Linear Algebra and its Applications 705 (2025) 207–229

Contents lists available at ScienceDirect

Linear Algebra and its Applications

journal homepage: www.elsevier.com/locate/laa

Quantum subspace controllability implying full controllability

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A R T I C L E   I N F O

Article history:
Received 30 July 2024
Received in revised form 30 October 2024
Accepted 1 November 2024
Available online 7 November 2024
Submitted by T. Damm

MSC:
81Q93
81R99
93B05
93B25
93B27

Keywords:
Subspace controllability
Controllability of quantum systems
Lie algebraic methods

A B S T R A C T

In the analysis of controllability of finite dimensional quantum systems, *subspace controllability* refers to the situation where the underlying Hilbert space splits into the direct sum of invariant subspaces, and, on each of such invariant subspaces, it is possible to generate any arbitrary unitary operation using appropriate control functions. This is a typical situation in the presence of symmetries for the dynamics.

We investigate whether and when if subspace controllability is verified, the addition of an extra Hamiltonian to the dynamics implies full controllability of the system. Under the natural (and necessary) condition that the new Hamiltonian connects all the invariant subspaces, we show that this is always the case, except for a very specific case we shall describe. Even in this specific case, a weaker notion of controllability, controllability of the state (*Pure State Controllability*) is verified.

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https://doi.org/10.1016/j.laa.2024.11.002

1. Introduction and main result

It is well known that the controllability properties of a finite dimensional quantum system can be assessed using the (*dynamical*) *Lie algebra* $\mathcal{L} := \{iH_1, ..., iH_m\}_{Lie}$ generated by the Hamiltonians $\{H_1, ..., H_m\}$ of the system, that is, the smallest Lie algebra (closed under commutation relation) which contains the skew-Hermitian matrices $\{iH_1, ..., iH_m\}$ [4], [7], [8], [9], [12]. In particular the set of reachable evolutions for the quantum system is (dense in) the connected Lie group associated with the Lie algebra $\mathcal{L}$. If $\mathcal{L} = u(n)$ ($su(n)$), the Lie algebra of $n \times n$ skew-Hermitian matrices (skew-Hermitian with zero trace), the set of reachable evolutions is the full set of unitary (special unitary) matrices and the system is said to be *operator controllable* [4] or also *completely controllable* [13]. We shall use the term '*fully controllable*' in this paper. If, up to an isomorphism, $\mathcal{L} := sp\left(\frac{n}{2}\right)$, the symplectic Lie algebra (with n necessarily even in this case), then the system is *pure state controllable*. In this case, the set of reachable evolutions is not the full unitary group but it is rich enough to allow transfer from any state to any other state. This is because the symplectic Lie group $Sp\left(\frac{n}{2}\right)$ is transitive on the complex unit sphere. Modulo the presence in the Lie algebra $\mathcal{L}$ of multiples of the identity matrix, which only add a multiplicative phase factor to the state, these are the only cases where arbitrary transfers between two states can be achieved [3], [7], [13].

It follows from the application of representation theory ideas [6] that, in the presence of a *group of symmetries*, that is, a group of matrices, which commute with all the Hamiltonians of the system, the Hilbert space of the system splits into the direct sum of a number of invariant subspaces. Therefore, in appropriate coordinates, the dynamics of the system appear in block diagonal form. As a simple example, consider two spin $\frac{1}{2}$ particles interacting via Ising interaction $H_1 = \sigma_z \otimes \sigma_z$, and subject to a common control magnetic field in the x direction which gives Hamiltonian $H_2 = \sigma_x \otimes \mathbf{1} + \mathbf{1} \otimes \sigma_x$ and in the y direction which gives Hamiltonian $H_3 = \sigma_y \otimes \mathbf{1} + \mathbf{1} \otimes \sigma_y$. Here $\mathbf{1}$ is the 2×2 identity matrix and $\sigma_{x,y,z}$ are the *Pauli matrices* defined by

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

The permutation group of two objects, which contains only the identity permutation and the exchange of 1 and 2, is a symmetry group for this system since all the Hamiltonians are invariant under the permutation of the 1 and 2 position. The Hilbert space splits into two invariant subspaces which are given, in this case, by the so-called *symmetric sector* spanned by $\left\{|00\rangle, |11\rangle, \frac{1}{\sqrt{2}}\left(|01\rangle + |10\rangle\right)\right\}$ and the *anti-symmetric sector* spanned by $\left\{\frac{1}{\sqrt{2}}\left(|01\rangle - 10\rangle\right)\right\}$. One can in fact immediately verify the invariance of these two subspaces under H_1, H_2, and H_3. We refer to [2] and [10] for the full case of symmetric networks of two level quantum systems (qubits) and to [5] for the treatment of symmetric networks of d-level systems for general d.

If a quantum system is fully controllable on each invariant subsystem the system is called *subspace controllable (SC)*. In the presence of subspace controllability one can think of performing universal quantum computation on one of the invariant subspaces and use the dynamics on the other spaces for other purposes, e.g., for quantum error correction and mitigation. Subspace controllability has been investigated and proved for various topologies of quantum networked systems in recent literature, in various contexts, (see, e.g., [2], [5], [10], [14], [15]).

The question we want to address in this paper is whether and when, in the presence of subspace controllability, the addition of one *extra Hamiltonian* to the dynamics would lead to full controllability of the quantum system, that is, the possibility of achieving any (special) unitary transformation on the whole Hilbert space. It is known that full controllability is, from a mathematical perspective, a *generic* property (see, e.g., [4], [11]). Therefore almost every extra Hamiltonian will do the job of giving full controllability. However, physical systems often present *symmetries*, which prevent full controllability. So to give a precise characterization of the set of extra Hamiltonians that do or do not re-establish full controllability is important from a physics perspective. We shall see that the set of Hamiltonians which do not lead to full controllability is, in fact, very slim, and we will describe it precisely.

Our investigation complements previous research in the literature where the considered vector space decomposition is as a *tensor product decomposition* of the underlying Hilbert space $\mathcal{H} = \otimes_j V_j$ and controllability is assumed on each space V_j. It is known [16] (cf. also [1] for the spin $\frac{1}{2}$ case) that controllability on each of the spaces V_j's, that is, *local* controllability together with the presence of an extra Hamiltonian which 'connects' the various subsystems in an appropriate sense, is sufficient to obtain full controllability. In this tensor-local case, there is no permutation symmetry in the system as local transformations are not required to be the same on each of the subsystems. On the other hand, the presence of a group of permutation symmetries is often the decisive factor which leads to the (direct sum) vector space splitting we are considering as in the example above described.

In studying subspace controllability we shall neglect the consideration of common phase factors (multiples of the identity) on each invariant subspace which determine the allowed phase differences between the various subspaces and we shall assume that the Lie algebra on each subspace of dimension n_j is $su(n_j)$. We shall remove this restriction at the end of the paper, in section 4. We shall also assume that the dimension n_j of each invariant subspace is ≥ 2. In the case where one subspace has dimension $n_j = 1$, one cannot in principle talk about subspace controllability since the Lie group $SU(1)$ which is just the identity matrix is not transitive on the one dimensional circle. Still we shall discuss some generalizations of the main theorem of this paper to this setting in section 4.

Subspace controllability comes in two flavors and variations of them. They were named *strong* and *weak* in [5] and we shall use this terminology here as well. In the strong case, not only $\mathcal{L}$ acts as $su(n_j)$ on every invariant subspace of dimension n_j, but the various elements in $su(n_j)$ can be chosen *independently* one from the other. Therefore, in the chosen coordinates, matrices in $\mathcal{L}$ appear as block diagonal matrices $\text{diag}(A_1, A_2, ..., A_M)$ with A_j arbitrary in $su(n_j)$, $j = 1, ..., M$, with n_j the dimension of the j-th invariant subspace. In the weak case, the matrices $\{A_1, A_2, ..., A_M\}$ are related to each other. A result proved in [5] (Lemma 8 therein) shows that if the dimension n_j and n_k are different then A_j and A_k must be independent of each other. Therefore, if the dimensions n_j are all different, only the strong case is possible. If two dimensions n_j and n_k are equal, then it is possible that A_j determines A_k and, in fact, modulo a coordinate transformation in one of the two subspaces we can assume $A_j = A_k$. Obviously, mixed cases are also possible between weak and strong with many possible situations. In this paper, we shall consider only the case of strong SC, that is, we will assume that $\mathcal{L}$ is spanned by matrices of the form $\text{diag}(A_1, A_2, ..., A_M)$ with A_j, $j = 1, ..., M$, arbitrary in $su(n_j)$, and independent of each other.[1]

