Lie Algebraic Analysis and Control of Quantum Dynamics
(extended abstract)

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The goal of this paper is to describe the Lie algebraic method for analysis of quantum control systems. The starting point of this method is the calculation of the dynamical Lie algebra associated with a quantum system. If the system is not fully controllable, then one decomposes the dynamical Lie algebra into its semisimple and solvable parts and then the semisimple part into its simple ideals. This dynamical decomposition highlights the main features of the dynamics and therefore simplifies the task of control. This method was already described in various parts of the book [2] but we present a unified treatment in this paper and fill some gaps in the presentation of [2], in particular for what concerns the algorithms involved in the computations of the dynamical decomposition. Moreover, we shall describe some examples of application of this methodology.

1 Introduction

It is well known (see, e.g, [2], [4]) that given a finite dimensional quantum system described by the Schrödinger operator (matrix) equation

\[ \dot{X} = -iH(u(t))X, \quad X(0) = 1, \quad (1) \]

the set of operators \( X \) reachable by varying the control \( u \) is the connected Lie subgroup of \( U(n) \) corresponding to the Lie algebra \( \mathcal{L} \) generated by the set

\[ \mathcal{F} := \{ iH(u) | u \in \mathcal{U} \}, \quad (2) \]

that is, the smallest Lie subalgebra of \( u(n) \) containing \( \mathcal{F} \). In (1), (2), \( H \) is the Hamiltonian of the system which is a Hermitian matrix function of a (classical) control \( u = u(t) \), varying in a set of functions which, we assume, contains piecewise constant functions, with values in a set \( \mathcal{U} \). The matrix \( 1 \) is the identity matrix of appropriate dimensions. The Lie algebra \( \mathcal{L} \) is called the dynamical Lie algebra associated with the system and the associated connected Lie subgroup of \( U(n) \) will be denoted here by \( e^{\mathcal{L}} \).1 There exists a very simple algorithm to calculate \( \mathcal{L} \): One starts with a basis of \( \mathcal{F} \), \( F_1, \ldots, F_r \). If \( r = n^2 \) or \( r = n^2 - 1 \), one stops because \( \mathcal{L} = u(n) \) or \( \mathcal{L} = su(n) \), respectively. In this case \( e^{\mathcal{L}} = U(n) \) or \( e^{\mathcal{L}} = SU(n) \) and the system is said to be controllable.2 If this is not the case, one performs the Lie brackets of depth 1 \([F_j, F_k]\), \( j \neq k \) and isolate the ones that are linearly independent together with \( \{F_1, \ldots, F_r\} \), say \( D_1, \ldots, D_s \), if any. Then one performs Lie brackets of depth 2 which are Lie brackets of \( D_1, \ldots, D_s \) with the \( F_j \)'s, \( j = 1, \ldots, r \) and isolate matrices that are linearly independent together with \( F_1, \ldots, F_r, D_1, \ldots, D_s \). One goes on this way until one does not find any new linearly independent matrices. The set of matrices

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1Extending this notation, we shall use the notation \( e^K \) for the connected Lie group associated with a Lie algebra \( K \).
2This type of controllability is often called complete controllability or operator controllability to distinguish it from controllability of the state [1], [6].
thus found is a basis of the dynamical Lie algebra $\mathcal{L}$. If the size of this set is $n^2$ or $n^2 - 1$, we are in the controllable case. Otherwise the system is not controllable.\(^3\) However the Lie algebra $\mathcal{L}$ gives us information about the nature of the dynamics as we shall see in the rest of this paper.

