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# CONTROLLABILITY OF OPEN QUANTUM SYSTEMS\*

A. GRIGORIU<sup>†</sup>, H. RABITZ<sup>‡</sup>, AND G. TURINICI<sup>§</sup>

**Abstract.** The problem of controllability of open quantum systems (i.e., quantum systems interacting with an environment), whose dynamics is described by a non-Markovian master equation is addressed. The manipulations of the dynamics is realized with both a laser field and a tailored nonequilibrium, and generally time-dependent, state of the surrounding environment. Lie algebra theory is used to characterize the structures of the reachable states sets and to prove controllability. The theoretical results are supported by examples.

**Key words.** quantum control; controllability of the Lindblad equation; open system controllability; Lie group controllability; controllability in a non-compact Lie group

**AMS subject classifications.** 81Q93 , 93B05

## 1. Introduction and examples.

**2. Introduction.** Since the first successful laboratory experiments obtained in the 1990s [4, 12], the control of quantum systems using laser fields has been subject to significant developments ([4, 7, 12, 14, 18] etc.). An important part of the associated theoretical work has been devoted to the investigation of closed quantum systems having with unitary dynamics. However, realistic physical situations include circumstances where the quantum system is not isolated, but interacting with an environment (e.g., a molecule in a solvent). Research on control of open quantum systems is motivated by many applications including quantum computing [8], laser cooling, quantum reservoir engineering, management of decoherence, chemical reactions and energy transfer in molecules [17].

The complexity of phenomena that arise during the interaction between the laser, the environment with the quantum system requires the introduction of theoretical methods as an important step to accompany experimental efforts. This type of analysis can reveal the set of objectives that can be achieved. For quantum systems coupled with an environment one of the main characteristics is that the the dynamics is non-unitary. Open systems are often described by the Markovian approximation, which usually leads to a master equation [6], a linear first order differential equation for the reduced density matrix  $\rho$  of the open system with a generator  $\mathcal{M}$

$$\frac{d}{dt}\rho = \mathcal{M}\rho(t). \quad (2.1)$$

We will suppose for all that follows that the quantum dynamics takes place in a finite dimensional space (either because it intrinsically does so or because a suitable large basis set approximation has been chosen). Thus  $\rho(t)$  is a  $N \times N$  complex matrix for some integer  $N > 0$ . The most general form of the generator  $\mathcal{M}$  of the quantum dynamical semigroup is written in the following way:

$$\mathcal{M}\rho = -i[H, \rho] + \sum_{k=1}^{N^2-1} \gamma_k \left( A_k \rho A_k^* - \frac{1}{2} A_k^* A_k \rho - \frac{1}{2} \rho A_k^* A_k \right). \quad (2.2)$$

For any matrix  $X$  we denote by  $X^*$  its adjoint (the transpose conjugate); here  $H$  is a  $N \times N$  Hermitian matrix (i.e.,  $H^* = H$ ).

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2 The first term represents the unitary part of the system dynamics, the second term is referred to as the dissipator. The operators  $A_k$  are called Lindblad operators, and the corresponding density matrix equation is called the Lindblad equation:

$$\frac{d}{dt}\rho = -i[H, \rho] + \sum_{k=1}^{N^2-1} \gamma_k \left( A_k \rho A_k^* - \frac{1}{2} A_k^* A_k \rho - \frac{1}{2} \rho A_k^* A_k \right). \quad (2.3)$$

The coefficients  $\gamma_k$  can usually be defined to represent coupling to the environment, functioning as the relaxation rates for different decay modes of the open system.

The formulation (2.3) includes the requirements of the conservation of probability and of the complete positivity of the dynamical map [11, 10], i.e. if  $\rho(0)$  is a positive semidefinite Hermitian operator having  $\text{tr}(\rho) = 1$  it will remain so for any  $t \geq 0$ . We assume that the Hamiltonian  $H$  is a sum of an Hermitian operator  $H_0$  describing the evolution of the open quantum system in the absence of the interaction with a laser field  $\epsilon(t)$  and another dipole moment operator  $H_1$  which models the interaction with a laser field  $\epsilon(t)$ :

$$\frac{d}{dt}\rho = -i[H_0 + \epsilon(t)H_1, \rho] + \sum_{k=1}^{N^2-1} \gamma_k \left( A_k \rho A_k^* - \frac{1}{2} A_k^* A_k \rho - \frac{1}{2} \rho A_k^* A_k \right). \quad (2.4)$$

A fundamental question involving the system above is whether for any couple of  $\rho_i$  and  $\rho_f$  (both positive, semidefinite, Hermitian) a control  $\epsilon(t)$  exists such that  $\rho(0) = \rho_i$  and  $\rho(T) = \rho_f$  for some  $T > 0$ . If the answer is positive the system is called controllable.