As anticipated, our goal is to study under what conditions, in the presence of strong subspace controllability, as defined above, and under the above assumptions, the addition of an extra Hamiltonian, which we will denote by H_{extra}, will result in full controllability for the system. Defined $\tilde{\mathcal{L}}$ the dynamical Lie algebra generated by $\mathcal{L}$ and the new extra Hamiltonian iH_{extra}, that is,

$$\tilde{\mathcal{L}} := \{\mathcal{L}, iH_{extra}\}_{Lie},$$

we investigate when $\tilde{\mathcal{L}} = su(n)$, with $n = n_1 + n_2 + \cdots + n_M$. The matrix iH_{extra} will, in principle, be completely general. However a necessary condition for full controllability will be that H_{extra} contains off diagonal nonzero blocks 'connecting' the various indexes (subspaces). In a graph with M edges each representing a block (that is a subspace), 1 through M, there exists a path from 1 to M such that for any edge (a, b) the corresponding block of H_{extra} is different from zero. We shall use a *connectivity graph* for the extra Hamiltonian where the nodes represent the subspaces 1 through M and an edge connects two nodes a and b if the corresponding blocks of H_{extra} (C_{ab} and $-C_{ab}^\dagger$ in (2) below) are different from zero. We shall assume such a graph to be connected. This excludes the possibility of bigger invariant subspaces. We shall call such a type of extra Hamiltonian a '*connecting*' Hamiltonian. Since $\mathcal{L}$ contains all matrices, which are block diagonal, i.e. $A = \text{diag}(A_1, \ldots, A_M)$, with $A_j \in su(n_j)$, without loss of generality we may assume that the extra Hamiltonian has the following block form:

[1] The above recalled splitting of the Hilbert space due to the presence of a group of symmetry S is a consequence of what is known as *Schur-Weyl duality.* The duality implies that irreducible representations of S of dimension m_S which appear with multiplicity d_S give rise to m_S isomorphic irreducible (standard) representations of $u(d_S)$, that is, the dimension and multiplicity of irreducible representations are exchanged between S and the unitary group (Lie algebra). The case where the representations of $u(n_S)$ appear with multiplicity 1 corresponds to irreducible representations of S of dimension 1, as for the case of *Abelian groups.* We refer to [6] for details.

$$iH_{extra} = \begin{pmatrix} 0 & C_{12} & C_{13} & \dots & C_{1M} \\ -C_{12}^\dagger & 0 & C_{23} & \dots & C_{2M} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ -C_{1M}^\dagger & -C_{2M}^\dagger & -C_{3M}^\dagger & \dots & 0 \end{pmatrix} + \begin{pmatrix} i\lambda_1 \mathbf{1}_{n_1} & 0 & 0 & \dots & 0 \\ 0 & i\lambda_2 \mathbf{1}_{n_2} & 0 & \dots & \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & & \dots & i\lambda_M \mathbf{1}_{n_M} \end{pmatrix} \tag{2}$$

where each C_{jk} is a general complex $n_j \times n_k$ matrix, $\mathbf{1}_{n_j}$ is the identity matrix of dimension n_j, $\lambda_1, \lambda_2, ..., \lambda_N$ real numbers with $\sum_{j=1}^M \lambda_j n_j = 0$.[2] We remark that the constants λ_j could be, in principle, experimentally obtained by measuring H_{extra} for any state $|\psi\rangle$ that belongs to the j-th invariant subspace. According to the postulates of quantum mechanics, the average of such a measurement would be $n_j \lambda_j = \langle\psi|H_{extra}|\psi\rangle$.

Our main result summarized below states that, in the presence of strong SC, the introduction of a connecting extra Hamiltonian gives full controllability *always* except in a very specific case, which we will describe. The special case concerns the situation where all the n_j are equal to 2 and the λ_j's in (2) are all zeros. In this special case, one defines a *weighted connectivity graph* with M nodes (representing the row or column blocks) and an edge connecting the node j to the node k if $C_{jk} \neq 0$ in (2). The weights on each edge are assigned as follows: For every block $C_{jk} \neq 0$, $1 \leq j < k \leq M$, in iH_{extra}, write its *singular value decomposition*

$$C_{jk} = U \begin{pmatrix} b_{jk} & 0 \\ 0 & m_{jk} e^{i\phi_{jk}} \end{pmatrix} V^\dagger, \tag{3}$$

for U and V matrices in $SU(2)$ and $m_{jk} \geq 0$, and 'phases' $\phi_{jk} \in \mathbb{R}$. We shall only need such connectivity graph for the case where $m_{jk} = b_{jk} \neq 0$. Therefore, the phases ϕ_{jk} are determined without ambiguity, up to multiples of 2π. Then the phase ϕ_{jk} is the weight assigned to the edge (j, k), for $j < k$.

Theorem 1. *Assume $\mathcal{L} = \bigoplus_{j=1}^M su(n_j)$, that is, strong subspace controllability, and let H_{extra} in (2) be a connecting Hamiltonian. Let $n := \sum_{j=1}^M n_j$, with $n_j \geq 2$, for $j = 1, 2, ..., M$.*

1. *If one of the n_j's, $j = 1, ..., M$ is greater than 2, then*

$$\tilde{\mathcal{L}} = \{\mathcal{L}, iH_{extra}\}_{Lie} = su(n) \tag{4}$$

2. *If $n_1 = n_2 = \cdots = n_M = 2$ full controllability in (4) is also true in all cases except when the following conditions are all simultaneously verified*

[2] Since we assume $iH_{extra} \in su(n)$ as well, and therefore, with zero trace.

(a) $\lambda_1 = \lambda_2 = \cdots = \lambda_M = 0$ *in (2).*
(b) $b_{jk} = m_{jk}$ *in (3) for all jk's.*
(c) *The associated weighed connectivity graph is such that for any loop the sum of the weighs is equal to a multiple of* 2π*, where in the loop* ϕ_{jk} *(for* $j < k$*) is taken with the* $+$ *sign if we go from* j *to* k *and with the* $-$ *sign if we go from* k *to* j*.*

In this case we have, up to conjugacy,

$$\tilde{\mathcal{L}} := \{\mathcal{L}, iH_{extra}\}_{Lie} = sp(\frac{n}{2}) = sp(M), \tag{5}$$

and pure state controllability [4] is verified.

We remark that, as a consequence of the above theorem controllability of the state is *always* verified in the presence of subspace controllability and an arbitrary connecting extra Hamiltonian. We highlight this fact in the following corollary.

Corollary 1.1. *Assume* $\mathcal{L} = \bigoplus_{j=1}^{M} su(n_j)$*, that is, strong subspace controllability, and let* H_{extra} *in (2) be a connecting Hamiltonian. Then for any couple of states,* $|\psi_0\rangle$ $|\psi_1\rangle$*, there exists a control driving from* $|\psi_0\rangle$ *to* $|\psi_1\rangle$ *(pure state controllability).*

Remark 2. A hint that the $sp(\frac{n}{2})$ (pure state controllability) case may occur in the direct sum decomposition case (considered here) and not in the tensor-local case of [16] can be obtained by considering for simplicity the low dimensional $2+2$ case. Recall that in appropriate coordinates $sp(2)$ is defined as the space of matrices A satisfying $AJ + JA^T = 0$ where J is the matrix $J := \begin{pmatrix} 0 & \mathbf{1}_2 \\ -\mathbf{1}_2 & 0 \end{pmatrix}$. By a permutation of rows and columns $(2 \leftrightarrow 3)$ we can replace J with $\tilde{J} := \begin{pmatrix} \sigma_y & 0 \\ 0 & \sigma_y \end{pmatrix}$, and the matrices in $sp(2)$ in these coordinates are the $\tilde{A}$ satisfying $\tilde{A}\tilde{J} + \tilde{J}\tilde{A}^T = 0$. These include *all* matrices $\tilde{A} := \begin{pmatrix} B & 0 \\ 0 & C \end{pmatrix}$ with arbitrary $B \in su(2)$, $C \in su(2)$. Therefore in the subspace controllable case $\mathcal{L} = su(2) \oplus su(2)$ is a Lie subalgebra of $sp(2)$ and the addition of an appropriate element (in $sp(2)$) may lead to a full Lie algebra $sp(2)$. In the local tensor case, $\mathcal{L}$ is again $su(2) \oplus su(2)$, but the representation of $\mathcal{L}$ is an irreducible one (no invariant subspaces) which is given, modulo a change of coordinates (often referred to as the 'magic basis'), by the standard representation of $so(4)$. Since $so(4)$ is maximal in $su(4)$ the addition of any extra element will lead to $su(4)$, that is, full controllability.

The rest of the paper is mostly devoted to proving the above Theorem 1. In the next section, we consider the first case of the theorem, that is, when one of the n_j's is greater than 2. In section 3 we prove the second part of the theorem, which concerns the case where all the n_j are equal to 2. We give here the necessary graph theoretic background. The last section 4 is devoted to some discussion and generalization of the results. We present a remark showing that the addition of an extra Hamiltonian may transform weak

SC to strong SC. We then examine how the result of the above theorem modifies when strong SC is verified with possibly a phase factor in some or all the invariant subspaces, that is, the dynamical Lie algebra $\mathcal{L}$ acts as $u(n_j)$ rather than $su(n_j)$ on some of the invariant subspaces. This is the content of Theorem 7. Lastly we discuss the case where some of the invariant subspaces have dimension 1. In this case in general Theorem 1 does not hold, that is, the connectivity assumption of the extra Hamiltonian is not sufficient to guarantee full controllability. We describe some necessary conditions and conjecture that these conditions are actually also sufficient.

