes, in the quantum control context, we can easily produce a unitary matrix U and its inverse $U^\dagger$, such that $UAU^\dagger = -A$. If we are not in one of these cases, we can use the following fact.

Proposition 3.2. *Let* $e^{-B|t|}$ *be an element of a compact Lie group* $e^{\mathcal{L}}$. *For every* $\epsilon > 0$ *there exists* $\bar{t} > 0$ *such that*[2]

$$\|e^{-B|t|} - e^{B\bar{t}}\| < \epsilon. \tag{11}$$

Proof. Consider $e^{-B|t|}$ and the sequence $e^{nB|t|}$, which, by compactness of $e^{\mathcal{L}}$, has a converging subsequence $e^{n(k)B|t|}$. We have $\lim_{k\to\infty} e^{(n(k+1)-n(k)-1)B|t|} = e^{-B|t|}$. Therefore there is $\bar{k}$ such that $\|e^{(n(\bar{k}+1)-n(\bar{k})-1)B|t|} - e^{-B|t|}\| < \epsilon$, and the proposition holds with $\bar{t} = (n(\bar{k}+1)-n(\bar{k})-1)|t|$. □

Remark 3.3. The proof given above follows the one given in [14]. A different, more concrete, proof can be given recalling that $e^{\mathcal{L}}$, being a compact Lie group of matrices, is a subgroup of $U(n)$ (cf [29, theorem 2.15]). From properties of the Frobenius norm, we have

$$\|e^{B\bar{t}} - e^{-B|t|}\| = \sqrt{2} \sqrt{n - \sum_{j=1}^{n} \cos(\omega_j(\bar{t} + |t|))}, \tag{12}$$

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[2] Whenever we do specific computations involving norms of matrices we use the Frobenius norm $\|A\| := \sqrt{\mathrm{Trace}(AA^\dagger)}$.

where $i\omega_j$, $j = 1, \ldots, n$ are the eigenvalues (possibly repeated) of B. If we can choose $\bar{t} > 0$ so that

$$[1 - \cos(\omega_j(\bar{t} + |t|))] < \frac{\epsilon^2}{2n}, \tag{13}$$

for every $j = 1, \ldots, n$, then (11) is certainly satisfied. If $g := \arccos\left(1 - \frac{\epsilon^2}{2n}\right)$, then, we satisfy condition (13) if we are able to find $\bar{t}$ and integers m_j, $j = 1, \ldots, n$, such that

$$|\omega_j(\bar{t} + |t|) - 2\pi m_j| < g. \tag{14}$$

However, according to Dirichlet's approximation theorem (see, e.g., [2]), given a natural number N and n reals $\alpha_1, \ldots, \alpha_n$, we can find positive integers $a, b_1, \ldots, b_n$, with $1 \leqslant a \leqslant N^n$ so that $|\alpha_j a - b_j| < \frac{1}{N}$, for every $j = 1, \ldots, n$. This result can be applied to satisfy condition (14) identifying α_j with $\frac{\omega_j |t|}{2\pi}$, choosing $\frac{1}{N} < \frac{g}{2\pi}$, choosing $m_j = b_j$, and $\bar{t}$ so that $\frac{\bar{t} + |t|}{|t|} = a$. Notice that since $a \geqslant 1$, $\bar{t} \geqslant 0$ as desired. For the problem to find a and b_j's, there are several algorithms in the literature (cf [15, 16]). Note, however, that we are only interested in a, which determines $\bar{t}$, and since a is bounded from above by N^n, it can be always found, in principle, by exhaustive search.

3.2. Summary of the method and remarks

We can summarize the given method as follows:

(i) Given $\mathcal{F} := \{A_1, \ldots, A_m\}$ find, via similarity transformations, $\dim \mathcal{L} - m$ more matrices $\{A_{m+1}, \ldots, A_{\dim(\mathcal{L})}\}$ so that $\{A_1, \ldots, A_{\dim(\mathcal{L})}\}$ is a basis for $\mathcal{L}$.

(ii) Take the (principal) logarithm of X_f, A, so that $e^A = X_f$.

(iii) Find M (sufficiently large) and $t_1, \ldots, t_{\dim(\mathcal{L})}$, so that

$$e^{\frac{A}{M}} = \prod_{j=1}^{\dim(\mathcal{L})} e^{A_j t_j}. \tag{15}$$

Then $X_f = e^A = \left(\prod_{j=1}^{\dim(\mathcal{L})} e^{A_j t_j}\right)^M$.

(iv) Replace the exponentials of the matrices $A_{m+1}, \ldots, A_{\dim(\mathcal{L})}$ with expressions involving the exponentials of $\{A_1, \ldots, A_m\}$ as obtained from step (i).

(v) Replace every exponential e^{Bt}, ($B \in \mathcal{F}$) involving negative t with its approximation involving positive t. This can be obtained with arbitrary accuracy according to proposition 3.2 and remark 3.3.

We have already discussed in remark 1 the problem of solving equation (15). We give few more remarks on this method.

Remark 3.4. The last step of the method can be achieved exactly (i.e., without involving an approximation) if the orbits associated with the given matrices $\mathcal{F} := \{A_1, \ldots, A_m\}$ are periodic. In this respect, note that, if this is the case, all the other matrices obtained by the method also have associated periodic orbits. In fact their eigenvalues are the same as those of the original matrices. Therefore, for a given matrix B, and negative $\bar{t}$, we can choose a positive t, such that $e^{Bt} = e^{B\bar{t}}$. This suggests to use the flexibility in the choice of the initial matrices $\mathcal{F}$ in (5) in order to be in this situation, if possible. The only requirement on $\mathcal{F}$ is in fact to be a set of linearly independent generators of $\mathcal{L}$. The procedure implies the following simple corollary.

Corollary 3.5. *If $\mathcal{F}$ is a set of generator matrices for a Lie algebra $\mathcal{L}$ then there exists a basis of $\mathcal{L}$ whose matrices have the same spectrum as the elements of $\mathcal{F}$.*

Remark 3.6. Step (v) of the procedure introduces an error in the approximation of $e^{\frac{A}{M}}$ which then is (possibly) amplified by repeating this approximation M times. In order to control the error one proceeds as follows. Assume δ is given which is the maximum tolerable error in the procedure. Moreover, step (3) of the procedure has given a value for M and there are r exponentials in the expression of $e^{\frac{A}{M}}$ with negative t. The choice of $\epsilon < \frac{\delta}{rM}$ in (11) and (13) guarantees that the final error is $< \delta$. In order to see this let us denote by $e^{\frac{A}{M}}{}_{\text{appr}}$ the approximation of $e^{\frac{A}{M}}$ where the exponentials with negative times are replaced with their approximations with positive times according to the above procedure. We approximate e^A with $\left[e^{\frac{A}{M}}{}_{\text{appr}}\right]^M$. Using formula (A.5), we have

$$\left\| e^A - \left[e^{\frac{A}{M}}{}_{\text{appr}} \right]^M \right\| \leqslant M \left\| e^{\frac{A}{M}} - e^{\frac{A}{M}}{}_{\text{appr}} \right\|. \tag{16}$$

Write $e^{\frac{A}{M}} := \prod_{j=1}^r P_j N_j$, where the Ps (Ns) denote exponentials with nonnegative (negative) times, and $e^{\frac{A}{M}}{}_{\text{appr}} := \prod_{j=1}^r P_j \tilde{N}_j$, where $\tilde{N}_j$ is the approximation of N_j. A straightforward induction argument[3] shows that

$$\left\| e^{\frac{A}{M}} - e^{\frac{A}{M}}{}_{\text{appr}} \right\| = \left\| \prod_{j=1}^r P_j N_j - \prod_{j=1}^r P_j \tilde{N}_j \right\| \leqslant \sum_{j=1}^r \left\| N_j - \tilde{N}_j \right\|. \tag{17}$$

Therefore by choosing $\epsilon < \frac{\delta}{rM}$ for all js we have $\left\| N_j - \tilde{N}_j \right\| < \frac{\delta}{rM}$, from (17) $\left\| e^{\frac{A}{M}} - e^{\frac{A}{M}}{}_{\text{appr}} \right\| < \frac{\delta}{M}$ and from (16) $\left\| e^A - \left[e^{\frac{A}{M}}{}_{\text{appr}} \right]^M \right\| < \delta$.