A first approach when controlling the system is to manipulate the control  $\epsilon(t)$  when the non-unitary part is absent, i.e.,  $\mathcal{M}$  is Hermitian and thus the system is isolated. Then  $\rho_i$  and  $\rho_f$  has to satisfy an additional compatibility relation i.e. some unitary matrix  $U$  has to exist such that

$$\rho_f = U \rho_i U^*. \quad (2.5)$$

If the controllability question is thus rephrased we know [9, 16, 1] that the system is controllable if the Lie algebra generated by  $iH_0$  and  $iH_1$  is of dimension at least  $N^2 - 1$ .

But, the system may either be not isolated or not controllable in the isolated setting; then one can rely on using specially tailored environments, which affect the system via the non-unitary evolution, with controls applied through the dissipative part of the dynamics, cf. [15]. In this approach, a suitably optimized non-equilibrium distribution function of an environment is employed as a control instrument to achieve the desired objective making the parameters  $\gamma_k$  time dependent controls.

This type of incoherent control by the environment (i.e., control by  $\gamma_k(t)$ ) may be combined with optimally tailored coherent fields (i.e., control through  $\epsilon(t)$ ) to allow for simultaneous control through both the Hamiltonian and dissipative parts of the system dynamics.

Unitary dynamics can achieve control only within sets of states satisfying the compatibility relation (2.5). Control by the environment affects a system through dissipative dynamics and can be used to steer the system from a pure or a mixed state into mixed and in some cases pure states (a familiar example is the cooling of a thermalized quantum system, which requires coupling to a reservoir). As a conclusion when the dissipative term is present then the controllability question has to be rephrased only asking that  $\rho_i$  and  $\rho_f$  are both positive Hermitian matrices.

The important question of controllability of open quantum systems has not been fully addressed, although some aspects of this problem have been considered. The problem of kinematic state controllability (KSC) of open quantum systems whose dynamics are represented by Kraus maps has been considered in [19]. The existence of a Kraus map that can move a finite-dimensional open quantum system from any initial state  $\rho_i$  to any final target state  $\rho_f$  has been proven. The complete KSC of finite-dimensional open quantum systems with Kraus-map dynamics is in contrast to restricted KSC of closed quantum systems where unitary dynamics can connect only states with the same density-matrix spectrum.

Another result [2, 3] established that when only the laser field  $\epsilon(t)$  is used as a control then some states will always be unreachable. This is a negative result that invites a precise redefinition of the setting. Two formulations are possible: either we ask what subset of states  $\rho_f$  can be reached or we introduce additional control to recover controllability for all  $\rho_f$ . We explore in this paper the second choice and consider the manipulation of the dynamics with both a laser field  $\epsilon(t)$  as well as a tailored nonequilibrium, and generally time-dependent, state of the surrounding environment  $\gamma(t)$ :

$$\frac{d}{dt}\rho = -i[H_0 + \epsilon(t)H_1, \rho] + \sum_{k=1}^{N^2-1} \gamma_k(t) \left( A_k \rho A_k^* - \frac{1}{2} A_k^* A_k \rho - \frac{1}{2} \rho A_k^* A_k \right). \quad (2.6)$$

We will study the controllability of equation (2.6).

Treating  $\gamma$  as time dependent has been considered before, but the sign of  $\gamma$  deserves attention. The derivation of the Lindblad equation suggests choosing each  $\gamma_k$  to be non-negative (see [6] for more details). Negative  $\gamma$  have however been considered in the literature, cf. [5].