2. $n_j > 2$ for some j

In this section we will prove the first statement of Theorem 1. The proof is by induction on the number of invariant subspaces M starting from $M = 2$, as the base step. We refer to formula (2) for the extra Hamiltonian H_{extra}.

Let $A = \text{diag}\,(A_1, \dots, A_M)$, and $B = \text{diag}\,(B_1, \dots, B_M)$, with A_j, $B_j \in su(n_j)$. The matrices $[A, iH_{extra}]$ and $[B, [A, iH_{extra}]]$, have the same block form as the first matrix in iH_{extra}, where now each matrix C_{jk} is replaced respectively by $\hat{C}_{jk}$ and $\tilde{C}_{jk}$, given by:

$$\begin{aligned} \hat{C}_{jk} &= A_j C_{jk} - C_{jk} A_k \\ \tilde{C}_{jk} &= B_j A_j C_{jk} - B_j C_{jk} A_k - A_j C_{jk} B_k + C_{jk} A_k B_k. \end{aligned} \tag{6}$$

Fix a pair (j, k) with $1 \le j < k \le M$, choosing the matrix A with all $A_l = 0$, for all $l \neq j$ and B with all $B_l = 0$, for all $l \neq k$, we have that the Lie algebra $\tilde{\mathcal{L}}$ contains all the partitioned matrices, where the only non-zero blocks are the ones in the places j and k, that is, matrices of the form

$$H_{jk} = \begin{pmatrix} 0 & \dots & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & -A_j C_{jk} B_k & \dots \\ \vdots & \vdots & \vdots & \vdots \\ \dots & B_k C_{jk}^\dagger A_j & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}. \tag{7}$$

Notice that since we have assumed $n_l \ge 2$ for all $l = 1 \dots, M$, if $C_{jk} \neq 0$ then $A_j C_{lk} B_k \neq 0$ also, for some choice of A_j and B_k, for example, we may take both matrices diagonal with all diagonal elements different from zero. (Notice that this does not hold if one of the dimensions n_j or n_k is equal to one since $su(1) = 0$.)[3]

[3] As it will be discussed in section 4, this is the only point where we use the assumption that all the n_j's are different from 1.

2.1. Case $M = 2$

In this case, the extra Hamiltonian can be written as

$$iH_{extra} = \begin{pmatrix} 0 & C_{12} \\ -C_{12}^{\dagger} & 0 \end{pmatrix} + \begin{pmatrix} i\lambda_1 \mathbf{1}_{n_1} & 0 \\ 0 & i\lambda_2 \mathbf{1}_{n_2} \end{pmatrix}, \tag{8}$$

with $C_{12} \neq 0$ because of the connectivity assumption.

We shall use the following fact:

Lemma 3. *Assume $\mathcal{L} = su(n_1) \oplus su(n_2)$, with $n_1 \geq 2$ and (without loss of generality) $n_1 \geq n_2$. Assume C_{12} in H_{extra} in (8) has a single element different from zero. Then $\{\mathcal{L}, iH_{extra}\}_{Lie} = su(n_1 + n_2)$*

The result of this Lemma was already proved in [5] for the case where such a nonzero element is a multiple of the imaginary unit i. Even if the proof in our more general case can be carried out similarly, we present it here for completeness. We remark that the lemma does not assume that n_1 *and* n_2 are different from 1. It is enough that one of them is, which is a natural assumption; otherwise $\mathcal{L}$ would be zero.

Proof. Since the second matrix in (8) commutes with all matrices of the type $A = \text{diag}(A_1, A_2)$, for $A_j \in su(n_j)$, by choosing $A = \text{diag}(D_1, 0)$, where D_1 is any diagonal matrix in $su(n_1)$ with all elements different from zero, we have that $\tilde{\mathcal{L}}$ contains the matrix:

$$H_{12} = \begin{pmatrix} 0 & D_1 C_{12} \\ C_{12}^{\dagger} D_1 & 0 \end{pmatrix}, \tag{9}$$

where the matrix $D_1 C_{12}$ has only one non-zero element. Write this non-zero element as $re^{i\phi}$. Since all the block diagonal matrices with blocks in $su(n_1)$ and $su(n_2)$ are in $\mathcal{L}$, we can, without loss of generality, replace H_{12} with $UH_{12}U^{\dagger}$ with arbitrary $U = \text{diag}(V_1, V_2)$, for any $V_j \in SU(n_j)$, $j = 1, 2$.[4] Choose $V_1 \in SU(n_1)$ to be diagonal with $ie^{-i\phi}$ in the position corresponding to the row of the nonzero element of $D_1 C_{12}$, and $V_2 = \mathbf{1}$, the identity matrix in $SU(n_2)$. Then $UH_{12}U^{\dagger}$ will be equal to the one in equation (9) with $D_1 C_{12}$ replaced by $V_1 D_1 C_{12} V_2$, where now the only nonzero element is equal to ir. After this modification, the proof follows the one in [5].

For $1 \leq a, b \leq n_1 + n_2$, $a \neq b$, we denote by X_{ab} (Y_{ab}) the matrix that is 0 everywhere and has the Pauli matrix $i\sigma_x$ ($i\sigma_y$) (cf., (1)) at the intersection of the rows and columns a and b. It can be verified that:

[4] To prove this fact, we argue as follows. For any $H \in \tilde{\mathcal{L}}$ and $U = \text{diag}(V_1, V_2)$, for any $V_j \in SU(n_j)$, $j = 1, 2$, we have that $V_j = e^{iW_j}$ for some $W_j \in su(n_j)$, so letting $W = \text{diag}(W_1, W_2)$ we have $UHU^{\dagger} = \sum_j \frac{1}{j!} ad_W^j H \in \tilde{\mathcal{L}}$ since $\tilde{\mathcal{L}}$ is a closed Lie algebra.

$$[X_{ab}, Y_{ac}] = X_{bc} \;\text{ and } [X_{ab}, Y_{bd}] = X_{ac}. \tag{10}$$

Notice that the matrices X_{ab} and Y_{ab} when $a, b \in \{1, \ldots, n_1\}$ or $a, b \in \{n_1+1, \ldots, n_1+n_2\}$ are block diagonal and therefore in $\mathcal{L}$.

Assume that the nonzero element of $V_1 D_1 C_{12} V_2$ is in the j row ($1 \leq j \leq n_1$) and in the l column ($n_1 + 1 \leq l \leq n_1 + n_2$), then $UH_{12}U^\dagger = rX_{jl}$. Take any $1 \leq k \leq n_1$ with $k \neq j$ and any $n_1 + 1 \leq m \leq n_1 + n_2$, with $m \neq l$, we have, using (10),

$$[X_{jl}, Y_{jk}] = X_{lk} \in \tilde{\mathcal{L}} \;\text{ and } [X_{lk}, Y_{lm}] = X_{km} \in \tilde{\mathcal{L}}$$

Since $1 \leq k \leq n_1$ and $n_1 + 1 \leq m \leq n_1 + n_2$ are arbitrary, we have that all matrices X_{km} are $\tilde{\mathcal{L}}$. Denote by Z_{km} the diagonal matrix which is zero everywhere except for the k element which is equal to i and the m element which is equal to $-i$. It holds $[Z_{km}, X_{kr}] \propto Y_{mr}$, where we write $A \propto B$, if the two matrices are proportional, with a nonzero proportionality factor. Since $\mathcal{L}$ contains all Z_{km} where $1 \leq k, m \leq n_1$ or $n_1 + 1 \leq k, m, \leq n_1 + n_2$, we have that, for $1 \leq k \leq n_1$ and $n_1 + 1 \leq m \leq n_1 + n_2$ all matrices Y_{km} are $\tilde{\mathcal{L}}$.

Thus the Lie algebra $\tilde{\mathcal{L}}$ contains all the block diagonal matrices with blocks in $su(n_1)$ and $su(n_2)$, and also all the matrices X_{km} and Y_{km} for $1 \leq k \leq n_1$ and $n_1+1 \leq m \leq n_1+n_2$. So, it is a Lie algebra of dimension at least $(n_1^2-1)+(n_2^2-1)+2n_1n_2 = (n_1+n_2)^2-2$.

