NOTIONS OF CONTROLLABILITY FOR BILINEAR MULTILEVEL QUANTUM SYSTEMS

Francesca Albertini [1] and Domenico D'Alessandro[2]

Abstract

In this paper, we define four different notions of controllability of physical interest for multilevel quantum mechanical systems. These notions involve the possibility of driving the evolution operator as well as the state of the system. We establish the connections among these different notions as well as methods to verify controllability.

1 Introduction

In this paper, we consider multilevel quantum systems described by a finite dimensional bilinear model [7], [20]

$$|\dot{\psi}> = (A + \sum_{i=1}^{m} B_i u_i(t))|\psi>, \tag{1}$$

where $|\psi>$[3] is the state vector varying on the complex sphere $S_{\mathbb{C}}^{n-1}$, defined as the set of n-ples of complex numbers $x_j + iy_j$, $j = 1, ..., n$, with $\sum_{j=1}^{n} x_j^2 + y_j^2 = 1$. The matrices A, $B_1, ..., B_m$ are in the Lie algebra of *skew-Hermitian* matrices of dimension n, $u(n)$. If A and B_i, $i = 1, ..., m$ have zero trace they are in the Lie algebra of skew Hermitian matrices with zero trace, $su(n)$. The functions $u_i(t)$, $i = 1, 2, ..., m$ are the controls. They are assumed to be piecewise continuous functions although this assumption is immaterial for most of the theory developed here. Models of quantum control systems different from the bilinear one (1) may be more appropriate in some cases (see e.g. [2], [8]). Infinite dimensional (quantum) bilinear systems have been studied in control theory in [3], [12].

The solution of (1) at time t, $|\psi(t)>$ with initial condition $|\psi_0>$, is given by:

$$|\psi(t)>= X(t)|\psi_0>, \tag{2}$$

where $X(t)$ is the solution at time t of the equation

$$\dot{X}(t) = (A + \sum_{i=1}^{m} B_i u_i(t))X(t), \tag{3}$$

with initial condition $X(0) = I_{n\times n}$. The matrix $X(t)$ varies on the Lie group of special unitary matrices $SU(n)$ or the Lie group of unitary matrices $U(n)$ according to whether or not the matrices A and B_i in (3) have all zero trace.

---

[1]Dipartimento di Matematica Pura ed Applicata, Universita' di Padova, via Belzoni 7, 35100 Padova, Italy. Tel. (+39) 049 827 5966 email: albertin@math.unipd.it

[2]Department of Mathematics, Iowa State University, Ames, IA 50011, USA, Tel. (+1) 515 294 8130, email: daless@iastate.edu

[3]We use Dirac notation $|\psi>$ to denote a vector on $\mathbb{C}^n$ of length 1, and $<\psi| := |\psi>^*$ where * denotes transposed conjugate

Equation (1) is the Schrödinger equation [22] which describes the dynamics of a quantum system. The Hamiltonian operator $H(t) := A + \sum_{i=1}^{n} B_i u_i(t)$ represents the energy of the system at time t. More specifically, assuming the $u_i(t)$ constant, $i = 1, ..., m$, the eigenvectors of the matrix H are the stationary states which are associated to the possible values for the energy of the system. These values for the energy are given by the corresponding eigenvalues of H. It is always possible to assume that A and the B_i's have zero trace, since this can be achieved by adding a multiple of the identity to H, which corresponds to shifting the values of the energy by a fixed amount. It is assumed in (1) that the Hamiltonian has an affine dependence on some functions of time, the controls u_i, $i = 1, .., m$, which can be varied in a given experimental set up. An example of a system that can be described by an equation of this type is a particle with spin in a time varying electro-magnetic field where the controls u_i represent the x, y and z components of the field. The problem of control for this particular system is treated in some detail in [7].

In several experiments, it is of interest to know whether or not fields u_i can be chosen so as to drive the state $|\psi>$ in (1) between two given configurations. This is the case for example in Molecular Control [6] where $|\psi>$ represents the state of a chemical reaction. In other contexts, it is important to know whether every unitary transformation between two states ($X(t)$ in (2)) can be implemented with a given physical set-up. This occurs, for example, in quantum computation [9] where the state of the system $|\psi>$ carries the *information* and the evolution operator X represents a *(logic) operation.*

In this paper, we shall define four different notions of controllability which are of physical interest for quantum mechanical systems of the form (1). Using general results on transitivity of transformation groups, we shall provide criteria to check these controllability notions and establish the connections among them.

The controllability of the system (1) is usually investigated by applying general results on bilinear right invariant systems on compact Lie groups [13] [20]. These results, applied to our model, give a necessary and sufficient condition for the set of states reachable for system (3) to be the whole Lie group $U(n)$ (or $SU(n)$). The condition is given in terms of the Lie algebra generated by the matrices A, B_1,...,B_m. Controllability results for quantum systems that do not use the Lie algebraic approach have been developed in [14], [28] [29]. Investigations related to the one presented here were carried out in [24]-[27] which also present some examples of applications.

2 Definitions of Notions of Controllability for Multilevel Quantum Systems

The following notions of controllability are of physical interest for quantum mechanical systems described in (1):

- **Operator-Controllability (OC)**. The system is *operator-controllable* if every desired unitary (or special unitary) operation on the state can be performed using an appropriate control field. From (2) and (3), this means that there exists an admissible control to drive the state X in (3) from the Identity to X_f, for any $X_f \in U(n)$ (or $SU(n)$).

