Sufficient conditions for controllability of finite level quantum systems via structure theory of semisimple Lie algebras

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Abstract

The controllability of the unitary propagator of a finite level quantum system is studied in this paper by analyzing the structure of the semisimple Lie algebra $\mathfrak{su}(N)$.

1 Introduction

The question of controllability for a finite level quantum system, see Ref. [6, 16, 18], is studied in this paper by analyzing the structure of the semisimple Lie algebra of its time evolution operator. For a compact semisimple Lie group like $SU(N)$, the testing of global controllability is the simplest of all noncommutative Lie groups. In fact, compactness implies that the accessibility property collapses into (global) controllability and semisimplicity implies that almost all pairs of vector fields span the corresponding Lie algebra. The first property means that purely algebraic tools, like the *Lie algebra rank condition* normally used in control theory provides necessary and *sufficient* conditions for controllability, while the second property affirms that controllability is generically verified with a single control. The main scope of this paper is to give the interpretation of these properties in terms of structure theory of semisimple Lie algebras, see Ref. [5, 10], and to provide alternative tests to the exhaustive computation of commutators that the Lie algebra rank condition requires. So genericity is interpreted in terms of regularity of the roots of the Lie algebra $\mathfrak{su}(N)$ and another property, regularity along the control vector field, immediately follows. The main tool we use, together with the regularity of the roots, is the connectivity of the graph of the control vector field. Both properties were classically used to analyze controllability of vector fields on semisimple Lie algebras (especially the noncompact ones, see Ref. [12, 9, 8]). For the same type of problem as ours, the properties of the graph were recently used also in [18]. The conditions we obtain, based only on the *a priori* knowledge of the two vector fields, are only sufficient but they allow us to avoid any computation of Lie brackets. From the generic case, physically representing a quantum system with all different transition values between its (nondegenerate) energy levels, these tools carry on to the singular case, where some of these levels might be equispaced.

This paper is an abridged version of [2], to which we refer for proofs of the results reported.

2 Quantum control system

Consider a finite level quantum system described by a state $|\psi\rangle$ evolving according to the time dependent Schrödinger equation

$$i\hbar|\dot{\psi}(t)\rangle = \left(\hat{H}_0 + u(t)\hat{H}_1\right)|\psi(t)\rangle \tag{2.1}$$

where the traceless Hermitian matrices $\hat{H}_0$ and $\hat{H}_1$ are respectively the internal (or free) Hamiltonian and the external Hamiltonian, this last representing the interaction of the system with a single control field $u(t)$. In the N-level approximation, the state $|\psi\rangle$ is expanded with respect to a basis of N orthonormal eigenstates $|\varphi_i\rangle$: $|\psi\rangle = \sum_{i=1}^{N} c_i|\varphi_i\rangle$ where the c_i are complex coefficients that satisfy the normalization condition $\sum_{i=1}^{N} |c_i|^2 = 1$. If we write the initial condition of (2.1) as $|\psi_0\rangle = \sum_{i=1}^{N} c_{0i}|\varphi_i\rangle$, then also the vector $c = [c_1 \dots c_N]^T$ satisfies a differential equation similar to (2.1):

$$\begin{aligned} i\hbar\dot{c}(t) &= \left(\tilde{H}_0 + u(t)\tilde{H}_1\right)c(t) \\ c(0) &= c_0 \end{aligned} \tag{2.2}$$

where now the traceless Hermitian matrix $\tilde{H}_0$ is diagonal. The real coefficients $\mathcal{E}_i$, $\mathcal{E}_1 \leq \dots \leq \mathcal{E}_N$, appearing along the diagonal of $\tilde{H}_0$ are eigenvalues, $\tilde{H}_0|\varphi_i\rangle = \mathcal{E}_i|\varphi_i\rangle$, and represent the energy levels of the system. If $\mathcal{E}_i = \mathcal{E}_j$ for some $i \neq j$, then the system is said *degenerate*. If, instead, some of the levels are equispaced, $\mathcal{E}_i - \mathcal{E}_j = \mathcal{E}_k - \mathcal{E}_l$ for $(i,\, j) \neq (k,\, l)$, $i \neq j$, $k \neq l$, then the system is said to have *degenerate transitions* (or resonances). The solution of (2.2) is $c(t) = X(t)c(0)$ with the unitary matrix $X(t)$ representing the time evolution operator. If we use atomic units ($\hbar = 1$), then instead of (2.2) we can study the right invariant bilinear control system evolving on the Lie group $SU(N)$ and characterized by the skew-Hermitian vector fields $A = -i\tilde{H}_0$ and $B = -i\tilde{H}_1$:

$$\begin{aligned} &\dot{X}(t) = (A + u(t)B)\,X(t) \qquad X(t) \in SU(N), \quad A,\, B \in \mathfrak{su}(N) \\ &X(0) = I \end{aligned} \tag{2.3}$$