Moreover, for $1 \leq k \leq n_1$ and $n_1 + 1 \leq m \leq n_1 + n_2$, we have $[X_{km}, Y_{km}] \propto Z_{km}$, which give an extra dimension (the possibility of having a block of nonzero trace in one (and therefore both) diagonal blocks). So $\tilde{\mathcal{L}}$, is a subalgebra of $su(n_1 + n_2)$ of dimension $(n_1 + n_2)^2 - 1$, therefore $\tilde{\mathcal{L}} = su(n_1 + n_2)$. □

By the singular value decomposition, and since C_{12} in (8) is non zero, we know that there exist unitary matrices $U \in SU(n_1)$ and $V \in SU(n_2)$, such that

$$UC_{12}V^\dagger = \begin{pmatrix} D_{n_2\times n_2} \\ 0_{(n_1-n_2)\times n_2} \end{pmatrix}, \tag{11}$$

with $D_{n_2\times n_2}$ diagonal and with the first element real and > 0. Letting $W = \text{diag}(U, V)$, with $U \in SU(n_1)$ and $V \in SU(n_2)$, we can replace H_{extra} in (8) with $WH_{extra}W^\dagger$ (see footnote 4) Thus we have the following fact:

Lemma 4. *Assume $\mathcal{L} = su(n_1) \oplus su(n_2)$, with $n_1 \geq 2$. Then we can assume, without loss of generality, C_{12} in (8) of the form $C_{12} := \begin{pmatrix} D_{n_2\times n_2} \\ 0_{(n_1-n_2)\times n_2} \end{pmatrix}$ with $D_{n_2\times n_2}$* diagonal and *with the first element real and* > 0.

The Lie algebra $\mathcal{L}$ is spanned by the matrices $\begin{pmatrix} A_{n_1\times n_1} & 0 \\ 0 & B_{n_2\times n_2} \end{pmatrix}$ with $A_{n_1\times n_1} \in su(n_1)$ arbitrary and $B_{n_2\times n_2} \in su(n_2)$ arbitrary.

Since we are assuming that one of the blocks has dimension different from (in fact greater than) 2, we can assume $n_1 \geq 3$. Let $A = \text{diag}(D_{12}, 0)$ and $B = \text{diag}(D_{13}, 0)$, where $D_{jk} \in su(n_1)$ is the diagonal matrix having i in position j and $-i$ in position k and zeros everywhere else. Then specializing (6), we obtain,

$$[B, [A, iH_{extra}]] = \begin{pmatrix} 0 & D_{13}D_{12}C_{12} \\ -C_{12}^{\dagger}D_{13}D_{12} & 0 \end{pmatrix}.$$

Since the matrix C_{12} has the form given by Lemma 4, the matrix $D_{13}D_{12}C_{12}$, has only the first element of $D_{n_2 \times n_2}$ (cf. Lemma 4) different from zero, so full controllability follows by applying Lemma 3.

2.2. *Case $M > 2$*

Assume $M > 2$. Let $\bar{j}$ be one of the blocks with $n_{\bar{j}} > 2$, which exists since we are assuming that not all the blocks have dimension 2. Since iH_{extra} is a connecting Hamiltonian, one of the blocks $C_{\bar{j}k}$, for $k = 1, \ldots, M$, $k \neq \bar{j}$, in equation (2) has to be different from zero. Assume $C_{\bar{j}\bar{k}} \neq 0$.

To simplify notation, we assume that the blocks corresponding to $\bar{j}$ and $\bar{k}$ are the first two, after possibly a permutation of the blocks and also $n_1 \geq n_2$.

The Lie algebra $\tilde{\mathcal{L}}$ contains all the block diagonal matrices $A = \text{diag}\,(A_1, A_2, 0, \ldots, 0)$, with $A_j \in su(n_j)$. Moreover $\tilde{\mathcal{L}}$ contains the matrix H_{12} of equation (7), i.e.,

$$H_{12} = \begin{pmatrix} 0 & -A_1C_{12}B_2 & 0 & \ldots & 0 \\ A_1C_{12}^{\dagger}B_2 & 0 & 0 & \ldots & \ldots \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & \ldots & 0 \end{pmatrix}. \tag{12}$$

Therefore we can apply the result for $M = 2$ to the first two blocks, and we get that $\tilde{\mathcal{L}}$ contains all the block diagonal matrices $A = \text{diag}\,(A_{12}, A_3, \ldots, A_M)$, where now $A_{12} \in su(n_1 + n_2)$ is arbitrary. So now we have the same model with $M - 1$ blocks, where the iH_{extra} Hamiltonian is still a connecting one, and again not all the blocks have dimension 2. Full controllability follows from the inductive assumption.

3. $n_1 = n_2 = \cdots = n_M = 2$

In this section, we shall prove the second statement of Theorem 1. In the proof, we shall use some notions and terminology of graph theory. Such notions are not necessary to understand and apply Theorem 1 but they facilitate the exposition of the proof. Given the fundamental and elementary nature of the notions we will describe, we assume they are known although we are not aware of a reference for them. The reader familiar with graph theory might recognize some known concepts with perhaps a different terminology.

3.1. Some graph theory

We are interested in connected graphs with M nodes labeled by the natural numbers 1 through M and weighted edges where each edge connecting nodes j and k, with $j < k$, has a weight $\phi_{jk} \in \mathbb{R}$. Every pair of nodes are joined by at most one edge and the ordering of the nodes naturally induces an orientation on the edges since if $j < k$ the edge is assumed oriented from j to k. A (non-oriented) path between node j and node k is a sequence of edges connecting j with k. The *length* of the path is the sum of the weights of the edges of the path taken with a positive sign if the path goes in the direction of the edge and with a negative sign if it goes in the opposite direction. Notice that, contrary to standard terminology in mathematics, the length of a path maybe a negative number. Notice also that we can assume a path to cross an edge only once, that is, it is a *simple path*. Paths that cross an edge more than once can in principle also be considered but their length will be the same as the one of a corresponding simple path since crossing an edge two times will give a zero net contribution to the length.

In analogy to the theory of path integrals, we shall call a graph of the above type a *potential graph* if every path between two nodes has the same length. For a potential graph, the *distance* between two nodes, j and k, $d(j,k)$, is the length of any path between j and k. Notice, again, that such a number can be a negative number. However, the distance from j to j itself is zero. An alternative, equivalent, definition of a potential graph is that the length of any cycle is zero. Furthermore, for a potential graph, given three points on a path, a, b, and c, $d(a,c) = d(a,b) + d(b,c)$. A basic example of a potential graph is a connected graph without cycles. In this case, given any two nodes there is only one (simple) path joining them.

Given a potential graph G we can define its completion G^c as another potential graph which is also *complete*, that is, every two nodes are connected by an edge. We use the following procedure: Start with G and pick two nodes that are not joined by an edge, say a and b, with $a < b$. Introduce an edge from a to b with a weight $\hat{\phi}_{ab} = d(a,b)$. The new graph is still a potential graph. To see this, take a simple path connecting two nodes r and s. If the path does not include the new edge (a,b), then its length is $d(r,s)$. If the path includes the new edge (a,b), its length is $l = d(r,a) + \hat{\phi}_{ab} + d(b,s) = d(r,a) + d(a,b) + d(b,s) = d(r,s)$. Thus every path between r and s has the same length and the new graph is therefore a potential graph also and the distances between nodes are unchanged. We can then proceed with the new graph adding a new edge between any two nodes not directly connected by an edge, and so on. The resulting final graph is a complete graph which is potential and such that all the distances are unchanged as compared to the original graph. Notice also that the final complete graph is independent of the way we perform such a completion procedure.

In the rest of this section, we shall consider the above construction with the only change that all the arithmetic (sums and difference of the weights of the edges) is done mod 2π. We start the proof of the second statement of Theorem 1 by considering the condition (b) of the statement and prove that if $b_{jk} \neq m_{jk}$ for one pair jk then full controllability is verified (Proposition 5). This leaves us with only the case where $b_{jk} = m_{jk}$ for all pairs jk. In subsection 3.3, we consider a Lie algebra $\hat{\mathcal{L}}$ which is constructed using the above graph theoretic ideas and it is such that $\mathcal{L} \subseteq \hat{\mathcal{L}} \subseteq \tilde{\mathcal{L}}$. We prove that such a Lie algebra is isomorphic to the symplectic Lie algebra $sp(M)$. Since $\tilde{\mathcal{L}}$ contains a subalgebra isomorphic to $sp(M)$ and we know that $sp(M)$ is *maximal* in $su(2M)$ (cf. [3]), we conclude the proof of the theorem in subsection 3.4 by using the fact that if (and only if) one or both the conditions (a) and (c) are violated, $\tilde{\mathcal{L}}$ contains an additional element not in $\hat{\mathcal{L}}$. Therefore, $\tilde{\mathcal{L}} = su(2M) = su(n)$ in these cases.

3.2. $m_{jk} \neq b_{jk}$ for some pair jk

Since all blocks have dimension 2, the C_{jk} blocks in the iH_{extra} Hamiltonian (see equation (2)) are 2×2 matrices. For $1 \leq j \leq M$, let A^j be the block diagonal matrix, with the j block equal to $i\sigma_z$ (cf. (1)) and all the other blocks equal to zero. Fix a pair jk, with $1 \leq j < k \leq M$, then the matrix $[A^k, [A^j, iH_{extra}]]$, has (cf., equation (7)) all the blocks equal to zero except the jk block which is equal to $-(i\sigma_z)C_{jk}(i\sigma_z)$. By repeating the same Lie bracket, we obtain again a partitioned matrix zero everywhere except in the jk block which is given by the matrix $(i\sigma_z)^2 C_{jk}(i\sigma_z)^2 = C_{jk}$. Thus the Lie algebra $\tilde{\mathcal{L}}$ contains all the following matrices, for pairs (jk) such that $C_{jk} \neq 0$, that is, for all (j,k) edges in the connectivity graph:

$$H_{jk} = \begin{pmatrix} 0 & \dots & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & C_{jk} & \dots \\ \vdots & \vdots & \vdots & \vdots \\ \dots & -C_{jk}^\dagger & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}. \tag{13}$$

By using the singular values argument as in (11), we may assume that the C_{jk}'s in (13) are diagonal. We will denote these matrices by (cf., (3))

$$C_{jk} = \begin{pmatrix} b_{jk} & 0 \\ 0 & m_{jk} e^{i\phi_{jk}} \end{pmatrix}, \tag{14}$$

with $b_{jk} \geq 0$ and $m_{jk} \geq 0$ and $\phi_{jk} \in \mathbb{R}$.