Remark 3.7. [6] It is interesting to analyze the problem of determining the number of factors involved in the factorization of e^A (and therefore M in (15)) and the related problem of determining the total time of control. This is a complicated problem in general whose solution depends on the specific situation at hand, i.e., set of available matrices $\mathcal{F}$ in (5) and the final condition X_f. To illustrate some of the issues involved, let us first consider the simplified case where all the matrices in $\mathcal{F}$ have associated periodic orbits in (6). Therefore we first neglect the problem of negative times. To simplify the discussion, we shall also assume that the period is the same for all matrices and we shall denote it by T. The number of exponentials involved in obtaining a neighborhood of the identity in $e^{\mathcal{L}}$ depends on how the matrices in $\mathcal{F}$ combine in Lie brackets to give a basis of $\mathcal{L}$. One may for example be able to generate $\dim \mathcal{L} - m$ new linearly independent matrices with only one Lie bracket among the elements in $\mathcal{F}$ or need *repeated* Lie bracket, in which case, the number of factors grows. In the worst case, we only produce one new linearly independent matrix at every step. In this case, the total number of exponentials at step j is [6] $d_j = 2d_{j-1} + d_{j-2}$, having defined recursively the numbers d_j as

$$d_0 = 1, \qquad d_1 = 3, \qquad d_j = 2d_{j-1} + d_{j-2}, \tag{18}$$

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[3] It is clear that $\| P_1 N_1 - P_1 \tilde{N}_1 \| = \| N_1 - \tilde{N}_1 \|$ from properties of the Frobenius norm since P_1 is unitary. If $r > 1$, we have

$$\left\| \left(\prod_{j=1}^{r-1} P_j \tilde{N}_j \right) P_r \tilde{N}_r - \left(\prod_{j=1}^{r-1} P_j N_j \right) P_r N_r + \left(\prod_{j=1}^{r-1} P_j N_j \right) P_r \tilde{N}_r - \left(\prod_{j=1}^{r-1} P_j N_j \right) P_r \tilde{N}_r \right\|$$

$$\leqslant \left\| \prod_{j=1}^{r-1} P_j \tilde{N}_j - \prod_{j=1}^{r-1} P_j N_j \right\| + \| N_r - \tilde{N}_r \| \leqslant \sum_{j=1}^r \| N_j - \tilde{N}_j \|,$$

where we used the fact that all the matrices are unitary and, in the last step, the inductive assumption.

and the number of exponentials required is $md_0 + \sum_{j=1}^{\dim \mathcal{L}-m} d_j$.[4] The sum of the times needed to obtain $e^{\frac{A}{M}}$ also grows with the number of steps (Lie brackets) needed to generate a basis of $\mathcal{L}$. Let us now assume for simplicity that only one Lie bracket (i.e., no repeated Lie bracket) is needed in order to obtain a basis of $\mathcal{L}$ and therefore we can generate a basis of $\mathcal{L}$ using elements in $\mathcal{F}$ and similarity transformations of the form (10) only (without iterating the procedure further). The interval of time used in the exponential of every element of $\mathcal{F}$ is at most T while for every element of the form F in (10) is at most $2T$ (T to implement the similarity transformation and at most T in the exponential of A_k in (10)). Therefore in a time at most $mT + 2(\dim \mathcal{L} - m)T$ we can 'cover' a neighborhood K of the identity in $e^{\mathcal{L}}$ and therefore implement $e^{\frac{A}{M}}$ for M sufficiently large. How large this M has to be depends on the 'size' of the neighborhood K. However, to the best of the author's knowledge, it is not known how to determine M in general. If it was, we could give a bound on the *order of generation* of a compact Lie group[5]. The problem of determining the order of generation has been the subject of much research but results are known only for special cases (e.g., $SU(2)$ [19]). Finally, if we do not assume periodic orbits, the total time of implementation is typically much larger because we might have to take $\bar{t}$ quite large in (13) in order to satisfy the bound on the error.

3.3. Example

We illustrate this method with a simple example of the quantum control of a two level system, i.e., a control problem on $SU(2)$, which is compact. Recall the definition of the Pauli matrices

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y := \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \qquad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{19}$$

Let $\mathcal{F} := \{A_1, A_2\}$, with $A_1 := i\sigma_z$ and $A_2 := i(\sigma_x + \sigma_y)$. Calculate $e^{A_1 \bar{t}} A_2 e^{-A_1 \bar{t}}$ which for $\bar{t} = -\frac{3}{8}\pi$ gives $A_3 = -i\sqrt{2}\sigma_y$, which is linearly independent of A_1 and A_2, and, along with them, forms a basis of $su(2)$. A straightforward calculation gives

$$e^{A_1 t_1} = \begin{pmatrix} e^{i t_1} & 0 \\ 0 & e^{-i t_1} \end{pmatrix}, \quad e^{A_2 t_2} = \begin{pmatrix} \cos(\sqrt{2}t_2) & e^{i\frac{3\pi}{4}} \sin(\sqrt{2}t_2) \\ -e^{-i\frac{3\pi}{4}} \sin(\sqrt{2}t_2) & \cos(\sqrt{2}t_2) \end{pmatrix}, \tag{20}$$

$$e^{A_3 t_3} = \begin{pmatrix} \cos(\sqrt{2}t_3) & \sin(\sqrt{2}t_3) \\ -\sin(\sqrt{2}t_3) & \cos(\sqrt{2}t_3) \end{pmatrix},$$

and the set

$$S_{1,2,3} := \left\{ e^{A_1 t_1} e^{A_2 t_2} e^{A_3 t_3} | t_1, t_2, t_3 \in \mathbf{R} \right\}, \tag{21}$$

---

[4] It must be remarked also that due to a result in [11, lemma IV.5.17] in general $\dim \mathcal{L} = \dim e^{\mathcal{L}}$ exponentials of elements of $\mathcal{F}$ are sufficient to obtain a neighborhood of the identity in $e^{\mathcal{L}}$. The author would like to thank R Zeier for pointing out this reference.