The system (2.3) is said (globally) *controllable* if the reachable set

$$\mathcal{R}_{\{A,\,B\}} = \{\bar{X} \in SU(N) \mid \text{ there exists an admissible input } u(\cdot) \text{ such that the integral curve of (2.3) satisfies } X(0) = I,\ X(t) = \bar{X} \text{ for some } t \geqslant 0\}$$

is all of the Lie group: $\mathcal{R}_{\{A,\,B\}} = SU(N)$. Given (any) $A,\, B \in \mathfrak{su}(N)$, call $\{A,\, B\}_{L.A.}$ the Lie algebra generated by A and B with respect to the Lie bracket. The literature on the subject of quantum control, see Ref. [7, 15, 1], has relied essentially on the condition of the following Theorem (originally due to [13]):

Theorem 2.1. *The system* (2.3) *is controllable if and only if* $\{A,\, B\}_{L.A.} = \mathfrak{su}(N)$.

Theorem 2.1 is a consequence of the following Lemma, which affirms that subsemigroups of compact groups are always subgroups:

Lemma 2.1. (Lemma 1, Ch.6 of [11]) *For the compact semisimple Lie group $SU(N)$*

$$\mathrm{cl}\left(\exp(tA,\ t<0)\right) \subset \mathrm{cl}\left(\exp(tA,\ t \geqslant 0)\right) \qquad \forall\, A \in \mathfrak{su}(N)$$

where $\exp\,:\,\mathfrak{su}(N) \to SU(N)$ *is the Lie group exponential map (and* cl *means closure).*

Consequently, the drift vector field A of (2.3) is not hampering controllability on the large and thus Theorem 2.1 follows. Furthermore, the semisimple character of $\mathfrak{su}(N)$ implies the following:

Lemma 2.2. (Theorem 12, Ch.6 of [11]) *The set of pairs $A, B \in \mathfrak{su}(N)$ such that $\{A,\ B\}_{L.A.} = \mathfrak{su}(N)$ is open and dense in $\mathfrak{su}(N)$.*

Putting together Theorem 2.1 and Lemma 2.2 then we have:

Corollary 2.1. *The system* (2.3) *is controllable for almost all pairs $A,\ B \in \mathfrak{su}(N)$.*

3 Roots and graphs

Consider the following basis of $\mathfrak{su}(N)$:

$$\{iH_i\,,\ i=1,\dots,N-1\} \cup \{X_{ij} = E_{ij} - E_{ji}\,,\ 1 \leqslant i < j \leqslant N\} \cup \{Y_{ij} = i(E_{ij}+E_{ji})\,,\ 1 \leqslant i < j \leqslant N\} \tag{3.4}$$

where E_{ij} has 1 in the $(i,\ j)$-th position and 0 elsewhere.

Definition 3.1. *An element $H \in \mathfrak{su}(N)$ is said* regular *if* $\dim(\ker \mathrm{ad}_H) = N-1$.

The set of regular elements H is open and dense in $\mathfrak{su}(N)$.

For the quantum system on $\mathfrak{su}(N)$, the *roots* α of the Lie algebra, see [2], admit the interpretation of transitions between energy levels of the system. In particular, the roots computed at $\tilde{H}_0$ are $\alpha_{ij}(\tilde{H}_0) = \mathcal{E}_j - \mathcal{E}_i$ ($i<j \Rightarrow \alpha_{ij} \geqslant 0$). Denote by Δ the set of nonzero roots, by Δ^+ the subset of positive roots, and by Φ the set of *fundamental roots* i.e. the set of positive roots that cannot be written as sums of two other positive roots.

We need a stronger version of the regularity property, see Ref. [11], p. 187.

Definition 3.2. *A regular $H \in \mathfrak{su}(N)$ is said* strongly regular *if all nonzero eigenvalues $\alpha(H)$ are distinct and have multiplicity 1.*

Also the set of strongly regular elements is open and dense in $\mathfrak{su}(N)$.