In the following proposition, we prove that if condition (b) of the second statement of Theorem 1 does not hold, then full controllability holds.

Proposition 5. *Assume that there exists a pair jk such that the matrix $C_{jk} \neq 0$ in (14) has $b_{jk} \neq m_{jk}$, then $\tilde{\mathcal{L}} = su(2M)$. Thus, the model is fully controllable.*

Proof. Consider the case $M = 2$ first. In this case, by the connectivity assumption of H_{extra}, necessarily $C_{12} \neq 0$. If one between b_{12} and m_{12} is equal to zero (and the other one is necessarily different from zero), full controllability follows from Lemma 3. Assume therefore that b_{12} and m_{12} are both different from zero. The Lie algebra $\tilde{\mathcal{L}} := \{\mathcal{L}, iH_{extra}\}_{Lie}$ also contains, for any U and V in $SU(2)$, the matrix $\begin{pmatrix} U & 0 \\ 0 & V \end{pmatrix} H_{12} \begin{pmatrix} U^\dagger & 0 \\ 0 & V^\dagger \end{pmatrix}$, where H_{12} is the matrix given in equation (13), specialized to the case $M = 2$. By choosing $U := \begin{pmatrix} 0 & e^{i\psi} \\ -e^{-i\psi} & 0 \end{pmatrix}$, $V = \begin{pmatrix} 0 & e^{i\eta} \\ -e^{-i\eta} & 0 \end{pmatrix}$ with $\eta - \psi = \phi_{12}$, we get another matrix of the form H_{12} as in (13), that is,

$$\tilde{H}_{12} = \begin{pmatrix} 0 & \hat{C}_{12} \\ -\hat{C}_{12}^\dagger & 0 \end{pmatrix}, \tag{15}$$

with $\hat{C}_{12} := \begin{pmatrix} -m_{12} & 0 \\ 0 & -b_{12}e^{i\phi_{12}} \end{pmatrix}$. Since $b_{12} \neq m_{12}$, the linear combination $H_{12} + \frac{m_{12}}{b_{12}}\tilde{H}_{12}$, gives a matrix where the block $C_{12} + \frac{m_{12}}{b_{12}}\hat{C}_{12}$ has a single element different from zero, and therefore full controllability follows again from Lemma 3.

Assume now $M > 2$. Without loss of generality (by performing a change of coordinate if necessary), we may assume that $b_{12} \neq m_{12}$. The Lie algebra $\tilde{\mathcal{L}}$ contains all the block diagonal matrices $A = \operatorname{diag}(A_1, A_2, 0, \dots, 0)$, with $A_1, A_2 \in su(2)$. Moreover $\tilde{\mathcal{L}}$ contains the matrix H_{12} of equation (13). Since we are assuming $b_{12} \neq m_{12}$, we may apply what we have just proved for $M = 2$, and we get that $\tilde{\mathcal{L}}$ contains all the block diagonal matrices $A = \operatorname{diag}(A_{12}, A_3, \dots, A_M)$, with $A_{12} \in su(4)$ and $A_j \in su(2)$, for $j = 3, ..., M$. The sum of all the H_{jk} except H_{12} in (13) (multiplied by i) is a new H_{extra} for a new system with M replaced by $M - 1$. This new H_{extra} is still a connecting Hamiltonian, and, in this system, we have one of the blocks with dimension greater than 2 (the first one has dimension 4). Thus we can conclude full controllability from section 2. □

3.3. A Lie algebra $\hat{\mathcal{L}}$ with $\mathcal{L} \subseteq \hat{\mathcal{L}} \subseteq \tilde{\mathcal{L}}$

In view of the above result, we shall now consider the case where each nonzero block C_{jk} in (14) has $b_{jk} = m_{jk}$. Fix jk such that $C_{jk} \neq 0$. Since the corresponding matrix H_{jk} in equation (13) is in $\tilde{\mathcal{L}}$, we may assume $b_{jk} = m_{jk} = 1$. Thus $\tilde{\mathcal{L}}$, contains all of the following matrices:

$$A = \begin{pmatrix} A_1 & 0 & \dots & 0 \\ 0 & A_2 & \vdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & A_M \end{pmatrix}, \quad \text{with } A_j \in su(2), \tag{16}$$

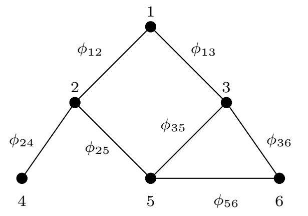

Fig. 1. Connectivity Graph.

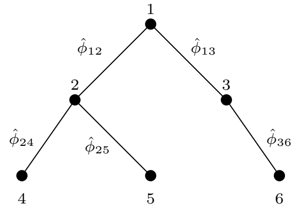

Fig. 2. Subgraph G.

$$H_{jk} = \begin{pmatrix} 0 & \ldots & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \ldots & \Phi_{jk} & \ldots \\ \vdots & \vdots & \vdots & \vdots \\ \ldots & -\Phi_{jk}^{\dagger} & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}, \quad \text{with } \Phi_{jk} := \begin{pmatrix} 1 & 0 \\ 0 & e^{i\phi_{jk}} \end{pmatrix}, \tag{17}$$

for all jk, $j < k$, such that $C_{jk} \neq 0$, with '*phases*' $\phi_{jk} \in \mathbb{R}$.

In the following lemma we shall study the Lie algebra $\hat{\mathcal{L}}$ generated by the matrices A in (16) and a *subset* of the matrices H_{jk} in (17). In particular we choose a subgraph G of the connectivity graph of the system which is both connected and without loops, that is, G is a *spanning tree* for the connectivity graph of the system. We pick the H_{jk}'s corresponding to the (j, k) edges of G. We shall denote matrices of the form H_{jk} in (17) in the Lie algebra $\hat{\mathcal{L}}$ by $\hat{H}_{jk}$ and the corresponding 'phases' by $\hat{\phi}_{jk}$, with the understanding that if (j, k) is an edge in G, then $\hat{H}_{jk} = H_{jk}$ and $\hat{\phi}_{jk} = \phi_{jk}$.

Figs. 1 and 2 give an example of these two graphs. In these pictures, we have $M = 6$. Fig. 1 is the *weighted* connectivity graph associated with H_{extra} where each edge represents a block different from zero in H_{extra}. Fig. 2 represents the associated spanning tree, i.e., the subgraph G, where the $\hat{\phi}_{jk} = \phi_{jk}$.

By doing Lie brackets among matrices $\hat{H}_{a,b}$ (of the form (17)) in $\hat{\mathcal{L}}$ we shall obtain new matrices of the same form with the phases related by a 'congruence relation'. The crucial observation is that the original graph G is, in the terminology of subsection 3.1, a *potential graph* and the procedure of taking Lie brackets corresponds to the graph completion procedure described in subsection 3.1.

Let $1 \leq j < k \leq M$ and $1 \leq l < m \leq M$. It is obvious that:

$$[\hat{H}_{jk}, \hat{H}_{lm}] = 0 \quad \text{if } \{j,k\} \cap \{l,m\} = \emptyset \text{ or } \{j,k\} = \{l,m\}. \tag{18}$$

In the case where $\{j,k\}$ and $\{l,m\}$ have a single element in common the Lie bracket $[\hat{H}_{jk}, \hat{H}_{lm}]$ depends on the relative ordering of j,k and l,m (recall that by definition $\hat{H}_{jk}$ and $\hat{H}_{lm}$ are defined with $j < k$ and $l < m$). In particular, consider $j < k < m$. By direct verification we obtain (we omit possible multiplicative $-$ signs in the resulting commutators which do not play any role in the argument that follows)

$$[\hat{H}_{jk}, \hat{H}_{km}] = \hat{H}_{jm}, \text{ with } \hat{\phi}_{jm} = \hat{\phi}_{jk} + \hat{\phi}_{km} \tag{19}$$

$$[\hat{H}_{jk}, \hat{H}_{jm}] = \hat{H}_{km}, \text{ with } \hat{\phi}_{km} = \hat{\phi}_{jm} - \hat{\phi}_{jk}; \tag{20}$$

$$[\hat{H}_{jm}, \hat{H}_{km}] = \hat{H}_{jk}, \text{ with } \hat{\phi}_{jk} = \hat{\phi}_{jm} - \hat{\phi}_{km}. \tag{21}$$