We shall use the term operator controllable for both the unitary case and the special unitary case pointing out the difference between the two cases wherever appropriate. Operator controllability in the unitary case is called 'Complete Controllability' in [24], [25].

- **Pure-State-Controllability (PSC)**. The system is *pure-state-controllable* if for every pair of initial and final states, $|\psi_0>$ and $|\psi_1>$ in $S^{n-1}_{\mathbb{C}}$ there exist control functions $u_1, ..., u_m$ and a time $t > 0$ such that the solution of (1) at time t, with initial condition $|\psi_0>$, is $|\psi(t)>=|\psi_1>$.
- **Equivalent-State-Controllability (ESC)**. The system is *equivalent-state-controllable* if, for every pair of initial and final states, $|\psi_0>$ and $|\psi_1>$ in $S^{n-1}_{\mathbb{C}}$, there exist controls $u_1, ..., u_m$ and a phase factor ϕ such that the solution of (1) $|\psi>$, with $|\psi(0)>=|\psi_0>$, satisfies $|\psi(t)>=e^{i\phi}|\psi_1>$, at some $t > 0$.

A density matrix ρ is a matrix of the form $\rho := \sum_{j=1}^{r} w_j |\psi_j><\psi_j|$, where the coefficients $w_j > 0$, $j = 1, 2, ..., r$, satisfy $\sum_{j=1}^{r} w_j = 1$ (see e.g. [22] Chp. 3). The state of a quantum system can be described by a density matrix. In particular, this is necessary when the system is an ensemble of non interacting quantum systems. The constant w_j, $j = 1, \ldots, r$, gives the proportion of systems in the state $|\psi_j>$.

- **Density-Matrix-Controllability (DMC)** The system is density matrix controllable if, for each pair of unitarily equivalent [4] density matrices ρ_1 and ρ_2, there exists a control $u_1, u_2, ..., u_m$ and a time $t > 0$, such that the solution of (3) at time t, $X(t)$, satisfies

$$X(t)\rho_1 X^*(t) = \rho_2. \tag{4}$$

Equivalent state controllability is of interest because, in quantum mechanics, states that differ by a phase factor are physically indistinguishable. Therefore, from a physics point of view, having ESC is as good as having PSC. Density matrix controllability is of interest when a mixed ensemble of different states is considered. In this case, the state at every time is represented by a density matrix which evolves as $\rho(t) = X(t)\rho(0)X^*(t)$, where $X(t)$ is solution of (3) with initial condition equal to the identity. Since $X(t)$ is unitary, only density matrices that are unitarily equivalent to the initial one can be obtained through time evolution.

In the following five sections we study the previous four notions of controllability, give criteria to check them in practice, and discuss the relations among them.

3 Operator Controllability

Operator controllability is the type of controllability considered in [20]. Operator controllability can be checked by verifying the *Lie algebra rank condition* [13], namely by verifying whether or not the Lie algebra generated by $\{A, B_1, B_2, ..., B_m\}$ is the whole Lie algebra $u(n)$ (or $su(n)$). More in general, recall that there exists a one to one correspondence between the Lie subalgebras of $u(n)$ and the connected Lie subgroups of $U(n)$. We will denote in the sequel by $\mathcal{L}$ the Lie algebra generated by $\{A, B_1, B_2, ..., B_m\}$ and by $e^{\mathcal{L}}$ the corresponding connected Lie subgroup of $U(n)$. The following result follows from the fact that $U(n)$ is a *compact* Lie group (its proof can be easily carried out by showing that I is a Poisson stable point and by applying Theorem 4.4 of [16]).

Theorem 1 *The set of states attainable from the Identity for system (3) is given by the connected Lie subgroup $e^{\mathcal{L}}$, corresponding to the Lie algebra $\mathcal{L}$, generated by $\{A, B_1, B_2, ..., B_m\}$.*

Corollary 3.1 System (3) is operator-controllable if and only if $\mathcal{L} = u(n)$ (or $\mathcal{L} = su(n)$).

[4] Two matrices A, $B \in U(n)$ are said to be unitarily equivalent if there exists a matrix $C \in U(n)$ such that $CAC^* = B$

4 Pure State Controllability

From the representation of the solution of Schrödinger equation (2), it is clear that the system is pure state controllable if and only if the Lie group $e^{\mathcal{L}}$ corresponding to the Lie algebra $\mathcal{L}$ generated by $\{A, B_1, ..., B_m\}$ is transitive on the complex sphere $S^{n-1}_{\mathbb{C}}$. Results on the classification of the *compact* and *effective* [5] Lie groups transitive on the (real) sphere were obtained in [4], [18], [23]. Applications to control systems were described in [5]. We will recall in Theorem 3 these results and then will provide further results and make the necessary connections for the application of interest here.