**3. The problem.** For simplicity we consider throughout the paper the circumstance when  $\gamma_2 = \dots = \gamma_{N^2-1} = 0$ , see Remark 4.2 for the general situation. Equation (2.6) becomes:

$$\frac{d}{dt}\rho = -i[H_0, \rho] - i\epsilon(t)[H_1, \rho] + \gamma(t) \left( A \rho A^* - \frac{1}{2} \rho A^* A - \frac{1}{2} A^* A \rho \right), \quad (3.1)$$

where  $H_0$  and  $H_1$  are real  $N$ -dimensional symmetric matrices (thus Hermitian) and  $\gamma$  a real time dependent function.

**3.1. Background on controllability on Lie groups.** As will be seen in the sequel, controllability results have to deal fundamentally with the loss of compactness that arises from the non-Hermitian nature of the generator  $\mathcal{M}$ . Let us consider a connected but not necessarily compact Lie group  $G$  with Lie algebra  $L(G)$  and control system

$$\frac{dX}{dt}(t) = \mathbb{X}_0(X(t)) + \sum_{i=1}^m u_i(t) \mathbb{X}_i(X(t)), \quad (3.2)$$

where  $\mathbb{X}_0$  and  $\mathbb{X}_i$  are right-invariant vector fields on  $G$ . If necessary we will denote this solution  $X(t; u; Y)$  to indicate its dependence on time, controls and initial state  $Y$ . Consider the set of all reachable states from  $Y$  at time  $t$ :

$$\mathcal{R}^t(Y) = \{X(t; u; Y) \mid X(t; u; Y) \text{ solution of (3.2), } X(0; u; Y) = Y\}. \quad (3.3)$$

It follows to see that

$$\mathcal{R}^t(Y) = \mathcal{R}^t(e)Y. \quad (3.4)$$

where we denote by  $e$  the identity of the Lie group  $G$ ; thus, describing the set  $\mathcal{R}^t(e)Y$  allows for completely describing all the other reachable sets. When the final time is not specified, we will use

$$\mathcal{R}(Y) = \cup_{t \geq 0} \mathcal{R}^t(Y). \quad (3.5)$$

We take the admissible controls  $u_i(t)$  to be the set of all locally bounded and measurable functions.

Consider  $\mathbb{L}$  to be the Lie algebra generated by  $X_0, X_1, \dots, X_m$  and  $\mathbb{S}$  its corresponding Lie group (Lie subgroup of  $G$ ). We **do not assume** that  $\mathbb{S}$  is compact.

The results proved below build on the following reformulation of a result in [13][Thm 6.6] (to which we refer for further details):

**THEOREM 3.1** (Jurdjevic and Sussmann 1972). *If there exists a constant control  $u = (u_1, \dots, u_m)$  and a sequence of positive numbers  $\{t_n\}$  with  $t_n > 0$  with the property that  $\lim_{n \rightarrow \infty} X(t_n, u, e)$  exists and belongs to  $\bar{\mathbb{S}}$  (the closure is relative to  $\mathbb{S}$ ) then  $\mathcal{R}(e) = \mathbb{S}$ .*

4 **4. Controllability.** We define the operators  $\mathcal{H}_0, \mathcal{H}_1$  and  $\mathcal{L}$  as follows:

$$\begin{aligned}\mathcal{H}_0 : \rho &\longrightarrow -i[H_0, \rho] \\ \mathcal{H}_1 : \rho &\longrightarrow -i[H_1, \rho] \\ \mathcal{L} : \rho &\longrightarrow A\rho A^* - \frac{1}{2}\rho A^* A - \frac{1}{2}A^* A\rho,\end{aligned}\tag{4.1}$$

and rewrite equation (3.1) as:

$$\frac{d}{dt}\rho = \mathcal{H}_0\rho + \epsilon(t)\mathcal{H}_1\rho + \gamma(t)\mathcal{L}\rho.\tag{4.2}$$

Introduce the sets of matrices:

$$\mathcal{H}_N = \{Z \in \mathbb{C}^{N \times N} \mid Z = Z^*\}, \quad \mathcal{H}_N^0 = \{Z \in \mathbb{C}^{N \times N} \mid Z = Z^*, \operatorname{tr}(Z) = 0\}.\tag{4.3}$$

Recall that  $\mathcal{H}_N$  (respectively  $\mathcal{H}_N^0$ ) has dimension  $N^2$  (respectively  $N^2 - 1$ ) when seen as a vector space over  $\mathbb{R}$ .