[5] Given a set of generators $\mathcal{F}$ of a Lie algebra $\mathcal{L}$, the order of generation is the number of factors, in the products of alternate exponentials of elements of $\mathcal{F}$, needed in order to express every element of the Lie group $e^{\mathcal{L}}$. Assume that with a certain number d of exponentials we can obtain all the elements in a neighborhood K of the identity. Therefore for every X_f we can find M so that $X_f^{\frac{1}{M}} \in K$. Assume now that we were able to associate with each X_f the minimum $M = M(X_f)$ for which this is possible. Such $M = M(X_f)$ has to be uniformly bounded over X_f because if it was unbounded this would contradict the known result about uniform finite generation of compact Lie group (cf [6]) (essentially a consequence of the compactness of $e^{\mathcal{L}}$). If $M_{\max}$ is this bound, $M_{\max}d$ is a bound on the order of generation.

covers a neighborhood of the identity in $SU(2)$. Assume now the target state X_f is

$$X_f := \begin{pmatrix} \frac{1}{\sqrt{2}} & i\frac{1}{\sqrt{2}} \\ i\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}. \tag{22}$$

We first try to see if X_f is in the set $S_{1,2,3}$ in (21). Therefore we must be able to choose t_1 and t_3 so that $P := e^{-A_1 t_1} X_f e^{-A_3 t_3}$ has the form $e^{A_2 t_2}$. This means in particular that the difference between the phases of the $P_{1,2}$ element and $P_{1,1}$ elements in P is $\frac{3\pi}{4}$. As a straightforward calculation shows, $P_{1,2} P_{1,1}^* = \frac{i}{2}$ independently of the choice of t_1 and t_3. Therefore $X_f \notin S_{1,2,3}$. We replace X_f with $X_f^{\frac{1}{2}}$. The same calculation shows that, for every t_1, $P_{1,2} P_{1,1}^* = \frac{\sqrt{2}}{2} \sin(2\sqrt{2} t_3) + i\frac{\sqrt{2}}{2}$ and, therefore, the choice $t_3 := \frac{3\pi}{4\sqrt{2}}$ achieves the desired phase difference. Then, we can choose t_1 to impose that the element $P_{1,1}$ has phase zero (it is real). This leads to $t_1 = \frac{9\pi}{8}$. With these choices, we have

$$e^{-A_1 t_1} X_f^{\frac{1}{2}} e^{-A_3 t_3} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} e^{i\frac{3\pi}{4}} \\ -\frac{1}{\sqrt{2}} e^{-i\frac{3\pi}{4}} & \frac{1}{\sqrt{2}} \end{pmatrix}. \tag{23}$$

Comparing this with $e^{A_2 t_2}$ in (20) leads to the choice $t_2 = \frac{\pi}{4\sqrt{2}}$. With these choices $X_f = (e^{A_1 t_1} e^{A_2 t_2} e^{A_3 t_3})^2$.

In terms of the original available matrices, A_1 and A_2, we have

$$X_f = \left(e^{A_1 t_1} e^{A_2 t_2} e^{-A_1 \frac{3\pi}{8}} e^{A_2 t_3} e^{A_1 \frac{3\pi}{8}} \right)^2, \tag{24}$$

where t_1, t_2, t_3 are those found above. The presence of the negative 'time' $-\frac{3\pi}{8}$ in the third exponential does not pose any problems since the one-dimensional subgroup associated with A_1 (as well as any other matrix in $su(2)$) is periodic.

A similar treatment shows that had we chosen to work with the set

$$S_{1,3,2} := \left\{ e^{A_1 t_1} e^{A_3 t_3} e^{A_2 t_2} | t_1, t_2, t_3 \in \mathbf{R} \right\}, \tag{25}$$

we would have achieved X_f with just three exponentials. This shows that the order in which the exponentials are chosen may be important.

It must be said that for the special case of $SU(2)$ there are many more techniques which may be preferable to that advocated here. For example, since one has available both $i\sigma_z$ and $i\sigma_y$ one could have applied a simple Euler decomposition. It is also possible, for general target matrices, to find the factorization with the minimum number of factors [5]. Our goal here was to illustrate the method on a simple, easily computable, case. We remark that even for large dimensional Lie groups, one can combine these ideas with Lie group decompositions for which there exists a large set of tools [9].

4. Method 2: constructive controllability with arbitrarily small error

In this and the following section, we illustrate methods which do not require the solution of nonlinear algebraic equations, such as (8), but can be implemented with simple linear algebraic techniques. The algorithms achieve control to the target with arbitrary small error.

Reconsider the available set of matrices $\mathcal{F}$ in (5). As before, we relax the requirement to use only elements in the semigroups (6) and use elements in the subgroups (7). We can then replace elements in the subgroups with elements in the semigroups as done in the previous section. We start with a definition.

Definition 4.1. *A matrix H is said to be simulable with the set $\mathcal{F}$ if there exist r continuous, strictly increasing, functions f_j, $j = 1, \ldots, r$, with $f_j(0) = 0$, defined in an interval $[0, \epsilon)$, such that*

$$\mathrm{e}^{Hx} = \prod_{j=1}^{r} \mathrm{e}^{L_j f_j(x)} + O(x^{1+\delta}), \tag{26}$$

for some matrices $L_j \in \mathcal{F} \bigcup -\mathcal{F}$ and[6] a $\delta > 0$.

Remark 4.2. This definition is reminiscent of the problem of *Hamiltonian quantum simulation* in quantum computation (cf [3, 22] and references therein). The problem of Hamiltonian simulation is the problem of implementing (or approximating) an evolution e^{Hx}, for every x, with a quantum circuit, i.e., with a sequence of unitary transformations. According to formula (26), if an Hamiltonian is simulable, we can approximate e^{Hx} with a sequence of unitary evolutions obtained by evolving according to L_j's. This approximation improves with x small at a rate better than linear in x, because $\delta > 0$.

Lemma 4.3. *Assume (26) holds. Then*

$$\lim_{n \to \infty} \left(\prod_{j=1}^{r} \mathrm{e}^{L_j f_j(\frac{1}{n})} \right)^n = \mathrm{e}^{H} \tag{27}$$

Proof. If (26) holds then

$$\lim_{n \to \infty} \left(\prod_{j=1}^{r} \mathrm{e}^{L_j f_j(\frac{1}{n})} \right)^n = \lim_{n \to \infty} \left[\mathrm{e}^{H \frac{1}{n}} - O\left(\frac{1}{n^{1+\delta}} \right) \right]^n. \tag{28}$$

However, we have this standard limit in matrix analysis (see [12, section 6.5])

$$\lim_{n \to \infty} \left[\mathrm{e}^{H \frac{1}{n}} - O\left(\frac{1}{n^{1+\delta}} \right) \right]^n = \mathrm{e}^{H}, \tag{29}$$

which proves the lemma.

$\square$

From the point of view of constructive controllability, this lemma says that, for each simulable H, we can put together a product of exponentials of elements in $\mathcal{F} \bigcup -\mathcal{F}$ which, repeated a large enough number of times, approximates, with arbitrary accuracy, e^{H}.

Theorem 2. *Every H in the dynamical Lie algebra $\mathcal{L}$ is simulable.*

Remark 4.4. This theorem along with lemma 4.3 and proposition 3.2 give an alternative proof of a slightly weaker form of the Lie algebra rank condition of theorem 1. Since $\mathrm{e}^{\mathcal{L}}$ is compact, for every X_f in $\mathrm{e}^{\mathcal{L}}$, there exists $H \in \mathcal{L}$ such that $\mathrm{e}^{H} = X_f$. Theorem 2 and lemma 4.3 say that we can find a sequence of reachable points converging to X_f for every X_f. Therefore the set of reachable states is dense in $\mathrm{e}^{\mathcal{L}}$.