We consider the canonical Lie group isomorphism between $U(n)$ and a Lie subgroup of $SO(2n)$. The correspondence between the matrices $X = R + iY$ in $U(n)$, with R and Y real, and the matrix $\tilde{X} \in SO(2n)$ is given by

$$\tilde{X} := \begin{pmatrix} R & -Y \\ Y & R \end{pmatrix}. \tag{5}$$

The same formula (5) provides the corresponding isomorphism between the Lie algebra $u(n)$ and a Lie subalgebra of $so(2n)$. As X acts on $|\psi > := \psi_R + i\psi_I$ on the complex sphere $S^{n-1}_{\mathbb{C}}$, $\tilde{X}$ acts on the vector $\begin{pmatrix} \psi_R \\ \psi_I \end{pmatrix}$ on the real sphere S^{2n-1}. Therefore, transitivity of one action is equivalent to transitivity of the other. Since $SO(2n)$ is effective on the real sphere S^{2n-1} so is each of its Lie subgroups and in particular the one obtained from $e^{\mathcal{L}}$ via the transformation (5). As for compactness, notice that the transformation (5) preserves compactness. Moreover, $e^{\mathcal{L}}$ is connected and we have the following facts (see [19] pg. 226, we state here this result in a form suitable to our purposes):

Theorem 2 *([19]) For every connected Lie group G which is transitive on the real sphere, there exists a compact connected Lie subgroup $H \subseteq G$ which is also transitive*[6].

Theorem 3 *([18], [23]) The only compact connected Lie subgroups of $SO(2n)$ that are transitive on the real sphere of odd dimensions S^{2n-1} are locally isomorphic to one of the following:*

1) $SO(2n)$ itself.

2) $U(n)$.

3) $SU(n)$, $n \geq 2$.

4) The symplectic group $Sp(\frac{n}{2})$, for n even and $n > 2$. [7]

5) The full quaternion-unitary group defined as the group generated by $Sp(\frac{n}{2})$ and the one dimensional group $\{K \in U(n) | K := e^{i\phi} I_n, \phi \in \mathbf{R}\}$, $n > 2$ and even.

6) The covering groups of $SO(7)$ and $SO(9)$ for $n = 4$ and $n = 8$, respectively.

Notice that Theorem 3 solves only partially the problem of determining which subgroups of $SO(2n)$ are transitive on the real sphere S^{2n-1}. In fact, it only gives a necessary condition for the

[5] Recall (see e.g. [19] pg. 40) that a transformation group G on a manifold M is called effective if the only transformation in G that leaves every element of M fixed is the identity in G.

[6] Connectedness is not explicitly mentioned in the result in [19] but it follows from the proof since H is in fact a maximal compact subgroup of G which is always connected (see [19] pg. 188).

[7] Recall the Lie group of symplectic matrices $Sp(k)$ is the Lie group of matrices X in $SU(2k)$ satisfying $XJX^T = J$, with J given by $J = \begin{pmatrix} 0 & I_k \\ -I_k & 0 \end{pmatrix}$.

Lie algebra to be isomorphic to one of the Lie algebras of the Lie groups listed in the theorem. It is known that, for example, the realification (5) of the symplectic group $Sp(\frac{n}{2})$ is transitive on S^{2n-1}, but nothing can be said from the Theorem for Lie groups that are only locally isomorphic (namely have isomorphic Lie algebra) to $Sp(\frac{n}{2})$, unless further information is supplied. In this paper we are interested only in the subgroups of $SO(2n)$ that are isomorphic via (5) to a subgroup of $SU(n)$ (or $U(n)$). We will solve the problem of giving necessary and sufficient conditions for pure state controllability in terms of the Lie algebra $\mathcal{L}$ generated by $A, B_1, B_2, ..., B_m$ in Theorem 4. In the following three Lemmas we use representation theory and structure theory (see e.g. [15]) to prove three properties of classical Lie groups and algebras which we will use in the proof of Theorem 4. We refer to [15] for the terminology and notions of Lie group theory used here. We relegate the proofs of the three lemmas to the Appendix.

Recalling that, by definition, the covering groups of $SO(7)$ and $SO(9)$ have Lie algebras isomorphic to $so(7)$ and $so(9)$ respectively, Lemma 4.1 will be used to rule out that such groups arise, after realification (5), as subgroups of $SU(4)$ (or $U(4)$) and $SU(8)$ (or $U(8)$).

Lemma 4.1 (a) There is no Lie subalgebra of $su(4)$ (or $u(4)$) isomorphic to $so(7)$.
(b) There is no Lie subalgebra of $su(8)$ (or $u(8)$) isomorphic to $so(9)$.

Lemma 4.2 Assume n even. All the subalgebras of $su(n)$ or $u(n)$ that are isomorphic to $sp(\frac{n}{2})$ are conjugate to $sp(\frac{n}{2})$ via an element of $U(n)$.

Lemma 4.3 Assume n even. Then, the only subalgebra of $su(n)$ containing $sp(\frac{n}{2})$ (or a Lie algebra isomorphic to $sp(\frac{n}{2})$) properly is $su(n)$ itself.

We are now ready to state a necessary and sufficient condition for pure state controllability in terms of the Lie algebra $\mathcal{L}$ generated by $\{A, B_1, B_2, ..., B_m\}$.