## 2 Decomposition of the Dynamics

In this section, we will see how a vector space decomposition of $\mathcal{L}$ induces a factorization of the Lie group $e^\mathcal{L}$ and therefore a decomposition of the dynamics of (1). Every Lie algebra $\mathcal{L}$ over the field of reals $\mathbb{R}$ is the semidirect sum of a semisimple Lie algebra $S$ and the maximal solvable ideal in $\mathcal{L}$, called the radical, $R$, that is,

$$\mathcal{L} = S \oplus R. \quad (3)$$

Semidirect sum means that

$$[S, S] \subseteq S, \quad [S, R] \subseteq R, \quad [R, R] \subseteq R. \quad (4)$$

This is known as Levi decomposition (see, e.g., [3]). While $R$ is unique the semisimple part $S$ is unique only up to isomorphisms of $\mathcal{L}$. It is called the Levi subalgebra. The Levi subalgebra $S$ is the direct sum of $p$ simple subalgebras $S_j$, $j = 1, \ldots, p$, i.e.,

$$S = \bigoplus_{j=1}^{p} S_j. \quad (5)$$

Direct sum means that

$$[S_f, S_b] = \{0\}, \quad \text{when } f \neq b. \quad (6)$$

In our case, the fact that the dynamical Lie algebra $\mathcal{L}$ is a subalgebra of $u(n)$ implies several important simplifications in the Levi’s decomposition of $\mathcal{L}$. In particular we have:\(^4\)

**Theorem 1** If $\mathcal{L} \subseteq u(n)$, then the semidirect sum in (3) is a direct sum, i.e.,

$$[S, R] = \{0\}, \quad (7)$$

and $R$ is Abelian, i.e., $[R, R] = \{0\}$.

The decomposition of the dynamical Lie algebra $\mathcal{L}$ (3) has immediate consequences for the Lie group of possible evolutions $e^\mathcal{L}$ and for the dynamics of the quantum system (1). For every control $u$, the solution of (1) $X = X(t)$ factorizes as

$$X(t) = R \prod_{j=1}^{p} S_j. \quad (8)$$

Here $S_j \in e^{S_j}$ and $R \in e^{R}$ and all the factors in (8) commute. Moreover $R$ is itself the product of elements belonging to one dimensional commuting subgroups. Write $R$ as the sum of one dimensional Lie algebras $R = \bigoplus_{l=1}^{q} R_l$, then $R = \prod_{l=1}^{q} R_l$, with $R_l \in e^{R_l}$. Controlling the system (1) means then controlling in parallel the systems

$$\dot{S}_j = -iH_{S_j}(u)S_j, \quad S_j(0) = 1, \quad j = 1, \ldots, p, \quad (9)$$

$$\dot{R}_l = -iH_{R_l}(u)R_l, \quad R_l(0) = 1, \quad l = 1, \ldots, q \quad (10)$$

where $-iH_{S_j}$ and $-iH_{R_l}$ are the components of $-iH(u)$ in $S_j$, $j = 1, \ldots, p$, and $R_l$, $l = 1, \ldots, q$, respectively.

\(^3\)See subsection 3.2.1 of [2] for further discussion of this procedure.

\(^4\)This fact is probably known but was not used in the treatment of [2]. A proof will be given in the final version of this paper.
In conclusion, every finite dimensional quantum mechanical control system has the structure of $p + q$ subsystems in parallel of Figure 1. The first $p$ subsystems vary on simple Lie groups for which a classification is known (cf. [5] and the references therein). The remaining $q$ subsystems vary on one dimensional Lie groups. The total evolution is the commuting product of the evolutions on the various smaller subgroups.

\[
\begin{align*}
\dot{S}_1 &= -iH_{S1}(u(t))S_1 \\
\vdots \\
\dot{S}_p &= -iH_{Sp}(u(t))S_p \\
\dot{R}_1 &= -iH_{R1}(u(t))R_1 \\
\vdots \\
\dot{R}_q &= -iH_{Rq}(u(t))R_q \\
X &= \prod_{l=1}^{q} R_l \prod_{j=1}^{p} S_j
\end{align*}
\]

Figure 1: Structure of a quantum control system. The control $u$ drives simultaneously $p + q$ systems on Lie groups (which are simple Lie groups or one-dimensional Lie groups). The total evolution $X$ is the commuting product of the evolutions on the various subgroups.

In order to obtain the decomposition of the dynamics, we need to find bases for the subalgebras, $S_j$ and $R_l$, $j = 1, \ldots, p$, $l = 1, \ldots, q$, of $\mathcal{L}$ starting from a basis of $\mathcal{L}$. Algorithms to calculate these bases exist for general Lie algebras over general fields [3]. However they can be significantly simplified in our specific case since $\mathcal{L}$ is a subalgebra of $u(n)$. Much of the treatment in the next section is based on [3], but we give simplified algorithms for these calculations.