Elaborating on the proof of theorem 2, we will also show how to choose the elements $L_j \in \mathcal{F} \bigcup -\mathcal{F}$ and the functions f_j in (26) so as to make the controllability result constructive. We shall discuss this after the proof.

---

[6] $-\mathcal{F}$ denotes the set $\{-A_1, -A_2, \ldots, -A_m\}$.

Proof. The proof is similar to that given in [4] in the context of quantum walks dynamics. In particular, we will show that the set of simulable elements is a Lie algebra containing $\mathcal{F}$ and this will be sufficient since $\mathcal{L}$ is the smallest Lie algebra containing $\mathcal{F}$, by definition.

First of all, it is clear that every element in $\mathcal{F}$ is simulable, since equation (26) holds with $r = 1$ and $O \equiv 0$. Therefore the set of simulable matrices contains $\mathcal{F}$.

Moreover if H satisfies equation (26), then we have

$$e^{-Hx} = \prod_{j=r}^{1} e^{-L_j f_j(x)} - \prod_{j=r}^{1} e^{-L_j f_j(x)} O(x^{1+\delta}) e^{-Hx}, \tag{30}$$

and by expanding the exponentials it follows that the last term is also $O(x^{1+\delta})$. Therefore $-H$ is also simulable. Moreover, for $a \geqslant 0$, (26) holds for aH with $f_j(x)$ replaced by $f_j(ax)$ and $O(x^{1+\delta})$ replaced by $O(a^{1+\delta}x^{1+\delta}) = O(x^{1+\delta})$. If (26) holds for H_1 and H_2, i.e., we have

$$e^{H_i x} = \prod_{j=1}^{r_i} e^{L_j^i f_j^i(x)} + O_i(x^{1+\delta_i}), \qquad i = 1, 2, \tag{31}$$

combining this with

$$e^{(H_1+H_2)x} + O(x^2) = e^{H_1 x} e^{H_2 x}, \tag{32}$$

gives[7]

$$e^{(H_1+H_2)x} = \prod_{j=1}^{r_2} e^{L_j^2 f_j^2(x)} \prod_{j=1}^{r_2} e^{L_j^1 f_j^1(x)} + O(x^{1+\delta}), \tag{33}$$

with $\delta = \min\{\delta_1, \delta_2, 1\}$. Therefore, if H_1 and H_2 are simulable, so is $H_1 + H_2$. These arguments show that the set of simulable matrices is a vector space.

To show that it is also a Lie algebra, we have to show that if H_1 and H_2 are both simulable so is $[H_1, H_2]$. In order to see this, write (31) in the form

$$e^{H_1 t} = T_1(t) + O_1(t^{1+\delta_1}), \qquad e^{H_2 t} = T_2(t) + O_2(t^{1+\delta_1}), \tag{34}$$

i.e., by replacing the products with the functions T_1 and T_2. This also gives (cf (30))

$$\begin{aligned} e^{-H_1 t} &= T_1^{-1}(t) - T_1^{-1}(t) O_1(t^{1+\delta_1}) e^{-H_1 t}, \\ e^{-H_2 t} &= T_2^{-1}(t) - T_2^{-1}(t) O_2(t^{1+\delta_2}) e^{-H_2 t}. \end{aligned} \tag{35}$$

We use the exponential formula (see, e.g., [12, section 6.5])

$$e^{[H_1, H_2]t^2} + O(t^3) = e^{-H_1 t} e^{-H_2 t} e^{H_1 t} e^{H_2 t}. \tag{36}$$

Using (34) and (35) in (36), we have

$$\begin{aligned} e^{[H_1, H_2]t^2} + O(t^3) = {} & \left(T_1^{-1} - T_1^{-1} O_1 e^{-H_1 t}\right) \left(T_2^{-1} - T_2^{-1} O_2 e^{-H_2 t}\right) \\ & \times (T_1 + O_1)(T_2 + O_2). \end{aligned} \tag{37}$$

Expanding the right-hand side, omitting terms that are clearly $O(t^\alpha)$, $\alpha > 2$, since they contain the product of two O functions, we have

$$\begin{aligned} e^{[H_1, H_2]t^2} + O(t^3) = {} & T_1^{-1} T_2^{-1} T_1 T_2 + T_1^{-1} T_2^{-1} T_1 O_2 + T_1^{-1} T_2^{-1} O_1 T_2 \\ & - T_1^{-1} T_2^{-1} O_2 e^{-H_2 t} T_1 T_2 + T_1^{-1} O_1 e^{-H_1 t} T_2^{-1} T_1 T_2 + O(t^\alpha). \end{aligned} \tag{38}$$

---

[7] Here and elsewhere, we use the notation O for a generic O-function and we use indices like in O_1 and O_2 when we want to highlight a particular O-function.

Expanding in McLaurin series the functions multiplying O_1 and O_2, we see that the terms corresponding to the first terms of the expansion cancel, leaving only terms of the form $O(t^{\beta'})$ with $\beta' > 2$. In conclusion, we have

$$\mathrm{e}^{[H_1,H_2]t^2} = T_1^{-1}(t)T_2^{-1}(t)T_1(t)T_2(t) + O(t^\beta), \qquad \beta > 2, \tag{39}$$

and by setting $t = \sqrt{x}$, we obtain

$$\mathrm{e}^{[H_1,H_2]x} = T_1^{-1}(\sqrt{x})T_2^{-1}(\sqrt{x})T_1(\sqrt{x})T_2(\sqrt{x}) + O(x^{\frac{\beta}{2}}), \qquad \beta > 0, \tag{40}$$

which shows that $[H_1, H_2]$ is simulable as well, and completes the proof.

$\square$

In order to use lemma 4.3 and theorem 2 for control, we need to show how, given H, one can find the matrices L_j in $\mathcal{F} \bigcup -\mathcal{F}$ so that (26) holds. We first find a basis of $\mathcal{L}$ by taking repeated Lie brackets of elements in $\mathcal{F}$. More precisely, set

$$\mathcal{D}_0 := \mathcal{F}, \tag{41}$$

a linearly independent set of elements of '*depth*' 0 (no Lie bracket necessary), and let

$$\tilde{\mathcal{D}}_1 := [\mathcal{D}_0, \mathcal{F}], \tag{42}$$

a set of elements of depth 1, which are Lie brackets of elements of depth 0 with elements of $\mathcal{F}$. From the set $\tilde{\mathcal{D}}_1$ we extract a, possibly smaller, set $\mathcal{D}_1$ such that $\mathcal{D}_0 \bigcup \mathcal{D}_1$ is a maximal linearly independent set in $\mathcal{D}_0 \bigcup \tilde{\mathcal{D}}_1$. We then calculate a set of Lie brackets of depth 2

$$\tilde{\mathcal{D}}_2 := [\mathcal{D}_1, \mathcal{F}], \tag{43}$$

and extract a subset $\mathcal{D}_2 \subseteq \tilde{\mathcal{D}}_2$ so that $\mathcal{D}_0 \bigcup \mathcal{D}_1 \bigcup \mathcal{D}_2$ is a maximal linearly independent set in $\mathcal{D}_0 \bigcup \mathcal{D}_1 \bigcup \tilde{\mathcal{D}}_2$. Proceeding this way, we obtain a set $\bigcup_{k=0}^r \mathcal{D}_k$, which spans all of $\mathcal{L}$. As a consequence of $\mathcal{L}$ being finite dimensional, the procedure will end at some finite depth r after which we cannot find any new linearly independent matrix. Consider now the basis of $\mathcal{L}$ which we have found with this procedure $\{A_1, \ldots, A_{\dim \mathcal{L}}\}$. With each A_j is associated a depth equal to $0, 1, \ldots, r$. We decompose H as

$$H = \sum_{k=1}^{\dim \mathcal{L}} \alpha_k A_k, \tag{44}$$

and write, following the theorem,

$$\mathrm{e}^{Hx} = \prod_{k=1}^{\dim \mathcal{L}} \mathrm{e}^{\alpha_k A_k x} + O(x^{1+\delta}). \tag{45}$$