B is expressed in terms of the components of the $\mathfrak{su}(N)$ basis as:

$$B = B_0 + \sum_{\alpha \in \Gamma^+ \subseteq \Delta^+} \left(b_\alpha^{\Re} X_\alpha + b_\alpha^{\Im} Y_\alpha\right) \tag{3.5}$$

where $B_0 \in i\mathfrak{h}$, $b_\alpha^{\Re}$ and $b_\alpha^{\Im}$ are real and $\Gamma^+ \subseteq \Delta^+$ is the subset of roots "touched" by B.

In this case, it is possible to use the connectivity properties of the graph of B to draw conclusions about controllability in the same spirit as it is done in [9] for *normal* (or *split*) *real forms*. Consider the *graph* $\mathcal{G}_B$ associated to a square matrix $B = [b_{ij}]$, i.e. the pair $\mathcal{G}_B = (\mathcal{N}_B, \mathcal{C}_B)$ where $\mathcal{N}_B$ represents a set of N ordered nodes $\mathcal{N}_B = \{1, \ldots, n\}$ and $\mathcal{C}_B$ the set of oriented arcs joining the nodes: $\mathcal{C}_B = \{(i, j) \mid b_{ij} \neq 0\}$. The graph $\mathcal{G}_B$ is said *strongly connected* if for all pairs of nodes in $\mathcal{N}_B$ there exists an oriented path in $\mathcal{C}_B$ connecting them. $\mathcal{G}_B$ is strongly connected if and only if B is permutation-irreducible (P-irreducible) [1], i.e. there exists no permutation matrix P such that

$$P^{-1}BP = \begin{bmatrix} B_1 & * \\ 0 & B_2 \end{bmatrix}$$

A square matrix is P-irreducible if and only if its graph does not contain any strongly disconnected subgraph. As long as we consider matrices B that are Hermitian or skew-Hermitian, the adjective "strong" (referring to the path being oriented) is irrelevant since $b_{ij} \neq 0$ if and only if $b_{ji} \neq 0$. $\mathcal{G}_{E_\alpha}$, $\alpha \in \Delta^+$, are called *elementary root graphs.* If $b_\alpha = b_\alpha^{\Re} + i b_\alpha^{\Im}$, rewriting B as

$$B = B_0 + B_1 = B_0 + \sum_{\alpha \in \Gamma^+} (b_\alpha E_\alpha - b_\alpha^* E_{-\alpha}) \tag{3.6}$$

where * is complex conjugate, then the (positive) *root graph* of B is $\mathcal{G}_B^+ = \bigcup_{\alpha \in \Gamma^+} \mathcal{G}_{E_\alpha}$ and $\mathcal{G}_{B-B_0}$ is "twice" $\mathcal{G}_B^+$.

The concepts of regular and strongly regular roots correspond to those of degenerate system and of system with degenerate transitions in the following way:

(i) if a system is degenerate then it has nonregular roots;

(ii) if a system is nondegenerate but has degenerate transitions then it has regular but not all strongly regular roots;

(iii) if a system is nondegenerate and has no degenerate transitions then it has only strongly regular roots.

In the basis (3.4), $b_\alpha = b_{ij}$, $1 \leqslant i < j \leqslant N$ and B_0 is simply the diagonal

$$B_0 = \sum_{k=1}^{N} b_{kk} E_{kk} = \sum_{k=1}^{N-1} \Big(\sum_{j=1}^{k} i b_{jj} \Big) (i H_K) \tag{3.7}$$

since $B_0 \in \mathfrak{su}(N)$ has to be traceless. The b_{jj} (which must be purely imaginary) correspond to loops on $\mathcal{G}_B$, i.e. to arcs beginning and ending on the same node. Thus they are irrelevant for the connectivity property. In the basis (3.4), A and B are:

$$A = \sum_{k=1}^{N-1} \Big(\sum_{j=1}^{k} \mathcal{E}_j \Big) (i H_k) \tag{3.8}$$

$$B = B_0 + \sum_{(i,j) \in \mathcal{C}_B^+} \big(b_{ij}^{\Re} X_{ij} + b_{ij}^{\Im} Y_{ij} \big) \tag{3.9}$$

[1] A permutation matrix P has elements that are 0 or 1, see [19]

The following lemma is the adaptation to our situation of Theorem 2 and Corollary 2 of [17]. Call $\mathfrak{f}_\alpha = \text{span}\{X_\alpha, Y_\alpha\}$.