Theorem 4 *The system is pure state controllable if and only if $\mathcal{L}$ is isomorphic (conjugate) to $sp(\frac{n}{2})$ or to $su(n)$, for n even, or to $su(n)$, for n odd (with or without the iI, where I is the identity matrix).*

Proof. If the system is pure state controllable then $e^{\mathcal{L}}$ is transitive on the complex sphere $S^{n-1}_{\mathbb{C}}$, therefore its realification (5) is transitive on the real sphere S^{2n-1}. Thus, from Theorem 2, it must contain a Lie group locally isomorphic to one of the groups listed in Theorem 3. As a consequence, the Lie algebra $\mathcal{L}$ must contain a Lie algebra isomorphic to one of the corresponding Lie algebras. Assume first n odd, then cases 4) 5) and 6) are excluded. Case 1) is also excluded since $\dim SO(2n) > \dim U(n)$, when $n \geq 2$ (recall that $SO(2)$ is the realification of $U(1)$). Therefore $\mathcal{L}$ must be either $su(n)$ or $u(n)$ in this case. If $n = 2$ then $su(2) = sp(1)$ so cases 3) and 4) and 2) and 5) coincide. If n is even and $n > 2$, then case 1) is excluded as above and cases 2) through 5) all imply that $sp(\frac{n}{2}) \subseteq \mathcal{L}$ up to isomorphism of $sp(\frac{n}{2})$, which from Lemma 4.3 gives $\mathcal{L} = sp(\frac{n}{2})$ or $\mathcal{L} = su(n)$ up to isomorphism (with or without the identity matrix). Case 6) is excluded by Lemma 4.1. This proves that the only possible Lie algebras $\mathcal{L}$ that correspond to a transitive Lie group are the ones given in the statement of the Theorem. The converse follows from the well known properties of transitivity of $SU(n)$ and $Sp(\frac{n}{2})$ as well as of any group conjugate to them via elements in $U(n)$, and from Lemma 4.2. □

A physically motivated model which is pure state controllable but not operator controllable was presented in [1]. This model describes three spin $\frac{1}{2}$ particles interacting with each-other via

Heisenberg interaction and with an external driving field. Particle 1 and 2 have the same $g-$factor (namely they interact in the same way with the external field) and the coupling constant between the two particles is equal to zero (they do not interact with each-other). Moreover the coupling constant between particle 3 and particle 1 is the negative of the coupling constant between particle 3 and particle 2. Networks of spins of this type arise as model of the dynamics of Molecular Magnets (see e.g. [17]).

5 Equivalent State Controllability

The notion of equivalent state controllability, although seemingly weaker, is in fact equivalent to pure state controllability. This can be proved as a consequence of the following Theorem given in [18].

Theorem 5 *([18]) Let G_1 and G_2 two compact and connected Lie groups and let $G := G_1 \times G_2$. If G is transitive on the real sphere S^n, then at least one of the groups G_1, G_2 is also transitive.*

If the system is ESC then for every pair of states $|\psi_0>$ and $|\psi_1>$ there exists a matrix X in $e^{\mathcal{L}}$ and a 'phase' $\phi \in \mathbf{R}$ such that

$$X|\psi_0>= e^{i\phi}|\psi_1> . \tag{6}$$

This can be expressed by saying that there exists an element Y in $e^{i\phi}e^{\mathcal{L}} := \{Y \in U(n)|Y = e^{i\phi}X, X \in e^{\mathcal{L}}, \phi \in \mathbf{R}\}$ such that $Y|\psi_0>=|\psi_1>$ and therefore $e^{i\phi}e^{\mathcal{L}}$ is transitive on the complex sphere. Now, if $span\{iI_n\} \subseteq \mathcal{L}$, then $e^{i\phi}e^{\mathcal{L}} = e^{\mathcal{L}}$ and therefore $e^{\mathcal{L}}$ is transitive and the system is PSC. If this is not the case, then from Theorem 2, there must exist a compact connected Lie group $G \subseteq e^{\mathcal{L}}$ such that $e^{i\phi}G$ is transitive. From Theorem 5, it follows, writing $e^{i\phi}G$ as $e^{i\phi}I_n \times G$, that one between the two groups $e^{i\phi}I_n$ and G, must be transitive. Therefore $G \subseteq e^{\mathcal{L}}$ is transitive. In conclusion, we have the following Theorem.

Theorem 6 *ESC and PSC are equivalent properties for quantum mechanical systems (1).*

Theorems 4 and 6 show that a necessary and sufficient condition to have pure state controllability or equivalent state controllability is that the Lie algebra $\mathcal{L}$ is the whole $su(n)$ or isomorphic to $sp(\frac{n}{2})$ (with or without iI). To check this isomorphism one can apply the structure theory of Lie algebras to $\mathcal{L}$. A more practical way to check equivalent state controllability will be presented in Section 7. This method only involves elementary matrix manipulations and can be extended to check density matrix controllability starting from a fixed given matrix.

6 Density Matrix Controllability

Notice that if $e^{\mathcal{L}} = SU(n)$ or $e^{\mathcal{L}} = U(n)$ then obviously the system is DMC. Moreover, in order for the system to be DMC, the model has to be equivalent state controllable (and therefore pure state controllable) as well, because transitions between pure states represented by matrices of the form $|\psi><\psi|$ must be possible. Therefore, to get DMC, $\mathcal{L}$ must be $su(n)$, or, for n even and $n > 2$ (see Theorem 4), it must be isomorphic (conjugate) to $sp(\frac{n}{2})$ (modulo multiples of the identity matrix). The next example shows that $Sp(\frac{n}{2})$ is not enough to obtain DMC. The example constructs a class of density matrices D with the property that