A simple computation indicates that for any  $Z \in \mathcal{H}_N : \mathcal{H}_0(Z), \mathcal{H}_1(Z), \mathcal{L}(Z) \in \mathcal{H}_N$ . Moreover all three operators are linear. Thus  $\mathcal{H}_0, \mathcal{H}_1, \mathcal{L} \in \operatorname{Lin}(\mathcal{H}_N, \mathcal{H}_N)$ , the space of linear operators from  $\mathcal{H}_N$  to  $\mathcal{H}_N$ . Also note that for any matrix  $Z$ :

$$\begin{aligned}\operatorname{tr}(\mathcal{H}_0 Z) &= \operatorname{tr}(-i[H_0, Z]) = 0 \\ \operatorname{tr}(\mathcal{H}_1 Z) &= \operatorname{tr}(-i[H_1, Z]) = 0 \\ \operatorname{tr}(\mathcal{L} Z) &= \operatorname{tr}(AZA^* - \frac{1}{2}ZA^*A - \frac{1}{2}A^*AZ) = 0.\end{aligned}$$

Thus we also have  $\mathcal{H}_0, \mathcal{H}_1, \mathcal{L} \in \operatorname{Lin}(\mathcal{H}_N^0, \mathcal{H}_N^0)$ . In particular the trace of  $\rho$  will not change during the evolution. This motivates the following definition:

**DEFINITION 4.1.** *The evolution (4.2) is density matrix controllable if for any positive semi-definite Hermitian matrices  $\rho_i$  and  $\rho_f$  with  $\operatorname{tr}(\rho_i) = \operatorname{tr}(\rho_f)$  there exists a time  $t \geq 0$  and locally bounded measurable controls  $\epsilon(\cdot), \gamma(\cdot)$  such that the solution of the evolution equation (3.1) starting at 0 from  $\rho_i$  reaches  $\rho_f$  at time  $t$ .*

We investigate controllability results in two distinct situations: when the matrix  $A$  is Hermitian or not.

**REMARK 4.1.** *The particular case of  $A$  being Hermitian corresponds to unital operator  $\mathcal{L}$ , i.e.  $\mathcal{L}I = 0$ , which is a situation frequently addressed in quantum information processing.*

**4.1. Situation I: Hermitian operator  $A$ .** Let us now consider the connected Lie group  $G_1$  of one-to-one linear transformations of  $\mathcal{H}_N^0$  that contains the identity operator. This group is isomorphic to  $GL^+(N^2 - 1)$  (the set of invertible matrices of dimension  $N^2 - 1$  with positive determinant). We know that  $G_1$  is connected but not compact. We will denote by  $\operatorname{Lie}(G_1)$  the Lie algebra of  $G_1$  which is isomorphic to  $\operatorname{Lin}(\mathcal{H}_N^0, \mathcal{H}_N^0)$ .

Denote by  $\mathcal{H}_0^{G_1}$  the element of  $\operatorname{Lie}(G_1)$  that is constructed from  $\mathcal{H}_0$  (and the same for  $\mathcal{H}_1$  and  $\mathcal{L}$ ). We associate to the evolution equation (4.2) the following evolution equation on the group  $G_1$ :

$$\begin{aligned}\frac{d}{dt}X(t) &= \left(\mathcal{H}_0^{G_1} + \epsilon(t)\mathcal{H}_1^{G_1} + \gamma(t)\mathcal{L}^{G_1}\right)X(t), \\ X(t=0) &= X_0.\end{aligned}\tag{4.4}$$

We will also write  $X(t; \epsilon, \gamma; X_0)$  when we will need to make explicit the dependence on the parameters; of course  $X(t; \epsilon, \gamma; X_0)$  belongs to the Lie group  $G_1$ . Then by definition  $\bar{\rho}(t) = X(t; \epsilon, \gamma; e)\bar{\rho}(0)$ .