These relations are, in fact, easily verified by noticing that only blocks corresponding to three indexes are involved in the commutators (the other blocks are zero) and therefore we can assume without loss of generality $j = 1$, $k = 2$ and $m = 3$. To verify the condition for $[\hat{H}_{jk}, \hat{H}_{jm}]$, for example, we calculate

$$\left[\begin{pmatrix} 0 & \hat{\Phi}_{12} & 0 \\ -\hat{\Phi}_{12}^{\dagger} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \begin{pmatrix} 0 & 0 & \hat{\Phi}_{13} \\ 0 & 0 & 0 \\ -\hat{\Phi}_{13}^{\dagger} & 0 & 0 \end{pmatrix} \right] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -\hat{\Phi}_{12}^{\dagger}\hat{\Phi}_{13} \\ 0 & \hat{\Phi}_{13}^{\dagger}\hat{\Phi}_{12} & 0 \end{pmatrix},$$

which gives the relation $\hat{\phi}_{23} = \hat{\phi}_{12} - \hat{\phi}_{13}$. Notice that all the three above relations can be summarized by the following *congruence relation*

$$\text{For all} \quad j < k < m, \qquad \hat{\phi}_{jm} = \hat{\phi}_{jk} + \hat{\phi}_{km} + 2s\pi. \tag{22}$$

Now, let us start with the potential graph G defined above (that is, the spanning tree of the weighted connectivity graph) and the matrices $\hat{H}_{jk}$ with (j,k) an edge in G. These are a subset (in $\hat{\mathcal{L}}$) of the H_{jk} in (17). For each edge (j,k), $\hat{\phi}_{jk} = \phi_{jk}$ is the distance on the graph between j and k. Consider now two nodes a and c, with $a < c$, which are not directly connected but are joined through a node b. By doing one of the commutators $[\hat{H}_{ab}, \hat{H}_{bc}]$, or $[\hat{H}_{ba}, \hat{H}_{bc}]$, or $[\hat{H}_{ab}, \hat{H}_{cb}]$, depending on the relative positioning of b with respect to a and c, we obtain $\hat{H}_{ac}$ where $\hat{\phi}_{ac}$ is, according to the above relations (22), the distance between a and c. We have therefore obtained a new matrix $\hat{H}_{ac} \in \hat{\mathcal{L}}$ and a new potential graph. We can continue the process of completing the graph G following the algorithm in subsection 3.1 adding new edges and by doing the corresponding Lie brackets. The end result is a set of all $\hat{H}_{jk}$ matrices, for $1 \leq j < k \leq M$ and a corresponding complete potential graph G^c with phases $\hat{\phi}_{jk}$ in $\hat{H}_{jk}$ corresponding to the weight (distance) $d(j,k)$ in G (and G^c).

Fig. 3 represents the complete graph G^c for the subgraph G given in Fig. 2. Here all nodes are connected, and the phases $\hat{\phi}_{jk}$ corresponding the edges that are not in

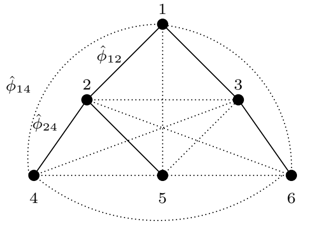

Fig. 3. Graph G^c.

G, like $\hat{\phi}_{14}$, are computed using (recursively) the congruence relation (22). For example $\hat{\phi}_{14} = \hat{\phi}_{12} + \hat{\phi}_{24}$.

There is also another set of linearly independent matrices in $\hat{\mathcal{L}}$. It is the set, defined, for each $j < k$, by

$$\hat{W}_{jk} = \begin{pmatrix} 0 & \dots & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \dots & \hat{\Phi}_{jk} F_{jk} & \dots \\ \vdots & \vdots & \vdots & \vdots \\ \dots & F_{jk}\hat{\Phi}_{jk}^\dagger & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}, \quad \text{with } F_{jk} \in su(2), \qquad \hat{\Phi}_{jk} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\hat{\phi}_{jk}} \end{pmatrix}, \tag{23}$$

where $\hat{\phi}_{jk}$ are the weights of the edges of the complete graph G^c (the distances from j to k). To obtain these matrices, it is sufficient to notice that, if we let A be the matrix of the form (16) with all zeros except the one in position k and $A_k = -F_{jk}$, then $[A, \hat{H}_{jk}] = \hat{W}_{jk}$. Here F_{jk} is arbitrary in $su(2)$.

If the A's in (16), the $\hat{H}_{jk}$'s corresponding to the edges of the complete graph G^c (cf, (17)) and the $\hat{W}_{jk}$'s in (23) were to span a Lie algebra (which would coincide with $\hat{\mathcal{L}}$) such a Lie algebra would have dimension $3M$ (matrices in (16)) + $\frac{M(M-1)}{2}$ (matrices $\hat{H}_{jk}$) (cf., (17)) + $\frac{3M(M-1)}{2}$ (matrices in (23)). This is equal to $M(2M+1)$ and it coincides with the dimension of $sp(M)$. Therefore, it is reasonable to expect that $\hat{\mathcal{L}}$ is isomorphic, which is the same as conjugate (see [3]), to the symplectic Lie algebra $sp(M)$. The following Lemma shows that this is indeed the case.

Lemma 6. *The Lie algebra $\hat{\mathcal{L}}$, generated by the matrices (16) and (17) for any pair $(j < k)$ in the graph G (the spanning tree extracted from the connectivity graph) is conjugate to the symplectic Lie algebra $sp(M)$.*

Proof. We need to show two things: 1) A in (16), $\hat{H}_{jk}$ and $\hat{W}_{jk}$ in (23) span a Lie algebra, that is, the span of these matrices is closed under commutation. This is the Lie algebra $\hat{\mathcal{L}}$; 2) Such a Lie algebra $\hat{\mathcal{L}}$ is isomorphic (conjugate) to $sp(M)$. Let us denote by $\mathcal{L}$

(consistently with the rest of the paper), $\hat{\mathcal{H}}$ and $\mathcal{W}$ the spans of the matrices in (16), (17) (hatted and considered for any $j < k$) and (23), respectively.

$[\mathcal{L}, \mathcal{L}] \subseteq \mathcal{L}$ is obvious while $[\mathcal{L}, \hat{\mathcal{H}}] \subseteq \mathcal{W}$ follows from the same argument we have used to prove that we can generate the matrices in (23) where we took in $\mathcal{L}$ a matrix with only one block different from zero. We can write any general matrix in $\mathcal{L}$ as a sum of such matrices. We now consider $[\mathcal{L}, \mathcal{W}]$. Given any $A = \text{diag}(A_1, \ldots, A_m)$, the matrix $[A, \hat{W}_{jk}]$ is a partitioned matrix as $\hat{W}_{jk}$ with $\hat{\Phi}_{jk} F_{jk}$ replaced by (see equation (6)) $A_j \hat{\Phi}_{jk} F_{jk} - \hat{\Phi}_{jk} F_{jk} A_k = \hat{\Phi}_{jk} \left(\hat{\Phi}_{jk}^{\dagger} A_j \hat{\Phi}_{jk} F_{jk} - F_{jk} A_k \right)$. Direct verification shows that given two matrices in $su(2)$, E and F,

$$EF = a\mathbf{1}_2 + L \tag{24}$$

for some a real and $L \in su(2)$.[5] Therefore by applying this to $\hat{\Phi}_{jk}^{\dagger} A_j \hat{\Phi}_{jk} F_{jk}$, and to $F_{jk} A_k$, we have $\left(\hat{\Phi}_{jk}^{\dagger} A_j \hat{\Phi}_{jk} F_{jk} - F_{jk} A_k \right) = \tilde{a}\mathbf{1}_2 + \tilde{F}_{jk}$, for some $\tilde{a}$ real and $\tilde{F}_{jk} \in su(2)$. Thus we have

$$[A, \hat{W}_{jk}] = \tilde{a}\hat{H}_{jk} + \tilde{W}_{jk},$$

for some $\tilde{W}_{jk}$ of the same form as $\hat{W}_{jk}$ in (23). Therefore $[\mathcal{L}, \mathcal{W}] \subseteq \hat{\mathcal{H}} \oplus \mathcal{W}$.

Formulas (19), (20) and (21) together with (18) imply that $[\hat{\mathcal{H}}, \hat{\mathcal{H}}] \subseteq \hat{\mathcal{H}}$.