Then we rewrite each of $\mathrm{e}^{\alpha_k H_k x}$ according to the procedure of the theorem. This is straightforward for depth equal to 0 and it has to be done iteratively for Lie brackets of higher depth. Summarizing the method is as follows:

(1) Find a basis for $\mathcal{L}$ by repeated Lie brackets of elements of $\mathcal{F}$.
(2) Expand H along this basis as in (44). Then one has (45).
(3) For each factor approximate the exponential with a product of exponentials involving elements in $\mathcal{F} \cup -\mathcal{F}$ according to the proof of theorem 2. In particular, the rules to obtain the approximating products are as follows.

   (a) If $A \in \mathcal{F} \cup -\mathcal{F}$, then the associated product is $T(x) = \mathrm{e}^{Ax}$ (only one factor).
   (b) If $T(x)$ is the product associated with A, then $T^{-1}(x)$ is the product associated with $-A$.

(c) If $T(x)$ is the product associated with A, then $T(ax)$ is the product associated with aA for any $a \geqslant 0$.

(d) If $T_A(x)$ and $T_B(x)$ are the products associated with A and B respectively, then $T_A^{-1}(\sqrt{x})T_B^{-1}(\sqrt{x})T_A(\sqrt{x})T_B(\sqrt{x})$ is the product associated with $[A, B]$.

(4) Combine all the products in a unique product, approximating e^{Hx}, which contains only exponentials of elements in $\mathcal{F}$ and $-\mathcal{F}$. By repeating this product for $x = \frac{1}{n}$ a large number of times n we obtain a matrix arbitrarily close to e^H.

(5) Replace every exponential e^{At} with $A \in \mathcal{F}$ and $t < 0$ in the approximating product with an approximating exponential of the form $e^{A\bar{t}}$ with $\bar{t} > 0$, according to proposition 3.2 and remark 3.3.

4.1. Example

We illustrate the previous procedure with an example taken from the theory of electrical networks. In particular, we consider the LC switching network in [32] whose dynamical equation is given by

$$\dot{x} = \begin{pmatrix} 0 & -\nu & 0 & 0 \\ \nu & 0 & 0 & 0 \\ 0 & 0 & 0 & -\beta \\ 0 & 0 & \beta & 0 \end{pmatrix} x + \begin{pmatrix} 0 & 0 & 0 & \gamma \\ 0 & 0 & \delta & 0 \\ 0 & -\delta & 0 & 0 \\ -\gamma & 0 & 0 & 0 \end{pmatrix} xu(t), \tag{46}$$

where ν, β, γ and δ are positive parameters depending on the inductances and capacitances of the electrical network. The vector x represents voltages and currents in the network and u is a switching control variable which takes values in $\{0, 1\}$. To make the discussion concrete, we choose the parameters $\nu = 1$, $\beta = 3$, $\gamma = 1$ and $\delta = 2$, so that the set of available matrices is[8]

$$\mathcal{F} := \left\{ A_1 := \begin{pmatrix} 0 & -1 & 0 & 1 \\ 1 & 0 & 2 & 0 \\ 0 & -2 & 0 & -3 \\ -1 & 0 & 3 & 0 \end{pmatrix}, \qquad A_2 := \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -3 \\ 0 & 0 & 3 & 0 \end{pmatrix} \right\}. \tag{47}$$

The solution to (46) is

$$x(t) = X(t)x(0), \tag{48}$$

where $X = X(t)$ is the solution of the matrix equation

$$\dot{X} = A(u)X, \qquad X(0) = \mathbf{1}, \quad A(1) = A_1, \quad A(0) = A_2. \tag{49}$$

Let us use the notation E_{jk} for the skew-symmetric, 4×4, matrix which has all the entries equal to zero except for the (jk)-th and (kj)-th ($1 \leqslant j < k \leqslant 4$) which are equal to 1 and -1, respectively. Therefore, we can write

$$A_1 = -E_{12} + E_{14} + 2E_{23} - 3E_{34}, \qquad A_2 = -E_{12} - 3E_{34}. \tag{50}$$

By calculating Lie brackets, at depth 1, we obtain

$$A_3 := [A_2, A_1] = -5E_{12} + 7E_{24}, \tag{51}$$

at depth 2

$$A_4 := [A_3, A_1] = 17E_{12} + 22E_{14} + 26E_{23} + 19E_{34}, \quad \text{and} \quad A_5 := [A_3, A_2] = 22E_{14} + 26E_{23}. \tag{52}$$

---

[8] Note that although the example is taken from the theory of electrical networks, it could also have been a model for a four-level quantum system where the control switches between two Hamiltonians A_1 and A_2. A_1 couples levels 1 and 2, and levels 3 and 4, 1 and 4, and, 2 and 3. A_2 couples only levels 1 and 2 and levels 3 and 4.

At depth 3, we obtain

$$A_6 := [A_4, A_1] = 145 E_{13} - 155 E_{24}. \tag{53}$$

As the matrices $\{A_l\}$, $l = 1, \ldots, 6$, are linearly independent, they span all of $so(4)$ and the state X of system (49) varies on the Lie group $SO(4)$, a compact Lie group.

Let us denote by $T_j = T_j(x)$ the products approximating $e^{A_j x}$, $j = 1, \ldots, 6$, and let us assume that the control problem is to transfer the state $[0, 0, 0, 1]^T$ to $[1, 0, 0, 0]^T$. We choose to drive the transition matrix X in (49) to the value

$$e^{A_5 \frac{\pi}{44}} = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & \cos(\frac{13\pi}{22}) & \sin(\frac{13\pi}{22}) & 0 \\ 0 & -\sin(\frac{13\pi}{22}) & \cos(\frac{13\pi}{22}) & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}. \tag{54}$$

We proceed using the composition rules illustrated in (a)–(d) above. Since $A_5 = [A_3, A_2]$, we have

$$T_5(x) = T_3^{-1}(\sqrt{x}) T_2^{-1}(\sqrt{x}) T_3(\sqrt{x}) T_2(\sqrt{x}). \tag{55}$$