**THEOREM 4.2.** *If the Lie algebra  $\operatorname{Lie}\{\mathcal{H}_0^{G_1}, \mathcal{H}_1^{G_1}, \mathcal{L}^{G_1}\}$  generated by  $\{\mathcal{H}_0^{G_1}, \mathcal{H}_1^{G_1}, \mathcal{L}^{G_1}\}$  has dimension  $(N^2 - 1)^2$  (as a vector space over the real numbers), then the system (4.2) is density matrix controllable.*

*Proof.* Without loss of generality we can suppose that  $tr(H_0) = 0$  and  $tr(H_1) = 0$ .

As a side remark, note that since  $A$  is Hermitian we can show by computation that  $\mathcal{L}$  is a Hermitian operator from  $\mathcal{H}_N^0$  to itself i.e.,  $\mathcal{L}^* = \mathcal{L}$ . However  $\mathcal{H}_0$  and  $\mathcal{H}_1$  are skew-Hermitian as operators from  $\mathcal{H}_N^0$  to itself.

We consider the following change of variables:

$$\bar{\rho} = \rho - \frac{tr(\rho(0))}{N}I. \quad (4.5)$$

Thus  $tr(\bar{\rho}(0)) = 0$  which implies  $\bar{\rho}(0) \in \mathcal{H}_N^0$ . By computation we obtain:

$$\begin{aligned} \dot{\bar{\rho}} &= \dot{\rho} = -i\left[H, \bar{\rho} + \frac{tr(\rho(0))}{N}I\right] + \mathcal{L}\left(\bar{\rho} + \frac{tr(\rho(0))}{N}I\right) \\ &= -i[H, \bar{\rho}] + \mathcal{L}(\bar{\rho}) + \mathcal{L}\left(\frac{tr(\rho(0))}{N}I\right). \end{aligned} \quad (4.6)$$

Since we are in the case when  $A$  is a Hermitian matrix :

$$\mathcal{L}\left(\frac{tr(\rho(0))}{N}I\right) = \frac{AA^* - A^*A}{N}(tr(\rho(0))) = 0. \quad (4.7)$$

Thus we obtain the equation for  $\bar{\rho}$  to be:

$$\dot{\bar{\rho}} = -i[H, \bar{\rho}] + \mathcal{L}(\bar{\rho}), \quad (4.8)$$

with  $\bar{\rho}$  Hermitian and  $tr(\bar{\rho})(0) = 0$ . But, since  $\mathcal{H}_0, \mathcal{H}_1, \mathcal{L} \in Lin(\mathcal{H}_N^0, \mathcal{H}_N^0)$  we can see them as vector fields on the manifold  $\mathcal{H}_N^0$  thus the evolution started on that manifold will remain there, which means that  $\bar{\rho}(t) \in \mathcal{H}_N^0$  for all  $t \geq 0$ , in particular  $tr(\bar{\rho})(t) = 0$  for all  $t \geq 0$ . Thus we always have  $\rho(t) = \bar{\rho}(t) + \frac{tr(\rho(0))}{N}I$ .

From the above relations we conclude that  $\mathcal{H}_0(\rho)$ ,  $\mathcal{H}_1(\rho)$  and  $\mathcal{L}(\rho)$  belong to  $Lin(\mathcal{H}_N^0, \mathcal{H}_N^0)$ .

The central question is to characterize  $\mathcal{R}(e)$  for the system (4.4). We will use the Thm. 3.1 with  $G = G_1$ . Then  $\mathbb{L} = Lie\{i\mathcal{H}_0^{G_1}, i\mathcal{H}_1^{G_1}, \mathcal{L}^{G_1}\}$  is the Lie algebra generated by  $\mathcal{H}_0^{G_1}$ ,  $\mathcal{H}_1^{G_1}$  and  $\mathcal{L}^{G_1}$ .

Since  $dim_{\mathbb{R}}(Lin(\mathcal{H}_N^0, \mathcal{H}_N^0)) = (N^2 - 1)^2$  (dimension as vector space over  $\mathbb{R}$ ) the higher possible dimension for  $\mathbb{L}$  is  $(N^2 - 1)^2$  (again over the real numbers) because  $\mathbb{L} \subset Lie(G_1)$ ; by hypothesis  $dim_{\mathbb{R}}(\mathbb{L}) = (N^2 - 1)^2$ , thus both have the same dimension  $(N^2 - 1)^2$  and  $\mathbb{L} = Lie(G_1)$  and  $\mathbb{S} = G_1$ . Take now  $\epsilon = 0, \gamma = 0$ , then equation (4.4) becomes:

$$\begin{aligned} \frac{d}{dt}X(t) &= \mathcal{H}_0^{G_1}X(t), \\ X(t=0) &= e, \end{aligned} \quad (4.9)$$

with solution  $X(t) = e^{t\mathcal{H}_0^{G_1}}$ ; take a sequence of positive numbers  $\{t_n\}$  with  $t_n > 0$ ; we need to prove that

$$\lim_{n \rightarrow \infty} e^{t_n \mathcal{H}_0^{G_1}} \in \bar{\mathbb{S}}. \quad (4.10)$$