$$\{WDW^* \mid W \in Sp(\frac{n}{2})\} \neq \{UDU^*|U \in SU(n)\}. \tag{7}$$

Example 6.1 Choose any $n > 2$ with n even, and let $|v>=\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \in \mathbb{C}^{\,n}$ and $|w>=\begin{pmatrix} -v_2 \\ v_1 \end{pmatrix} \in \mathbb{C}^{\,n}$, with $v_1, v_2 \in \mathbf{R}^{\,n/2}$, $||v|| = 1$. Then $||w|| = 1$, $< v|w >= 0$, thus, in particular, these two vectors are independent. Let

$$D = \frac{1}{2}\left(|v >< v| + |w >< w|\right).$$

It is easy to verify that $DJ = JD$ (where $J = \begin{pmatrix} 0 & I_n \\ -I_n & 0 \end{pmatrix}$). Thus, if $W \in Sp(\frac{n}{2})$ then we still have that:

$$(WDW^*)\,J = J\overline{(WDW^*)}.$$

Choose any two orthonormal vectors $|v' >$, $|w' > \in \mathbb{C}^{\,n}$, such that:

$$D' = \frac{1}{2}\left(|v' >< v'| + |w' >< w'|\right),$$

satisfies $D'J \neq J\bar{D}'$ (it is easy to see that two such vectors exist), and let $U \in U(n)$ be any unitary matrix such that $Uv = v'$ and $Uw = w'$, then, for all $W \in Sp(\frac{n}{2})$,

$$UDU^* = D' \neq WDW^*.$$

From the above discussion and example, we can conclude that *DMC is equivalent to OC*. Given a density matrix D, it is of interest to give a criterion on the Lie algebra $\mathcal{L}$ for the two orbits

$$\mathcal{O}_{\mathcal{L}} := \{WDW^* | W \in e^{\mathcal{L}}\} \quad \text{and} \quad \mathcal{O}_U := \{UDU^* | U \in U(n)\} \tag{8}$$

to coincide. To this aim, notice that since D is Hermitian, iD is skew-Hermitian so that $iD \in u(n)$, and a matrix commutes with iD if and only if it commutes with D. The *centralizer* of iD is by definition, the Lie subalgebra of $u(n)$ of matrices that commute with iD. Call this subalgebra $\mathcal{C}_D$ and the corresponding connected Lie subgroup of $U(n)$, $e^{\mathcal{C}_D}$. Analogously, the centralizer of iD in $\mathcal{L}$ is $\mathcal{C}_D \cap \mathcal{L}$ and we denote by $e^{\mathcal{C}_D \cap \mathcal{L}}$ the corresponding subgroup of $U(n)$ (which is also a subgroup of $e^{\mathcal{L}}$). For a given density matrix D, it is sufficient to calculate the dimensions of $\mathcal{L}$, $\mathcal{C}_D$ and $\mathcal{C}_D \cap \mathcal{L}$ to verify the equality of the two orbits $\mathcal{O}_{\mathcal{L}}$ and $\mathcal{O}_U$ defined in (8). We have the following result.

Theorem 7 *Let D be a given density matrix, then $\mathcal{O}_{\mathcal{L}} = \mathcal{O}_U$ if and only if*

$$\dim u(n) - \dim \mathcal{C}_D = \dim \mathcal{L} - \dim(\mathcal{L} \cap \mathcal{C}_D). \tag{9}$$

Proof. We have the following isomorphisms between the two coset spaces $U(n)/e^{\mathcal{C}_D}$ and $e^{\mathcal{L}}/e^{\mathcal{C}_D \cap \mathcal{L}}$ and the two manifolds $\mathcal{O}_U$ and $\mathcal{O}_{\mathcal{L}}$, respectively:

$$U(n)/e^{\mathcal{C}_D} \simeq \{UDU^* \mid U \in U(n)\}, \tag{10}$$

$$e^{\mathcal{L}}/e^{\mathcal{C}_D \cap \mathcal{L}} \simeq \{WDW^* \mid W \in e^{\mathcal{L}}\}, \tag{11}$$

where $\simeq$ means isomorphic. Therefore if the two orbits coincide, we must have that the two coset spaces must coincide as well. So, in particular, their dimensions have to be equal which gives (9).

Conversely assume that (9) is verified. Then the dimensions of the two coset spaces on the left hand sides of (10) and (11) are the same and so are the dimensions of the manifolds on the right hand side namely $\mathcal{O}_U$ and $\mathcal{O}_{\mathcal{L}}$. Notice also that these two manifolds are connected since both $U(n)$ and $e^{\mathcal{L}}$ are connected. Since $e^{\mathcal{C}_D}$ is closed in $U(n)$ and therefore compact, from Proposition 4.4 (b) in [11] we have that $e^{\mathcal{L}}/e^{\mathcal{L}\cap\mathcal{C}_D}$ is closed in $U(n)/e^{\mathcal{C}_D}$. On the other hand, since the two coset spaces have the same dimensions, $e^{\mathcal{L}}/e^{\mathcal{L}\cap\mathcal{C}_D}$ is open in $U(n)/e^{\mathcal{C}_D}$. By connectedness, we deduce that the two coset spaces must coincide, and therefore the two orbits coincide as well. $\square$