Lemma 3.1. *B is P-irreducible* $\iff \{\mathfrak{f}_\alpha,\ \alpha \in \Gamma^+\}_{L.A.} = \mathfrak{su}(N)$

The condition of Lemma 3.1 is "minimally" satisfied by a set of fundamental roots, although due to the nonuniqueness of the selection of the fundamental roots, not all the $\alpha \in \Phi$ have to be in Γ^+ for $\mathcal{G}_B$ to be connected.

Corollary 3.1. *If $\Phi \subseteq \Gamma^+$ then B is P-irreducible.*

4 Sufficient conditions for controllability in the generic case

Considerations similar to those used in the controllability analysis of normal real forms of classical Lie algebras (see [12, 9, 8, 17]) can be employed for our compact real form as well. In the case of free Hamiltonian of diagonal type, the connectivity property of the graph of the forced term B can replace the Lie algebraic rank condition, see [9].

Lemma 4.1. *If A is diagonal, a necessary condition for controllability is that $\mathcal{G}_B$ connected.*

In the case of $\mathcal{G}_B$ disconnected, the quantum system is decomposable into noninteracting subsystems [2].

The equivalence between $\{A, B\}_{L.A.} = \mathfrak{su}(N)$ and $\mathcal{G}_B$ connected is not exact: while $\mathcal{G}_B$ connected is a necessary condition for controllability, alone it is not a sufficient condition, but requires extra assumptions to be made on the diagonal matrix A. The simplest case corresponds to the drift term A being strongly regular and corresponds to all nondegenerate transitions.

Theorem 4.1. *Given A and B as in* (3.8) *and* (3.9)*, assume that $\mathcal{G}_B$ is connected. If A is strongly regular, then the system* (2.3) *is controllable.*

A weaker property than strong regularity is B-strong regularity, introduced in [17].

Definition 4.1. *Given B as in* (3.5)*, A is said* B-strongly regular *if the elements $\alpha(\tilde{H}_0)$, $\alpha \in \Gamma^+$, are nonzero and distinct.*

Unlike strong regularity, which requires all roots of Δ to be nonnull and distinct when computed in A, B-strong regularity requires the root decomposition determined by A to be strongly regular only along the roots Γ^+ entering into the decomposition of B: $\alpha_{ij}(\tilde{H}_0) = \mathcal{E}_j - \mathcal{E}_i \neq 0$ if $b_{ij} \neq 0$. Obviously, A strongly regular means A is B-strongly regular for all B.

Theorem 4.1 is a particular case of the following:

[2]In Turinici [18] it is required that $\tilde{H}_1$ is off-diagonal. The interpretation in terms of root decomposition offered here shows that this assumption is irrelevant for controllability: the diagonal terms of $\tilde{H}_1$ belong to the Cartan subalgebra and as such they commute with A.

Theorem 4.2. *Given A and B as in* (3.8) *and* (3.9)*, assume that $\mathcal{G}_B$ is connected. If A is B-strongly regular, then the system* (2.3) *is controllable.*

An alternative extension of Theorem 4.1 is mentioned in [18]. If Π_A^+ is the set of positive roots $\alpha(\tilde{H}_0)$ that are strongly regular for A, call $\Theta_A^+ = \Gamma^+ \cap \Pi_A^+$ the subset of positive strongly regular roots of Γ^+ when computed in A and Ω_A^+ the corresponding complementary set in Γ^+ (i.e. the set of non strongly regular roots of Γ^+): $\Omega_A^+ = \Gamma^+ \setminus \Theta_A^+$. So B splits into $B = B_r + B_s$ with $B_r = B_0 + \sum_{\alpha\in\Theta_A^+} \left(b_\alpha^{\Re} X_\alpha + b_\alpha^{\Im} Y_\alpha\right)$, the intersection of B with the strongly regular roots, and $B_s = \sum_{\alpha\in\Omega_A^+} \left(b_\alpha^{\Re} X_\alpha + b_\alpha^{\Im} Y_\alpha\right)$.

Theorem 4.3. *Given A and B as in* (3.8) *and* (3.9)*, assume that $\mathcal{G}_B$ is connected. If $\mathcal{G}_{B_r}$ is connected, then the system* (2.3) *is controllable.*

For controllability, it is sufficient that Θ_A^+ contains the fundamental roots, as in this case $\mathcal{G}_{B_r}$ is connected by Corollary 3.1.