Moreover, since $A_3 = [A_2, A_1]$ we have

$$T_3(x) = T_2^{-1}(\sqrt{x}) T_1^{-1}(\sqrt{x}) T_2(\sqrt{x}) T_1(\sqrt{x}), \tag{56}$$

and replacing into (55), we obtain

$$T_5(x) =$$
$$T_1^{-1}(\sqrt[4]{x}) T_2^{-1}(\sqrt[4]{x}) T_1(\sqrt[4]{x}) T_2(\sqrt[4]{x}) T_2^{-1}(\sqrt{x}) T_2^{-1}(\sqrt[4]{x}) T_1^{-1}(\sqrt[4]{x}) T_2(\sqrt[4]{x}) T_1(\sqrt[4]{x}) T_2(\sqrt{x}). \tag{57}$$

The product approximating $e^{A_5 \frac{\pi}{44} t}$ is $T_5(\frac{\pi}{44} t)$ which we can express in terms of exponentials of A_1 and A_2 only by replacing T_1 and T_2 (and T_1^{-1} and T_2^{-1}) according to the rules in (a) and (b) above. In conclusion, we have

$$T_5\left(\frac{\pi}{44} t\right) = e^{-A_1(\frac{\pi}{44} t)^{\frac{1}{4}}} e^{-A_2(\frac{\pi}{44} t)^{\frac{1}{4}}} e^{A_1(\frac{\pi}{44} t)^{\frac{1}{4}}} e^{A_2(\frac{\pi}{44} t)^{\frac{1}{4}}} e^{-A_2(\frac{\pi}{44} t)^{\frac{1}{2}}} \tag{58}$$

$$\times e^{-A_2(\frac{\pi}{44} t)^{\frac{1}{4}}} e^{-A_1(\frac{\pi}{44} t)^{\frac{1}{4}}} e^{A_2(\frac{\pi}{44} t)^{\frac{1}{4}}} e^{A_1(\frac{\pi}{44} t)^{\frac{1}{4}}} e^{A_2(\frac{\pi}{44} t)^{\frac{1}{2}}}.$$

I calculated the error

$$\text{Err}^2(n) = \left\| e^{A_5 \frac{\pi}{44}} - \left[T_5\left(\frac{\pi}{44} \frac{1}{n}\right) \right]^n \right\|^2 = 8 - 2\text{Tr}\left[\left(T_5\left(\frac{\pi}{44} \frac{1}{n}\right) \right)^n e^{A_5^T \frac{\pi}{44}} \right], \tag{59}$$

numerically, for various values of n and the behavior of this error as a function of the number of iterations n is reported in table 1. The error goes to zero as predicted by the above treatment. In a log–log scale the behavior is essentially linear.

To conclude the example we have to solve the problem that negative times are not allowed (point (5) of the above procedure) and therefore we have to replace terms of the form $e^{-A_1 x_1}$ and $e^{-A_2 x_2}$, with $x_{1,2} > 0$, in the expression of T_5, with approximations of the form $e^{A_1 \tilde{x}_1}$ and $e^{A_2 \tilde{x}_2}$, $\tilde{x}_{1,2} > 0$, respectively. In the case of A_2, since $\{e^{A_2 t} | t \in \mathbf{R}\}$ is periodic we can always find $\tilde{x}_1 > 0$ such that $e^{-A_2 x_1} = e^{A_2 \tilde{x}_1}$ for every $x_1 > 0$, and we can simply replace the exponential with x_1 with the exponential with $\tilde{x}_1$ in T_5, without changing the error. For the exponentials of A_1, however, we need to find an approximation and this is always possible with arbitrary accuracy according to proposition 3.2 and remark 3.3. We present a numerical treatment of the example in the appendix.

Table 1. Results of numerical experiments for the method in section 4.

Number of iterations, n	Error, Err
2	3.1531
10	2.3964
20	2.0500
30	1.8604
100	1.3761
500	0.9089
1000	0.7599
5000	0.5022
50 000	0.2791
100 000	0.2341
500 000	0.1558
1 000 000	0.1301
5 000 000	0.0873
10 000 000	0.0733
50 000 000	0.0490
100 000 000	0.0411

5. Combination of the two methods

The main ideas in the two methods of control described in the previous sections can be combined in a third method. The main idea of the method in section 3 was to use similarity transformations to generate a basis of the dynamical Lie algebra $\mathcal{L}$ starting from the given matrices in $\mathcal{F}$ in (5) (cf (10)). The main idea of the method in section 4 is the use of the limit in lemma 4.3, once (26) holds. This allows us to control to the target, by repeating a given sequence of available exponentials, with arbitrary accuracy. We can combine the two ideas. We first use similarity transformations to obtain a basis of $\mathcal{L}$, $A_1, \ldots, A_{\dim \mathcal{L}}$. Then, if e^H is the target and $H = \sum_{j=1}^{\dim \mathcal{L}} \alpha_j A_j$, we use the fact that

$$e^{Hx} = e^{\sum_{j=1}^{\dim \mathcal{L}} \alpha_j A_j x} = \prod_{j=1}^{\dim \mathcal{L}} e^{\alpha_j A_j x} + O(x^2), \tag{60}$$

along with lemma 4.3 to approximate with arbitrary accuracy the target state, i.e.,

$$e^H = \lim_{n \to \infty} \left[\prod_{j=1}^{\dim \mathcal{L}} e^{\alpha_j A_j \frac{1}{n}} \right]^n. \tag{61}$$

At the end of the process, if necessary, we replace all the exponentials of the form $e^{A_j t}$ with $t < 0$ with approximating exponentials of the form $e^{A_j \bar{t}}$ with $\bar{t} > 0$.

I tested this method on the example in section 4.1. Given A_1 and A_2 in (47) we have

$$F := e^{A_2 \frac{\pi}{2}} A_1 e^{-A_2 \frac{\pi}{2}} = \begin{pmatrix} 0 & -1 & 0 & 2 \\ 1 & 0 & 1 & 0 \\ 0 & -1 & 0 & -3 \\ -2 & 0 & 3 & 0 \end{pmatrix}. \tag{62}$$

Our target is $e^{A_5 \frac{\pi}{44}}$ in (54). We have the decomposition

$$A_5 = 10A_1 + 6F - 16A_2, \tag{63}$$

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Table 2. Results of numerical experiments for the method in section 5.

Number of iterations, n	Error, Err
2	2.2819
10	0.4544
20	0.2267
50	0.0906
100	0.0453
1000	0.0045
10 000	0.0005

so that

$$e^{A_5 \frac{\pi}{44} x} = R_5(x) + O(x^2), \tag{64}$$

with

$$R_5(x) := e^{10A_1 \frac{\pi}{44} x} e^{6F \frac{\pi}{44} x} e^{-16A_2 \frac{\pi}{44} x}. \tag{65}$$

We have, according to lemma 4.3,

$$\lim_{n \to \infty} \left[R_5 \left(\frac{1}{n} \right) \right]^n = e^{A_5 \frac{\pi}{44}}. \tag{66}$$

Table 2 shows the results of numerical experiments with this scheme displaying the error Err as a function of the number of iterations. Compared with table 1, it is clear that this method converges much faster. Another advantage is that all the exponentials e^{At} with negative t are for $A = A_2$ (cf (65) and (62)) and the one-dimensional subgroup associated with A_2 is closed. Therefore no further approximation is needed.

For the method presented in this section a simple upper bound on the error can be obtained by extending the bound for the Trotter's formula given in [20].[9] Let us assume that there is no error due to the approximation of exponentials e^{At} with negative t. Therefore the only source of error is the approximation of the exponential of a sum with the product of exponentials. Recall that we have that $e^{\mathcal{L}}$ is a subgroup of the unitary group.