3 Algorithms

Consider a basis $\{L_1, \ldots, L_s\}$ of $\mathcal{L}$. The calculation of bases of the two subspaces $\mathcal{S}$ and $\mathcal{R}$ in (3) is very much simplified in the case of interest here. It is easily seen that $\mathcal{R}$ is the center of $\mathcal{L}$, and therefore it is the space of the solutions of the system of $s = \dim \mathcal{L}$ equations

\[
[R, L_j] = 0, \quad j = 1, \ldots, s,
\]
in the variable \( R \in \mathcal{L} \). Moreover, using the fact that for every semisimple Lie algebra \( \mathcal{S}, \mathcal{S} = [\mathcal{S}, \mathcal{S}] \), along with \([\mathcal{S}, \mathcal{R}] = 0\) and that \( \mathcal{R} \) is Abelian, we have

\[
[\mathcal{L}, \mathcal{L}] = [\mathcal{S} \oplus \mathcal{R}, \mathcal{S} \oplus \mathcal{R}] = [\mathcal{S}, \mathcal{S}] = \mathcal{S}.
\]

Therefore the set of \( \begin{pmatrix} s \\ 2 \end{pmatrix} \) matrices, \([L_j, L_k], j \neq k\), spans \( \mathcal{S} \). In fact one can take a subspace complementary to \( \mathcal{R} \) in \( \mathcal{L} \) and a basis there of elements \( G_1, \ldots, G_{s - \dim \mathcal{R}} \) and calculate the space spanned by the \( \begin{pmatrix} s - \dim \mathcal{R} \\ 2 \end{pmatrix} \) Lie brackets \([G_j, G_k], j \neq k\).

The calculation of the simple ideals of \( \mathcal{S}, \mathcal{S}_j, j = 1, \ldots, \rho \), is more complicated. A preliminary step is the calculation of the so-called primary decomposition of \( \mathcal{S} \) which is also of interest to understand the structure of \( \mathcal{S} \). Therefore we treat this problem first.\(^5\)

### 3.1 Calculation of the primary decomposition of \( \mathcal{S} \)

The following definition is of interest for general Lie algebras.

**Definition 3.1** A Cartan subalgebra of a Lie algebra \( \mathcal{S} \) is a nilpotent subalgebra \( \mathcal{A} \) which is equal to its normalizer, that is

\[
\mathcal{A} = \{ S \in \mathcal{S} | [S, \mathcal{A}] \subseteq \mathcal{A} \}. \quad (13)
\]

The following algorithm calculates the Cartan subalgebra for \( \mathcal{S} \) semisimple and \( \mathcal{S} \subseteq u(n) \).

**Algorithm 1**

1. Given the semisimple Lie algebra \( \mathcal{S} \), set \( \mathcal{A} = \{0\} \).
2. Select an element \( X \neq 0 \) in \( \mathcal{S} \).
3. Calculate the space of elements in \( \mathcal{S} \) which commute with \( X \). Call this space \( \mathcal{D} \).
   
   Notice \( \mathcal{D} \) is also a subalgebra of \( u(n) \).\(^6\) Therefore (just like \( \mathcal{L} \) above), it has a Levi decomposition in its semisimple part which is equal to \([\mathcal{D}, \mathcal{D}]\) and the center, \( C(\mathcal{D}) \). This justifies the next step.
4. Write \( \mathcal{D} = [\mathcal{D}, \mathcal{D}] \oplus C(\mathcal{D}) \) where \( C(\mathcal{D}) \) is the center of \( \mathcal{D} \).
5. Set \( \mathcal{A} = \mathcal{A} \oplus C(\mathcal{D}) \).
6. If \([\mathcal{D}, \mathcal{D}] = 0\) Stop and return \( \mathcal{A} \) as Cartan subalgebra otherwise set \( \mathcal{S} = [\mathcal{D}, \mathcal{D}] \) and go to step 2.