Special cases of the above Theorem, are density matrices representing pure states or completely random states. In the first case, the density matrix D has the form, $D = |\psi><\psi|$ and, in an appropriate basis, it can be written as a diagonal matrix with the $(1,1)$ entry equal to one and all the remaining entries equal to zero. The analysis in Section 4 shows that the only Lie algebras $\mathcal{L}$ satisfying condition (9) are $su(n)$ or, for n even, isomorphic to $sp(\frac{n}{2})$ (with or without iI). For completely random states, the density matrix D is a real scalar matrix with trace equal to one, and therefore its centralizer in $\mathcal{L}$, $\mathcal{L}\cap\mathcal{C}_D$, is all of $\mathcal{L}$, for every subalgebra $\mathcal{L}$. Thus the condition (9) holds with $\dim\mathcal{L} - \dim\mathcal{L}\cap\mathcal{C}_D = 0$ for every $\mathcal{L}$. The interpretation, from a physics point of view, is the obvious fact that a completely random ensemble of quantum systems remains completely random after any evolution. The paper [26] contains a complete classification of density matrices as well as additional results on density matrix controllability.

7 Test of Controllability

As we have shown in the previous sections, the two notions of operator-controllability (in the special unitary case) and density-matrix-controllability are equivalent and they are the strongest among the controllability notions we have defined. On the other hand, pure state-controllability and equivalent-state-controllability are equivalent. These facts are summarized in the following diagram:

$$\text{DMC} \quad \Leftrightarrow \quad \text{OC} \quad \Rightarrow \quad \text{PSC} \quad \Leftrightarrow \quad \text{ESC} \ .$$

From a practical point of view, it is of great interest to give criteria on the Lie algebra $\mathcal{L}$ to ensure that the corresponding group is transitive on the complex sphere. In this case the system is pure state controllable. As we have seen from the analysis in Section 4, the Lie algebra $\mathcal{L}$ has to be $su(n)$ or $u(n)$ or, for n even, conjugate and therefore isomorphic to $sp(\frac{n}{2})$ (modulo multiples of the identity). To check this isomorphism, one can apply the Cartan theory of classification of semisimple Lie algebras [11]. A simpler and self contained test can be derived from Theorem 7. To this purpose, notice that pure state controllability is the same as equivalent state controllability (see Theorem 6) and this can be easily seen to be equivalent to the possibility of steering the matrix

$$D = \text{ diag } (1, 0, 0, ..., 0) \tag{12}$$

to any unitarily equivalent matrix. The centralizer $\mathcal{C}_D$ of the matrix iD in (12) in $u(n)$, is given by the set of matrices of the form

$$M := \begin{pmatrix} ia & 0 \\ 0 & H \end{pmatrix}, \tag{13}$$

with a any real and H a matrix in $u(n-1)$. The dimension of $\mathcal{C}_D$ is $(n-1)^2+1$ and therefore the number on the right hand side of (9) is $n^2 - ((n-1)^2+1) = 2n-2$. In conclusion as a consequence of Theorems 7 and 6 we have the following easily verifiable criterion for pure state controllability.

Theorem 8 *With the above notations and definitions, the system (3) is pure state controllable if and only if the Lie algebra $\mathcal{L}$ generated by $\{A, B_1, B_2, \ldots, B_m\}$ satisfies*

$$\dim \mathcal{L} - \dim(\mathcal{L} \cap \mathcal{C}_D) = 2n - 2. \tag{14}$$

We remark here that similar criteria can be given for different density matrices according to Theorem 7.

Example 7.1 Assume that the Lie algebra $\mathcal{L}$ is given by the matrices of the form

$$F := \begin{pmatrix} L + Z & T + C \\ -\bar{T} + \bar{C} & -L + Z^T \end{pmatrix}, \tag{15}$$

with L diagonal and purely imaginary, T diagonal, and Z, C having zeros on the main diagonal, all of them 2×2 matrices. This Lie algebra is in fact conjugate to $sp(2)$. Verifying this fact directly can be cumbersome. However to prove that the associated system is pure state controllable, one can verify that the Lie subalgebra of matrices of $\mathcal{L}$ that have the form (13), namely $\mathcal{L} \cap \mathcal{C}_D$, has dimension 4. Since the dimension of $\mathcal{L}$ is 10, we have (recall $n = 4$) $\dim \mathcal{L} - \dim \mathcal{L} \cap \mathcal{C}_D = 6 = 2n - 2$. Therefore the criterion of Theorem 8 is verified.

8 Conclusions

For bilinear quantum mechanical systems in the multilevel approximation a number of concepts concerning controllability can be considered. One can ask whether it is possible to drive the evolution operator or the state to any desired configuration. One typically represents the state with a vector with norm 1 or using the density matrix formalism. The possibility of driving a pure state between two arbitrary configurations is in general a weaker property than the controllability of the evolution operator. All the controllability properties of a given quantum system can studied by studying the Lie algebra generated by the matrices $\{A, B_1, \ldots, B_m\}$ of the system (1). This Lie algebra has to be the full Lie algebra $su(n)$ (or $u(n)$) for controllability of the operator while, for controllability of the state, it can be conjugate and therefore isomorphic to the Lie algebra of symplectic matrices of dimension n modulo a phase factor. We have also given a practical test to check this isomorphism. This test can be extended for density matrices of rank different from one and only requires elementary algebraic manipulations involving the centralizer of the given density matrix.

References

[1] F. Albertini and D. D'Alessandro, The Lie algebra structure and controllability of spin systems, *Linear Algebra and its Applications*, (350), (2002) pp. 213-235.