The calculations for $[\hat{\mathcal{H}}, \mathcal{W}]$ and $[\mathcal{W}, \mathcal{W}]$ are similar to each other, the former being, in some sense, a special case of the latter. Let us consider the latter and then we shall mention how to modify the calculation to consider the former. Analogously to (18), we have $[\hat{W}_{jk}, \hat{W}_{lm}] = 0$ if $\{j, k\} \cap \{l, m\} = \emptyset$ or $\{j, k\} = \{l, m\}$. So the only nonzero case is when only one index for the $\hat{W}$'s is in common. Fix $1 \leq j < k < m \leq M$. There are three cases analogously to (19), (20) and (21). Consider, as an example, the case corresponding to (19). We have,

$$[\hat{W}_{jk}, \hat{W}_{km}] = \begin{pmatrix} 0 & \ldots & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & \ldots & -\hat{\Phi}_{jk} F_{jk} \hat{\Phi}_{km} F_{km} & \ldots \\ \vdots & \vdots & \vdots & \vdots \\ \ldots & F_{km}^{\dagger} \hat{\Phi}_{km}^{\dagger} F_{jk}^{\dagger} \hat{\Phi}_{jk}^{\dagger} & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}, \tag{25}$$

for matrices F_{jk} and F_{km} in $su(2)$. We have:

$$-\hat{\Phi}_{jk} F_{jk} \hat{\Phi}_{km} F_{km} = -\hat{\Phi}_{jk} \hat{\Phi}_{km} \left(\hat{\Phi}_{km}^{\dagger} F_{jk} \hat{\Phi}_{km} F_{km} \right)$$

[5] To check this, write a general matrix in $su(2)$ as $\begin{pmatrix} ib & \beta \\ -\beta^* & -ib \end{pmatrix}$, with b real and β a general complex number.

Using equation (24) we have that $\hat{\Phi}_{km}^{\dagger} F_{jk} \hat{\Phi}_{km} F_{km} = \tilde{a}\mathbf{1}_2 + F_{jm}$ for some $\tilde{a}$ real and $F_{jm} \in su(2)$. Thus we have:

$$-\hat{\Phi}_{jk} F_{jk} \hat{\Phi}_{km} F_{km} = -\tilde{a}\hat{\Phi}_{jk}\hat{\Phi}_{km} - \hat{\Phi}_{jk}\hat{\Phi}_{km} F_{jm}.$$

Since

$$\hat{\Phi}_{jk}\hat{\Phi}_{km} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i(\hat{\phi}_{jk}+\hat{\phi}_{km})} \end{pmatrix}, \tag{26}$$

we have from (22) that $\hat{\Phi}_{jk}\hat{\Phi}_{km} = \hat{\Phi}_{jm}$. Thus

$$-\tilde{a}\hat{\Phi}_{jk}\hat{\Phi}_{km} - \hat{\Phi}_{jk}\hat{\Phi}_{km} F_{jm} = \tilde{a}\hat{\Phi}_{jm} - \hat{\Phi}_{jm} F_{jm} \;\Rightarrow\; [\hat{W}_{jk}, \hat{W}_{km}] = -\tilde{a}\hat{H}_{jm} - \hat{W}_{jm}.$$

Similar calculations hold in the other cases showing that $[\mathcal{W}, \mathcal{W}] \subseteq \hat{\mathcal{H}} \oplus \mathcal{W}$. When considering $[\hat{\mathcal{H}}, \mathcal{W}]$, the calculations are similar but if, for instance, we replace $\hat{W}_{jk}$ with $\hat{H}_{jk}$ in (25), in the right hand side F_{jk} has to be replaced by the identity. These considerations lead to conclude that $[\hat{\mathcal{H}}, \mathcal{W}] \subseteq \mathcal{W}$.

We are left with proving that the Lie algebra $\hat{\mathcal{L}}$ is isomorphic to $sp(M)$. A quick test for this is given in Corollary 3.3.13 in [4]. One takes the (density) matrix ρ which is zero everywhere except for 1 in position $(1,1)$ (this corresponds to a pure state) and calculate the dimension of $[\rho, \hat{\mathcal{L}}]$ which should be $2(2M-1)$. We look at the elements of the first row (and column) of a general matrix in $\hat{\mathcal{L}}$. There are 3 parameters coming from the first diagonal block (in $su(2)$) + $4(M-1)$ parameters coming from the off diagonal blocks. One parameter cancels in the commutator (the one corresponding to the first diagonal element of the commutator), so that the total number of free parameters is $3 + 4(M-1) - 1 = 2(2M-1)$ as desired. □

3.4. Conclusion of the proof

We are now ready to complete the proof of the second statement of Theorem 4. We have already proved in Proposition 5 that if condition (b) is not satisfied, then full controllability follows. So we assume that (b) holds. By construction we have that $\hat{\mathcal{L}} \subseteq \tilde{\mathcal{L}}$, so we know that $\tilde{\mathcal{L}}$ contains a subalgebra which is conjugate to $sp(M)$.

First, we assume that conditions (a) and (c) hold. Since (a) holds, the extra Hamiltonian has only the first matrix in the right hand side of (2). This matrix together with the matrices A of equation (16), generate all the matrices H_{jk} such that $C_{jk} \neq 0$. Under the assumption (c), the connectivity graph is a subgraph, with matching weights, of G^c and therefore the matrices H_{jk} in (17) are a *subset* of the matrices $\hat{H}_{jk}$ defined for *all* $1 \leq j < k \leq M$. Therefore $\tilde{\mathcal{L}} \subseteq \hat{\mathcal{L}}$, which implies $\tilde{\mathcal{L}} = \hat{\mathcal{L}} = sp(M)$ from Lemma 6. If condition (a) is not verified, then $\tilde{\mathcal{L}}$ contains an element different from zero which is not contained in $\hat{\mathcal{L}}$. It is a diagonal matrix having (at least two) blocks different from zero on the diagonal and multiples of the identity. Since $\hat{\mathcal{L}} = sp(M)$ is a *maximal subalgebra* in $su(2M)$ this implies that $\tilde{\mathcal{L}}$ is equal to $su(2M)$. Analogously, if condition (c) is not verified, one of the matrices H_{jk} in (17) is not contained in $\hat{\mathcal{L}}$, and full controllability holds.

4. Discussion and extensions

4.1. An extra Hamiltonian may transform weak into strong subspace controllability

The introduction of an extra Hamiltonian may have the effect of transforming weak SC to strong SC. To see this, consider a system with (purely) weak SC where the Lie algebra $\mathcal{L}$ is given by block diagonal matrices of the form $\text{diag}(A, A, ..., A)$ with A arbitrary in $su(d)$. We can write an arbitrary matrix in $\mathcal{L}$ as $\mathbf{1}_M \otimes A$, with $A \in su(d)$. Assume we add to the system an extra Hamiltonian of the form $H_{extra} := B \otimes C$ where $C \neq \mathbf{1}_d$ and B a Hermitian $M \times M$ matrix with all the eigenvalues $\lambda_1, \lambda_2, ..., \lambda_M$ of multiplicity 1. We shall show that this new extra Hamiltonian leads to strong SC.

Notice that, in this case, the new dynamical Lie algebra $\tilde{\mathcal{L}} = \{\mathcal{L}, iH_{extra}\}_{Lie}$, contains all the matrices of the form $B \otimes D$ with D arbitrary in $su(d)$. To see this, notice that by taking (repeated) Lie brackets of $B \otimes (iC)$ with elements of the form $\mathbf{1}_M \otimes A$ with A in $su(d)$ we can obtain all matrices of the form $B \otimes D$ where D is an arbitrary element in the ideal generated by $i(C - \frac{Tr(C)}{d}\mathbf{1}_d)$ in $su(d)$. Since C is not a multiple of the identity such an ideal cannot be zero, and, since $su(d)$ is a *simple* Lie algebra,[6] it must be $su(d)$ itself. The new dynamical Lie algebra $\tilde{\mathcal{L}}$ will also contain matrices of the form $B^2 \otimes D$ with arbitrary $D \in su(d)$, obtained by doing Lie brackets of element $B \otimes D_1$ and $B \otimes D_2$, with D_1 and D_2 in $su(d)$, since $su(d)$ is a semisimple Lie algebra $[su(d), su(d)] = su(d)$. Thus every arbitrary $D \in su(d)$, in $B^2 \otimes D$ can be achieved. Extending this argument, we find that $\tilde{\mathcal{L}}$ contains matrices $B^k \otimes D$ for arbitrary $D \in su(d)$ and arbitrary $k = 0, 1, 2, 3, ...$ After a change of coordinates, we may diagonalize B (and therefore B^k for any k), so we assume $B = \text{diag}(\lambda_1, \ldots, \lambda_M)$. Thus, for any arbitrary $X_0, X_1, ..., X_{M-1}$ in $su(d)$, we have all the block diagonal matrices $\text{diag}(\lambda_1^k X_k, \lambda_2^k X_k, ..., \lambda_M^k X_k)$, for $k = 0, 1, ..., M-1$. Then the linear system with unknowns $X_0, X_1, ..., X_{M-1}$ in $su(d)$ given by

$$\sum_{k=0}^{M-1} \lambda_1^k X_k = A_1, \quad \sum_{k=0}^{M-1} \lambda_2^k X_k = A_2, \qquad \cdots \qquad \sum_{k=0}^{M-1} \lambda_M^k X_k = A_M,$$

has a matrix of coefficients which is given by a Vandermonde matrix which is nonsingular since all the λ_j's are assumed different from each other. Therefore $\tilde{\mathcal{L}}$ contains all matrices of the form $\text{diag}(A_1, A_2, ..., A_m)$, with arbitrary $A_j \in su(d)$ and strong subspace controllability is achieved.