Corollary 4.1. *If $\Phi \subseteq \Theta_A^+$, then the system* (2.3) *is controllable.*

Notice that the condition of Theorem 4.1 is the one traditionally used in the literature to show that a generic pair of vector fields on compact semisimple Lie algebras are generating, see [14, 4, 3]. For this purpose, given A strongly regular, B is constructed such that ad_A is cyclic on $\bigoplus_{\alpha\in\Delta^+} \mathfrak{f}_\alpha$, for example by having $b_\alpha \neq 0\ \forall \alpha \in \Delta^+$. This means that $\bigoplus_{\alpha\in\Delta^+} \mathfrak{f}_\alpha$ can be spanned by "A-brackets" and thus all $\mathfrak{su}(N)$ is generated by adding the elements of the Cartan subalgebra. However, here the method is not directly applicable because some of the b_{ij} elements of B are allowed to be zero. In this case, from $\bigoplus_{\alpha\in\Gamma^+} \mathfrak{f}_\alpha$, the missing subspaces must be reached by means of "B-brackets" $[C,\, B]$, $[[C,\, B],\, B]$ etc. and then their span completed by single "A-brackets" $[A,\, [C,\, B]\,]$, $[A,\, [[C,\, B],\, B]\,]$, etc.

5 Sufficient conditions for controllability in a few singular cases

The use of "B-brackets" is the *leit motif* of all other sufficient conditions which are based on properties weaker than the strong regularity and B-strong regularity of the diagonal vector field A. These conditions belong to the first two cases of the classification of Section 3 and, from Corollary 4.1, they correspond to at least a pair of fundamental roots being equal. If new diagonal terms can be provided to compensate for the degenerate transitions, then controllability can be recovered. From (3.6), the level two bracket $[C,\, B]$ is

$$D = [C,\, B] = [C,\, B_0] + [C,\, B_1]$$

If B_0 is nonnull and linearly independent from A, it constitutes the simplest candidate to provide the missing fundamental roots. From (3.7), the fundamental roots at B_0, $\alpha(B_0)$, are equal to $\beta_{i,i+1} = b_{ii} - b_{i+1,i+1}$ when expressed in the basis (3.4). Restricting to the case (ii) of Section 3, i.e. assuming that the system is nondegenerate but with possibly degenerate transitions, equivalent versions of Theorems 4.1 and 4.2 hold for B_0 and C instead of A and B.

Theorem 5.1. *If A regular and $\mathcal{G}_B$ connected, then either of the following conditions is sufficient for controllability of* (2.3)*:*

1. *B_0 is strongly regular*

2. *B_0 is C-strongly regular*

One can think of weakening further the hypothesis of Theorem 5.1 by combining together strongly regular pieces from both A and B_0. To this end, analogously to what was done for the diagonal matrix A, call Θ_B^+ the set of positive strongly regular roots $\alpha(B_0)$ of Γ^+ and C_r the corresponding part of C: $C_r = \sum_{\Theta_B^+} \alpha(A) \left(b_\alpha E_\alpha + b_\alpha^* E_{-\alpha} \right)$.

Theorem 5.2. *Assume A regular and $\mathcal{G}_B$ connected. If $\mathcal{G}_{B_r} \cup \mathcal{G}_{C_r}$ is connected then the system* (2.3) *is controllable.*

As last, we treat the case of Cartan subalgebras from level two brackets of A and B. Since C is off-diagonal, the only useful bracket in this respect is $[C, B]$.
If D_0 is the diagonal part of D, then $D = D_0 + D_1$ and we can reformulated Theorem 5.1 with D_0 replacing B_0.

Theorem 5.3. *If A regular and $\mathcal{G}_B$ connected, then any of the following conditions is sufficient for controllability of* (2.3)*:*

1. *D_0 is strongly regular*

2. *D_0 is B-strongly regular*

3. *D_0 is C-strongly regular*

The practical situations in which Theorems 5.1-5.3 apply are when the system has resonant modes (which, again, corresponds to the case (ii) in the classification of Section 3). The extreme case is when $\mathcal{E}_{i+1} - \mathcal{E}_i = \text{const} \ \forall \ i = 1, \ldots n-1$ (nondegenerate system with all equally spaced energy levels). It is treated for example in [16].

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