[2] O. Atabek, C. Dion, A. D. Bandrauk, A. Keller, H. Umeda and Y. Fujimura, Two-frequency IR laser orientation of polar molecules. Numerical simulations for *HCN*, *Chem. Phys. Letters*, 1999, 302, 215-223.

[3] J. M. Ball, J. E. Marsden and M. Slemrod, Controllability for distributed bilinear systems, *SIAM J. Control and Optimization*, vol. 20, (4) (1982) 575-597.

[4] A. Borel, Some remarks about transformation groups transitive on spheres and tori, *Bull. Amer. Math. Soc.* **55**, pp. 580-586, 1949.

[5] R. Brockett, Lie theory and control systems defined on spheres, *SIAM J. Appl. Math.* Vol. 25. No. 2, September 1973.

[6] M. Dahleh, A. Peirce, H. A. Rabitz and V. Ramakrishna, Control of Molecular Motion, *Proceedings of the IEEE,*, Vol. 84, No. 1, January 1996.

[7] D. D'Alessandro and M. Dahleh, Optimal control of two-level quantum systems, in *IEEE Transaction on Automatic Control,* vol. 46. No. 6, June 2001, pp. 866-876.

[8] C. Dion, A. Keller, O. Atabek and A. D Bandrauk, Laser-induced alignment dynamics of HCN : roles of the permanent dipole moment and the polarizability, *Phys. Rev. A*, 59, p. 1382, 1999.

[9] D. DiVincenzo, Quantum Computation, *Science* Vol. 270, 13 October, 1995.

[10] E. B. Dynkin, Maximal subgroups of the classical groups, *Transl. Amer. Math. Soc.* (2) **6**, 245-378, (1957).

[11] S. Helgason, *Differential Geometry, Lie Groups and Symmetric Spaces*, Academic Press, New York, 1978.

[12] G. M. Huang, T. J. Tarn and J. W. Clark, On the controllability of quantum mechanical systems, *J. Math. Phys.* **24**, 11, November 1983, pg. 2608-2618.

[13] V. Jurdević and H. Sussmann, Control systems on Lie groups, *Journal of Differential Equations*, **12**, 313-329, 1972.

[14] K. Kime, Control of transition probabilities of the quantum-mechanical harmonic oscillator, *Appl. Math. Lett.* 6 (3), (1993) 11-15.

[15] A. Knapp, *Representation Theory. An Overview Based on Examples*, Princeton University Press, Princeton New Jersey, 1986.

[16] H. Kunita, Supports of diffusion processes and controllability problems, in K. Ito editor, *Proceedings Int. Symp. Stochastic. Diff. Eqn.,* pp. 163-185. Wiley, 1978.

[17] M. Luban, F. Borsa, S. Bud'ko, P. Canfield, S. Jun, J. K. Jung, P. Kögerler, D. Mentrup, A. Müller, R. Modler, D. Procissi, B. J. Suh and M. Torikachvili, Heisenberg spin triangles in V_6-type magnetic molecules: Experiment and theory, *Physical Review B*, **66**, 054407, 2002.

[18] D. Montgomery and H. Samelson, Transformation groups of spheres. *Ann. of Math.* **44**, 1943, pp. 454-470.

[19] D. Montgomery and L. Zippin, *Topological Transformation Groups*, Interscience Tracts in Pure and Applied Mathematics, Vol. 1, New York, N.Y. 1955.

[20] V. Ramakrishna, M. Salapaka, M. Dahleh, H. Rabitz and A. Peirce, Controllability of molecular systems, *Physical Review A*, Vol. 51, No. 2, February 1995.

[21] A. A. Sagle and R. E. Walde, *Introduction to Lie Groups and Lie Algebras,* Academic Press, 1973.

[22] J. J. Sakurai, *Modern Quantum Mechanics*, Addison-Wesley Pub. Co., Reading, Mass. 1994.

[23] H. Samelson, Topology of Lie groups, *Bull. Amer. Math. Soc.*, **58**, 1952, pp. 2-37.

[24] S. Schirmer, H. Fu and A. Solomon, Complete controllability of quantum systems, *Physical Rev. A* 63 (2001) 063410, arXiv quant-ph/0010031.

[25] S. G. Schirmer, H. Fu amd A. I. Solomon, Complete controllability of finite level quantum systems, *J. Phys. A*, **34** (2001) 1679, arXiv quant-ph/0102017.

[26] S. G. Schirmer, A. I. Solomon and J. V. Leahy, Dynamical Lie group action on kinematical equivalence classes and criteria for reachability of states for quantum systems, arXiv:quant-ph/0110171

[27] S. G. Schirmer, A. I. Solomon and J. V. Leahy, Degrees of controllability for quantum systems and application to atomic systems, arXiv:quant-ph/0108114

[28] G. Turinici, Controllable quantities in bilinear quantum systems, *Proceedings of the 39-th IEEE Conference on Decision and Control*, Sydney, Australia, Dec. 2000, pp. 1364-1369.