Proposition 5.1. *Let*

$$H := \sum_{j=1}^{k} A_j. \tag{67}$$

Then

$$\left\| e^H - \left(\prod_{j=1}^{k} e^{\frac{A_j}{m}} \right)^m \right\| \leqslant \frac{1}{2m} \sum_{j=1}^{k-1} \left\| \left[\sum_{l=1}^{j} A_l, A_{j+1} \right] \right\|. \tag{68}$$

In the application of the method, we have some freedom in choosing the matrices A_j in the expansion (67). The right-hand side of formula (68) shows that the error can be decreased by choosing as few matrices as possible and as many commuting matrices as possible. The error increases when we have to employ several non-commuting matrices and with the size of the commutators.

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[9] This bound can also be used in the method of section 4, but in that case it will have to be complemented by more estimates since the error is not only due to approximating the exponential of a sum with the product of exponentials. Errors are introduced in the approximation of the exponential of (nested) Lie brackets.

Proof. We prove that for every m,

$$\left\| e^{\frac{H}{m}} - \prod_{j=1}^{k} e^{\frac{A_j}{m}} \right\| \leqslant \frac{1}{2m^2} \sum_{j=1}^{k-1} \left\| \left[\sum_{l=1}^{j} A_l, A_{j+1} \right] \right\|, \tag{69}$$

and the result follows using formula (A.5). In fact, this result is already proven in [20, appendix B][10] for the case $k = 2$ and it follows by induction for general $k > 2$. In particular, write

$$\left\| e^{\frac{A}{m}} - \prod_{j=1}^{k} e^{\frac{A_j}{m}} \right\| = \left\| e^{\frac{A}{m}} - e^{\sum_{l=1}^{k-1} \frac{A_l}{m}} e^{\frac{A_k}{m}} + e^{\sum_{l=1}^{k-1} \frac{A_l}{m}} e^{\frac{A_k}{m}} - \prod_{j=1}^{k} e^{\frac{A_j}{m}} \right\| \tag{70}$$

$$\leqslant \left\| e^{\frac{A}{m}} - e^{\sum_{l=1}^{k-1} \frac{A_l}{m}} e^{\frac{A_k}{m}} \right\| + \left\| e^{\sum_{l=1}^{k-1} \frac{A_l}{m}} - \prod_{j=1}^{k-1} e^{\frac{A_j}{m}} \right\|,$$

where we have used the property that the Frobenius norm does not change by multiplication with a unitary matrix. By applying the inductive assumption to both terms of the last two terms above (in the first case the decomposition $A = (\sum_{l=1}^{k-1} A_l) + A_k$ is used) we obtain formula (69).

$\square$

6. Concluding remarks

The methods described in this paper can be seen as a constructive proof of the Lie algebra rank condition of theorem 1. They allow us to control any finite-dimensional right invariant system on a compact Lie group such as quantum systems subject to coherent control. It is expected that the ideas described above can be extended and improved by using more sophisticated exponential formulae [20] and by exploiting in various cases the inherent flexibility of the methods proposed. These, at every step, involve choices that when tailored to the problem at hand may significantly improve the performance of the control algorithms. It is also expected that it will be possible to obtain more estimates of the convergence rate and of the errors in various cases (as in proposition 5.1), by combining estimates known for exponential formulae.

Many techniques have been proposed for the coherent control of quantum-mechanical systems of the form (1) which apply to models with various assumptions. These techniques include Lie group decompositions (see, e.g., [7, 17, 26]), Lyapunov control (see, e.g., [30, 31]), optimal control (see, e.g., [28]) and several techniques of molecular control [24, 27]. These techniques assume additional structure in equation (1), often suggested by physical considerations, and/or require numerical solutions of differential equations, two points boundary value problems, numerical tuning of specific parameters, etc. One of the main motivations of these approaches was that the controllability result of theorem 1 is not constructive. In this paper, we have removed this obstacle and made this proof constructive so giving algorithms that can be applied *always*. In particular, the algorithms of sections 4 and 5 do not present any special difficulties from a mathematical point of view as they involve very well studied linear algebra operations such as calculating the exponential and the logarithm of a matrix and expanding a vector along a given basis. While I have not considered the problems which would arise in specific physical implementations, the strength of the proposed approach is in its generality and on the fact that, from a purely mathematical point of view, it always offers an alternative for any system of the form (1). One can also combine the methods

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[10] See in particular the proof of theorem 5, there noticing that Θ is zero in our case.

presented here with the other approaches in the literature above recalled. For example, using Lie group decompositions, one can decompose the target matrix X_f into the product of several factors for which the application of the method is particularly simple and/or efficient.

In the future, it will be of interest to improve the algorithms of the last two sections by minimizing the number of switches in the control laws. This mainly depends on the number of iterations. In this respect, the algorithm of section 5 is expected to be faster than the algorithm in section 4, as a consequence of the exponent 2, in $O(x^2)$ in (60) as opposed to the exponent $1+\delta$ (with δ typically < 1) in (26). If our main concern is however the time of implementation, the effect of an increasing number of iterations n in (28) is balanced by the $\frac{1}{n}$ exponents inside the limit. The main problem, in terms of time, is the approximation of matrices of the form e^{At} with $t < 0$ with matrices of the form e^{At}, with $t > 0$, in the case of non-closed subgroups (7). In fact, we might have to 'travel' for a long time inside the Lie group $e^{\mathcal{L}}$ before we get close enough to the original e^{At}. In special situations, however, it might be possible to transform A into $-A$ via available similarity transformations, or reduce ourselves to a smaller dimensional Lie subgroup where the problem is more easily tractable. Nevertheless, it is always possible to find such an approximation and therefore the control. Remark 3.3 shows how this problem can be reduced to a standard problem of Diophantine approximation in number theory for which there exists a vast literature and that can always be solved, in principle.

In conclusion, I would like to comment on the assumption of compactness and how this affects applications in quantum control. The assumption of compactness of the Lie group $e^{\mathcal{L}}$ is used in the paper only in two instances. It is used to have a surjective exponential map and to be able to approximate an exponential of the form e^{At} with t negative with an exponential of the same type with t positive. Whenever these two properties hold, the methods of this paper can still be applied to more general Lie groups. For finite-dimensional closed quantum-mechanical systems, the dynamical Lie algebra $\mathcal{L}$ is always a subalgebra of $u(n)$ and as a consequence it is always the direct sum of an Abelian Lie algebra and a semisimple one (cf, e.g., [8, 23]) and this ensures that the exponential map is still surjective. Moreover, although the Lie group $e^{\mathcal{L}}$ may not be compact (due to the presence of a nontrivial Abelian part in the Lie algebra $\mathcal{L}$) the considerations on approximating elements of the type e^{At} with $t < 0$ with elements of the type e^{At} with $t > 0$ can still be repeated, in the topology induced by the one of $U(n)$ which is compact. Therefore, these algorithms can be applied to the coherent control of finite-dimensional quantum systems in all cases.