[6] It contains no ideal beside zero and the Lie algebra itself.

4.2. Addition of phase factors

The term 'strong subspace controllability' also refers to the case where on each or some of the invariant subspaces, the j-th one, it is possible to have general unitary transformations in $U(n_j)$ not just any special unitary in $SU(n_j)$. In Lie algebraic terms, this means that $\mathcal{L}$ contains not only $\bigoplus_{j=1}^{M} su(n_j)$ by also the span of a basis of block diagonal matrices where the blocks are some multiples of the identity matrix. These matrices span the *center* of the dynamical Lie algebra $\mathcal{L}$ and are responsible, in quantum control theory problems, for our ability, to change the relative phase between the various subspaces (cf. [10]). If $\mathcal{L}$ has a nonzero center, this does not affect the situation of the first part of Theorem 1 since in that case we already have full controllability even without such matrices. As for the second part of Theorem 1, assume we have the situation where all conditions (a) (b) and (c) are verified and $\tilde{\mathcal{L}} = sp\left(\frac{n}{2}\right)$. We have used above the fact that the addition of an extra nonzero matrix in $su(n)$ to $sp\left(\frac{n}{2}\right)$ generates the whole $su(n)$. Therefore, adding the nonzero center of $\mathcal{L}$ to the $\tilde{\mathcal{L}}$ in part 2 of Theorem 1 results, again, in full controllability. Therefore, we can conclude with the following theorem.

Theorem 7. *Assume that a quantum system is strongly subspace controllable with Lie algebra $\mathcal{L}$ having a nontrivial center. Then the addition of any connecting extra Hamiltonian H_{extra}, gives*

$$\tilde{\mathcal{L}} = \{\mathcal{L}, iH_{extra}\}_{Lie} = su(n)$$

4.3. Presence of invariant subspaces of dimension 1

In the above treatment we have used the fact that all n_j are ≥ 2 only in section 2, and in particular in formula (7) to separate the various blocks C_{jk} of the extra Hamiltonian. In that situation, we needed the A_j's and B_k's (cf. formula (7)) to be different from zero, which is not possible for n_j or n_k equal to 1 since $su(1) = 0$. If we were able to separate blocks $C_{jk} \neq 0$ for couples $1 \leq j < k \leq M$ giving a connected graph, the result of the first part of Theorem 1 would still hold by replacing 'greater than 2' with 'different from 2'. One tool to separate such blocks are the matrices in the *center* of $\mathcal{L}$. In particular, if the center contains a block diagonal matrix which is all zeros except in the block j and in the block k which are $i\mathbf{1}_{n_j}$ and $-i\frac{n_j}{n_k}\mathbf{1}_{n_k}$, respectively, it is possible to repeat the argument in formula (7) with $A_j = i\mathbf{1}_{n_j}$ and $B_k = -i\frac{n_j}{n_k}\mathbf{1}_{n_k}$ and separate the block C_{jk}. The block diagonal part of H_{extra} in (2) does not play any role in this argument as its Lie bracket with any block diagonal matrix would be zero.

The most unfavorable case is when the center of $\mathcal{L}$ is zero, and, in that case, the first part of Theorem 1 is not true in general, that is, it is not possible to replace 'greater than 2' with 'different from 2', under the only assumption of H_{extra} being connecting. To see this, consider the case of a single block of dimension $n_1 > 1$ and m blocks of dimension 1. The matrices in $\mathcal{L}$ have the form $\begin{pmatrix} A & 0 \\ 0 & \mathbf{0}_m \end{pmatrix}$ with A arbitrary in $su(n_1)$

and $H_{extra} := \begin{pmatrix} \mathbf{0}_{n_1\times n_1} & C_{n_1\times m} \\ -C^{\dagger}_{n_1\times m} & D_{m\times m} \end{pmatrix}$. If the columns of the sub-matrix $\begin{pmatrix} C_{n_1\times m} \\ D_{m\times m} \end{pmatrix}$ are linearly dependent, then there exists a nonzero vector $\vec{v} := \begin{pmatrix} 0 \\ \vec{v}_1 \end{pmatrix}$ such that both $\mathcal{L}\vec{v} = 0$ and $H_{extra}\vec{v} = 0$ and therefore $\tilde{\mathcal{L}}\vec{v} = 0$. Thus $\vec{v}$ is a fixed vector for the dynamics and the system is not even pure state controllable. Therefore a necessary condition even for pure state controllability is that such a matrix $\begin{pmatrix} C_{n_1\times m} \\ D_{m\times m} \end{pmatrix}$ has full rank. This argument can be extended directly to the case where there is more than one block of dimension > 1. First we may put together all the blocks j with dimension $n_j > 1$ which are connected by H_{extra}, neglecting the connections that occur via the blocks of dimension 1. In practice, we remove from the connectivity graph all the nodes and edges corresponding to blocks with dimension 1. The resulting 'reduced' connectivity graph will have one or more connected components to which we can apply the analysis of sections 2 and 3. By reordering the rows and columns, we can always assume that the blocks of dimension 1 are the last ones, and we need that the corresponding columns of H_{extra} are linearly independent, i.e. the submatrix of H_{extra} formed by these last columns has full rank.

It is possible that this full rank condition is not satisfied but the connectivity graph of H_{extra} is connected. Consider for example again the case where there is only one block of dimension > 1, and m blocks of dimensions 1. Then, assume that the matrix $\begin{pmatrix} C_{n_1\times m} \\ D_{m\times m} \end{pmatrix}$ has $D_{m\times m} = 0$ and $C_{n_1\times m}$ has only one row different from zero, with all the elements different from zero. Then the rank is 1, but the connectivity graph is connected. Here, the connectivity graph has a star shape with the node corresponding to the first block connected to all the nodes corresponding to blocks of dimension 1, however the full rank condition, in this case, is satisfied if and only if there is only one block of dimension 1. On the other hand, it is also possible that the full rank condition is satisfied but the connectivity condition is not. Consider for example the case $n_1 = 2$ and $m = 2$ in the above notation with $C_{2\times 2} = \mathbf{0}_2$ and $D_{2\times 2} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}$.

In summary, these two conditions, *full rank* and *connectivity*, are in general independent, and both necessary for pure state controllability. We have not found any example where these two conditions were both satisfied and the resulting system with dynamical Lie algebra $\tilde{\mathcal{L}}$ was not (at least) pure state controllable. Therefore we conjecture that such two conditions are also sufficient. We conclude by briefly describing a few cases where we were able to prove controllability. For simplicity, we assume that there is only one block of dimension $n_1 > 1$ and m blocks of dimension 1, with $M = m + 1$. The first block may be the result of a single connected component in the reduced connectivity graph once all the nodes and edges corresponding to the blocks of dimension 1 are removed. Extensions to the general situation of several connected components are possible.

In the case $m = 1$, one can, in general use Lemma 3 to conclude full controllability. Let us therefore consider the case $m \geq 2$. Let us assume $n_1 \geq m$ and $C_{n_1\times m}$ (in the above notations) with full rank m. In this case, both the linear independence and connectivity are satisfied even if $D_{m\times m}=0$. We can do a global change of coordinates, that is, a similarity transformation with a block diagonal matrix $\begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}$ with V_1 and V_2 in $U(n_1)$ and $U(m)$, respectively, so that, by the singular value decomposition, $C_{n_1\times m}=\begin{pmatrix} \hat{D}_{m\times m} \\ \mathbf{0}_{(n_1-m)\times m} \end{pmatrix}$ with $\hat{D}_{m\times m}$ diagonal and full rank (with positive numbers on the diagonal). Even in this context, the case $n_1=2$ is somehow special. Consider the case $m=2$ and $C_{n_1\times m}=C_{2\times 2}=\mathbf{1}_2$. In this case a direct calculation similar to the ones done in section 3.3 shows that $\tilde{\mathcal{L}}=sp(2)$ (independently of $D_{2\times 2}$). If one (and therefore at least two) of the λ_j's in (2) are different from zero, one can use the maximality of $sp(2)$ in $su(4)$ argument to conclude full controllability. If $n_1\geq 3$, the Lie bracket of matrices of the type $\begin{pmatrix} A & 0 \\ 0 & 0 \end{pmatrix}$ with A diagonal with i and $-i$ only in two positions and zeros everywhere else, breaks down the matrix $C_{n_1\times m}=\begin{pmatrix} \hat{D}_{m\times m} \\ \mathbf{0}_{(n_1-m)\times m} \end{pmatrix}$ into matrices where only one element is nonzero. Successive applications of Lemma 3 shows by induction that $\tilde{\mathcal{L}}$ contains $su(n_1+1)$, $su(n_1+2)$ and so on up to $su(n_1+m)=su(n)$, and therefore full controllability is satisfied in this case as well.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgement

The research of D. D'Alessandro was supported by the ARO MURI grant W911NF-22-S-0007. The authors are indebted to an unknown referee of a previous paper [5] who suggested the question that has been answered in the present work.

Data availability

No data was used for the research described in the article.

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