The algorithm converges because at each step \( \mathcal{S} \) is semisimple and \( \mathcal{D} \) is a proper subspace of \( \mathcal{S} \), otherwise \( \mathcal{S} \) would have an element which commutes with all of \( \mathcal{S} \) which contradicts semisimplicity.

The following definition refers to a general Lie algebra over a general field (cf. [3] (Definitions 3.1.1 and 3.1.9)).

**Definition 3.2** A *collected primary decomposition* of a semisimple Lie algebra \( \mathcal{S} \) with respect to a Cartan subalgebra \( \mathcal{A} \) is a vector space decomposition of the form

\[
\mathcal{S} := \mathcal{A} \oplus \mathcal{V}_1 \oplus \mathcal{V}_2 \oplus \cdots \mathcal{V}_r, \quad (14)
\]

where

\(^5\)Proofs for the algorithms will be given in a complete version of this paper.

\(^6\)The fact that it is a Lie algebra, i.e., \([D_1, D_2] \in \mathcal{D}, \text{ for } D_1, D_2 \in \mathcal{D}\) follows immediately from an application of the Jacobi identity. We have \([\mathcal{D}_1, \mathcal{D}_2], X] = -[\mathcal{D}_2, X], D_1] - [[X, D_1], D_2] = 0.\]
1. The subspaces \( \mathcal{V}_j \)'s, \( j = 1, \ldots, r \), are invariant under \( \text{ad}_X \), for every \( X \in \mathcal{A} \), that is
\[
[\mathcal{A}, \mathcal{V}_j] \subseteq \mathcal{V}_j, \quad j = 1, \ldots, r.
\]
2. For every \( X \in \mathcal{A} \), and every \( \mathcal{V}_j \), the minimum polynomial of \( \text{ad}_X \) restricted to \( \mathcal{V}_j \) is the power of an irreducible polynomial.\(^7\)
3. For any two subspaces \( \mathcal{V}_j \) and \( \mathcal{V}_k \), there exists an \( X \in \mathcal{A} \) such that the minimum polynomials of \( \text{ad}_X \) restricted to \( \mathcal{V}_j \) and \( \mathcal{V}_k \) are powers of two different irreducible polynomials.

Given \( \mathcal{A} \) such a decomposition exists and is unique (Theorem 3.1.10 of [3]).

In our case, for every \( X \), the minimum polynomial of \( \text{ad}_X \) restricted to \( \mathcal{V}_j \) must be of the type \( (\lambda^2 + a_j^2) \), otherwise \( \text{ad}_X \) would have eigenvalues with nonzero real parts and-or eigenvalues with geometric multiplicity greater than one. This is not possible because we have (in an appropriate basis) \( \text{ad}_X^2 = -\text{ad}_X \).

An algorithm to calculate the collected primary decomposition is given below.

**Algorithm 2**

1. Select an element \( X \in \mathcal{A} \) such that \( \text{ad}_X \) has \( \dim \mathcal{L} - \dim \mathcal{A} + 1 \) different eigenvalues. That is, except for the 0 eigenvalue (which has eigenspace equal to \( \mathcal{A} \)), \( \text{ad}_X \) is non-degenerate.

   Such elements are called *splitting elements* and they exist (Corollary 4.11.3 of [3]). To find such an \( X \), notice that, if \( \{A_1, \ldots, A_m\} \) is a basis of \( \mathcal{A} \) then \( \text{ad}_{A_1}, \ldots, \text{ad}_{A_m} \) all commute and they can be simultaneously diagonalized. It is easier then to select real coefficients \( c_j \), such that \( \sum_{j=1}^{m} c_j \text{ad}_{A_j} \) has the desired property, and \( X = \sum_{j=1}^{m} c_j A_j \). For higher dimensional problems it may be more convenient to use randomized algorithms.

   Let \( X \) be the selected element, the minimum polynomial is of the form
\[
m_{\text{ad}_X}(\lambda) = \prod_{j=1}^{f} (\lambda^2 + a_j^2),
\]
with the \( a_j \) all \( \in \mathbb{R} \), all different from each other and with one of them equal to zero (0 is always an eigenvalue of \( \text{ad}_X \), \( X \) being an eigenvector).