Acknowledgments

Appendix. Numerical treatment of the error in the example of section 4.1

To be concrete let us assume that the maximum error we can tolerate is 0.4. From table 1, we choose $n = 10^5$. Fix $x := \frac{\pi}{44}10^{-5}$. We have (cf (59) and table 1)

$$\text{Err}(10^5) = \left\| e^{A_5 \frac{\pi}{44}} - (T_5(x))^{10^5} \right\| < 0.235. \tag{A.1}$$

Let $\tilde{T}_5$ be the approximation of T_5 in (58) where we only use positive values in the exponentials, appropriately replacing the exponentials of A_1. In particular, by rewriting $T_5(x)$ in (58) as

$$T_5(x) = \mathrm{e}^{-A_1 x^{\frac{1}{4}}} \Pi_1(x) \, \mathrm{e}^{-A_1 x^{\frac{1}{4}}} \Pi_2(x), \tag{A.2}$$

with $\Pi_1(x) = \mathrm{e}^{-A_2 x^{\frac{1}{4}}} \mathrm{e}^{A_1 x^{\frac{1}{4}}} \mathrm{e}^{A_2 x^{\frac{1}{4}}} \mathrm{e}^{-A_2 x^{\frac{1}{2}}} \mathrm{e}^{-A_2 x^{\frac{1}{4}}}$ and $\Pi_2(x) = \mathrm{e}^{A_2 x^{\frac{1}{4}}} \mathrm{e}^{A_1 x^{\frac{1}{4}}} \mathrm{e}^{A_2 x^{\frac{1}{2}}}$, we have

$$\tilde{T}_5 := \tilde{T}_5(x_1, x) = \mathrm{e}^{A_1 x_1} \Pi_1(x) \, \mathrm{e}^{A_1 x_1} \Pi_2(x). \tag{A.3}$$

Therefore the actual error $\tilde{E}rr$ is given by

$$\tilde{E}rr = \left\| \mathrm{e}^{A_5 \frac{\pi}{44}} - \left[\tilde{T}_5(x, x_1) \right]^{10^5} \right\| \leqslant \left\| \mathrm{e}^{A_5 \frac{\pi}{44}} - \left[T_5(x) \right]^{10^5} \right\| + \left\| \left[T_5(x) \right]^{10^5} - \left[\tilde{T}_5(x, x_1) \right]^{10^5} \right\|$$

$$< 0.235 + \left\| \left[T_5(x) \right]^{10^5} - \left[\tilde{T}_5(x, x_1) \right]^{10^5} \right\|, \tag{A.4}$$

where we used (A.1). Using the formula for A and B unitary matrices[11]

$$\|A^n - B^n\| \leqslant n \|A - B\|, \tag{A.5}$$

we write

$$\tilde{E}rr = < 0.235 + 10^5 \|T_5(x) - \tilde{T}_5(x, x_1)\|. \tag{A.6}$$

In view of our bound on the error of 0.4, we need to find $x_1 > 0$ so that $\|T_5(x) - \tilde{T}_5(x, x_1)\| \leqslant 0.165 \times 10^{-5}$. Now, we have

$$\left\| T_5 - \tilde{T}_5 \right\| = \left\| \mathrm{e}^{-A_1 x^{\frac{1}{4}}} \Pi_1 \, \mathrm{e}^{-A_1 x^{\frac{1}{4}}} \Pi_2 - \mathrm{e}^{A_1 x_1} \Pi_1 \, \mathrm{e}^{A_1 x_1} \Pi_2 \right\| = \left\| \Pi_1 - \mathrm{e}^{A_1 (x^{\frac{1}{4}} + x_1)} \Pi_1 \, \mathrm{e}^{A_1 (x^{\frac{1}{4}} + x_1)} \right\|. \tag{A.7}$$

Therefore we have

$$\left\| T_5 - \tilde{T}_5 \right\| \leqslant \left\| \Pi_1 - \mathrm{e}^{A_1 (x^{\frac{1}{4}} + x_1)} \Pi_1 \right\| \tag{A.8}$$

$$+ \left\| \mathrm{e}^{A_1 (x^{\frac{1}{4}} + x_1)} \Pi_1 - \mathrm{e}^{A_1 (x^{\frac{1}{4}} + x_1)} \Pi_1 \, \mathrm{e}^{A_1 (x^{\frac{1}{4}} + x_1)} \right\| = 2 \left\| \mathbf{1} - \mathrm{e}^{A_1 (x^{\frac{1}{4}} + x_1)} \right\|.$$

Therefore, we need to find $x_1 \geqslant 0$ so that

$$\left\| \mathbf{1} - \mathrm{e}^{A_1 (x^{\frac{1}{4}} + x_1)} \right\| \leqslant \frac{0.165 \times 10^{-5}}{2}. \tag{A.9}$$

We calculate explicitly the eigenvalues of A_1 which are given by $\pm i r$ and $\pm i l$, with r and l given by

$$r := \sqrt{\frac{15 + \sqrt{125}}{2}}, \qquad l := \sqrt{\frac{15 - \sqrt{125}}{2}}. \tag{A.10}$$

We have

$$\left\| \mathbf{1} - \mathrm{e}^{A_1 (x^{\frac{1}{4}} + x_1)} \right\| = 2 \sqrt{1 - \cos(r(x^{\frac{1}{4}} + x_1)) + 1 - \cos(l(x^{\frac{1}{4}} + x_1))}. \tag{A.11}$$

Therefore, setting $t := x^{\frac{1}{4}} + x_1$, formula (A.9) is certainly satisfied if

$$1 - \cos(rt) < 8 \times 10^{-14} \tag{A.12}$$

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[11] This formula is proved by writing $A^n - B^n = \sum_{k=1}^{n} A^{n-k} (A - B) B^{k-1}$, which gives

$$\left\| A^n - B^n \right\| \leqslant \sum_{k=1}^{n} \left\| A^{n-k} (A - B) B^{k-1} \right\| = n \|A - B\|,$$

since multiplication (right or left) by a unitary matrix does not modify the Frobenius norm.

and

$$1 - \cos(lt) < 8 \times 10^{-14}. \tag{A.13}$$

Setting $\epsilon := \arccos(1 - 8 \times 10^{-14})$, we need to find $t > x^{\frac{1}{4}}$, positive integers p and q such that

$$|rt - 2\pi p| < \epsilon, \qquad |lt - 2\pi q| < \epsilon. \tag{A.14}$$

One way to do this is as follows. Fix an integer $k > 0$ large enough so that

$$\frac{1}{k} < \frac{\epsilon}{2\pi}. \tag{A.15}$$

According to Dirichlet's approximation theorem (see, e.g., [25, theorem 1.3]) we can find p and q, with $1 \leqslant p \leqslant k$ positive integers so that

$$\left| \frac{l}{r} p - q \right| < \frac{1}{k}. \tag{A.16}$$

Choose p and q this way [2, 16] and

$$t = \frac{2\pi p}{r}. \tag{A.17}$$

Using this value of t, the first one of (A.14) is verified because the left-hand side becomes zero. Replacing this value of t in the second one of (A.14) and using (A.15) and (A.16) we obtain that the second inequality is satisfied as well. Moreover, since $q \geqslant 1$, we have that

$$t \geqslant \frac{2\pi}{r} \approx 1.7366 > x^{\frac{1}{4}} = \left(\frac{\pi}{44} 10^{-5} \right)^{\frac{1}{4}} \approx 0.0291. \tag{A.18}$$

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