[29] G. Turinici and H. Rabitz, Quantum wave function controllability, *Chem. Phys.*, (267), 1-9, (2001)

Appendix: Proofs of Lemmas 4.1, 4.2 and 4.3

Proof of Lemma 4.1

First notice that neither $so(7)$ nor $so(9)$ have an element which commutes with all the algebra, therefore if there exists a subalgebra of $u(4)$ (resp. $u(8)$) isomorphic to $so(7)$ (resp. $so(9)$), it must be also a subalgebra of $su(4)$ (resp. $su(8)$).

Statement (a) of the Lemma can be checked by calculating the dimensions of $su(4)$ and $so(7)$. We have $dim(su(4)) = 15 < dim(so(7)) = 21$. As for statement (b), assume there exists a subalgebra of $su(8)$, call it $\mathcal{F}$, isomorphic to $so(9)$, namely a (faithful) representation of $so(9)$. Assume first this representation to be irreducible. Then there is an highest associated weight by the fundamental theorem of representation theory (see e.g. [15], Theorem 4.28). The basic weights are given by $w_1 = (0,0,0,0)$, $w_2 = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, $w_3 = (1,0,0,0)$, $w_4 = (1,1,0,0)$, $w_5 = (1,1,1,0)$, $w_6 = (1,1,1,1)$. w_1 corresponds to the trivial representation which is obviously not faithful. For each one of the others the underlying vector space V on which the representation acts has dimension that can be calculated using Weyl formula (see e.g. [21] pg 332). This calculation gives the following values for $dim(V)$, for the cases w_2, w_3, w_4, w_5, w_6, respectively, 16, 9, 36, 84, 252. In any case, the dimension is bigger than 8 which is the maximum allowed by the fact that $\mathcal{F}$ is a subalgebra of $su(8)$. All the other irreducible transformations can be calculated as tensor products of the basic representations ([15] Pr.11 pg. 111, [21] Corollary 15.18 pg, 330) and therefore the dimension of V in this case is the product of the dimensions of the basic representations and therefore > 8. If the representation is not irreducible then it is the direct sum of irreducible transformations ([15] pg. 15 Corollary 1.7) and therefore the vector space V has dimension which is the sum of sum above given. In this case, the only possibility to have $dim(V) \leq 8$ is that $V = \oplus_{j=1}^{r} V_j$ and the representation acts as the trivial representation on any V_j, which makes it not faithful. $\square$

Proof of Lemma 4.2

Consider a subalgebra $\mathcal{F} \subseteq u(n)$ isomorphic to $sp(\frac{n}{2})$. It follows immediately from the fact that $\mathcal{F}$ is semisimple that $iI \notin \mathcal{F}$ and therefore $\mathcal{F} \subseteq su(n)$. Thus, $\mathcal{F}$ is a faithful representation of $sp(\frac{n}{2})$. Assume first that this representation is irreducible. Consider the parametrizations of the finite dimensional representations of $sp(\frac{n}{2})$ given by the theorem of the highest weight (see e.g. [15] Theorem 4.28). The $n-dimensional$ basic weight vectors are $w_1 = (0, 0, ..., 0)$, $w_2 = (1, 0, ..., 0)$,$w_3 = (1, 1, 0, ..., 0)$,...,$w_{\frac{n}{2}+1} = (1, 1, 1, ..., 1)$. w_1 gives the trivial representation which is not faithful; the representation corresponding to w_2 acts on a vector space V of dimension n. All the other representations act on vector spaces V of dimension $> n$. The same is true for the other irreducible representations whose weights are sums of some w_j, $j = 1, ..., \frac{n}{2} + 1$. As for reducible representations they are sums of the irreducible ones and therefore the dimension of the underlying vector space V is $> n$ except for the sum of a number $l \leq n$ of trivial representations which is a (higher dimensional) trivial representation and clearly not faithful. Therefore the only possible representations of dimensions n are all equivalent to each other and in particular they are equivalent to the basic representation of $sp(\frac{n}{2})$. In conclusion there exists a nonsingular matrix E such that

$$\mathcal{F} = Esp(\frac{n}{2})E^{-1}. \tag{16}$$

Notice that E is defined up to a multiplicative constant. It remains to show that E can be chosen in $U(n)$. The connected Lie subgroup of $SU(n)$ with Lie algebra $\mathcal{F}$ is a unitary representation of $Sp(\frac{n}{2})$ that assigns to an element $g \in Sp(\frac{n}{2})$ an element $\Phi(g)$ and, from (16), we have

$$E = \Phi^*(g)Eg, \tag{17}$$

from which it follows

$$EE^* = \Phi^*(g)EE^*\Phi(g) \quad \Rightarrow \quad \Phi(g)EE^* = EE^*\Phi(g). \tag{18}$$

The matrix EE^* commutes with all the elements of a unitary irreducible representation and therefore from Schur's Lemma (see e.g. [15] Proposition 1.5) it must be a scalar matrix αI, with α real > 0. Thus, scaling E by a factor $\sqrt{\alpha}$ we can make E unitary. $\square$

Proof of Lemma 4.3

It follows from the results in [10] that the complexification of $sp(\frac{n}{2})$ is a maximal subalgebra in the complexification of $su(n)$. Now, if there exists a proper subalgebra $\mathcal{F}$ of $su(n)$ properly containing $sp(\frac{n}{2})$, then its complexification will be a proper subalgebra of the complexification of $su(n)$ properly containing the complexification of $sp(\frac{n}{2})$ (cfr. [21] Section 9.3) which contradicts the maximality of $sp(\frac{n}{2})$. $\square$