   Moreover, from the choice of \( X \) being splitting \( f = \frac{\dim \mathcal{S} - \dim \mathcal{A}}{2} + 1 \) and is equal to the characteristic polynomial except (possibly) for the power of the monomial associated to the eigenvalue 0.\(^8\)

2. Take as \( \mathcal{V}_j \) the (two-dimensional) eigenspaces associated with the pair of purely imaginary eigenvalues corresponding to \( a_j^2 \). That is
\[
\mathcal{V}_j = \{ V \in \mathcal{L} | (\text{ad}_X^2 + a_j^2) V = 0 \}, \quad j = 1, \ldots, \frac{\dim \mathcal{S} - \dim \mathcal{A}}{2}.
\]

### 3.2 Calculation of the decomposition in simple ideals

The primary decomposition is a fundamental tool to explore the structure of a semisimple Lie algebra \( \mathcal{S} \). Using it, one can directly obtain the decomposition into simple ideals (5). The algorithm is as follows.

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\(^7\)An irreducible polynomial is a polynomial that is not factorized or cannot be factorized further in products of polynomials. The property of a polynomial to be irreducible depends crucially on the field we are considering. In the complex field, there is only one type of irreducible polynomials which are the ones written as \( \lambda + \alpha \), with \( \alpha \) complex. In the real field, which is the one which interests us the most there are only two types \( (\lambda - a) \) with \( a \in \mathbb{R} \) and \( (\lambda^2 + 2\zeta\lambda + \beta^2) \), with \( \zeta^2 - \beta^2 < 0 \), \( \zeta \) and \( \beta \) real. Notice that the last polynomial is not irreducible over the complex field.

\(^8\)Notice in particular that the difference between the dimension of \( \mathcal{L} \) and that of \( \mathcal{A} \) must be an even number.
Algorithm 3

1. For every $j = 1, \ldots, r$, calculate the spaces

$$I_j := + \infty_{k=0}^\infty \text{ad}_{S}^k \mathcal{V}_j,$$

where $\mathcal{V}_j$ are defined in (14).

$I_j$ is the smallest ideal containing $\mathcal{V}_j$. \text{ad}_{S}^k \mathcal{V}_j$ is defined inductively, where $\text{ad}_{S}^0 \mathcal{V}_j = \mathcal{V}_j$, and $\text{ad}_{S}^k \mathcal{V}_j = [S, \text{ad}_{S}^{k-1} \mathcal{V}_j]$.

2. The simple ideals $\mathcal{S}_l$, $l = 1, \ldots, p$ in (5) are given by the ideals $I_j$. Notice that some ideals may be coinciding.

4 Conclusion

This talk will conclude by presenting three physical examples of application of the above algorithms for decomposition of the dynamics: The first example concerns two spin $\frac{1}{2}$ particles subject to a single component of a magnetic field. The second example concerns two spin $\frac{1}{2}$ particles subject to only local operations and the third example is a quantum walk on a cycle. This is in fact a discrete time system but it is amenable of the same type of dynamical decomposition advocated here. The complete version of the paper will give a background of concepts from Lie algebras theory.

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References

[1] F. Albertini and D. D’Alessandro, Notions of controllability for bilinear multilevel quantum systems, *IEEE Transactions on Automatic Control*, 48, No. 8, 1399-1403 (2003).

[2] D. D’Alessandro, *Introduction to Quantum Control and Dynamics*, CRC Press, Boca Raton, FL, 2007.

[3] W. A. de Graaf, *Lie Algebras; Theory and Algorithms*, North-Holland, 2000.

[4] V. Jurdjević and H. Sussmann, Control Systems on Lie groups, *Journal of Differential Equations*, 12, 1972 313-329.

[5] A. Knapp, *Lie Groups: Beyond an Introduction*, 2nd ed., Birkhauser Beston, 2002.

[6] S. G. Schirmer, J. V. Leahy and A. I. Solomon, Degrees of controllability for quantum systems and applications to atomic systems, *J. Phys. A.*35, 4125-4141 (2002).