But as  $\mathcal{H}_0^{G_1}$  is a skew-Hermitian map which means that  $e^{t_n \mathcal{H}_0^{G_1}}$  belongs to the group of the orthogonal transformations of  $\mathcal{H}_N^0$  (isomorphic to the unitary matrix group  $U(N^2 - 1)$ ) which is a subgroup of  $G_1$ . Since the orthogonal group is compact it implies that up to extracting a subsequence  $\lim_{n \rightarrow \infty} e^{t_n \mathcal{H}_0^{G_1}}$  exists and belongs to  $\bar{\mathbb{S}}$ . Therefore  $\mathcal{R}(e) = \bar{\mathbb{S}}$ . In particular  $X$  can reach any orthogonal transformation from  $\mathcal{H}_N^0$  to itself. For any  $\rho_i$  and  $\rho_f$  with  $tr(\rho_i) = tr(\rho_f)$  we can find an orthogonal transformation to map  $\rho_i - \frac{tr(\rho_i)}{N}I \in \mathcal{H}_N^0$  to  $\rho_f - \frac{tr(\rho_f)}{N}I = \rho_f - \frac{tr(\rho_i)}{N}I \in \mathcal{H}_N^0$  i.e. we have controllability for  $\bar{\rho}$  thus for  $\rho$ .  $\square$

6 **4.2. Situation II: arbitrary operator A.** Let us now consider the connected Lie group  $G_2$  of one-to-one linear transformations of  $\mathcal{H}_N$  that contains the identity operator and preserves the trace. This group is isomorphic with

$$\{X \in GL(N^2) \mid \det(X) \geq 0, \operatorname{tr}(X(Z)) = \operatorname{tr}(Z), \forall Z \in \mathbb{R}^{N \times N}\}. \quad (4.11)$$

We know that  $G_2$  is connected but not compact. We will denote by  $Lie(G_2)$  the Lie algebra of  $G_2$ . Note that if  $\frac{d}{dt}\rho(t) = M(\rho(t))$  then  $\rho(t) = \exp(Mt)\rho(0)$ . If  $\operatorname{tr}(\rho(t)) = \text{const}$  it implies  $\frac{d}{dt}\operatorname{tr}(\rho(t)) = 0$ . Since  $\frac{d}{dt}\operatorname{tr}(\rho(t)) = \operatorname{tr}(\frac{d}{dt}\rho(t))$  it follows:

$$\operatorname{tr}(M(\rho(t))) = 0, \quad \forall \rho(t) \in \mathcal{H}_N. \quad (4.12)$$

Since  $\operatorname{tr}(\rho)$  is a linear operation and if  $\rho$  is viewed as a vector in  $\mathbb{R}^{N^2}$  then  $\operatorname{tr}(\rho) = \langle \alpha, \rho \rangle$  with  $\alpha$  a vector with "1" on a position corresponding to  $\rho_{ii}$ ,  $i = 1, \dots, N^2$  and zero elsewhere. In this case the Lie algebra is thus isomorphic with the set (endowed with its canonical Lie algebra structure):

$$\left\{ M \in \mathbb{R}^{N^2 \times N^2} \mid M^T \alpha \equiv 0_{\mathbb{R}^{N^2}} \text{ i.e. } \sum_{j=1}^{N^2} M_{ji} \alpha_j = 0, \quad \forall i = 1, \dots, N^2 \right\} \quad (4.13)$$

We have thus  $N^2$  constraints on  $\mathbb{R}^{N^2 \times N^2}$ , that means the dimension over  $\mathbb{R}$  of the Lie algebra is  $(N^2 - 1)N^2$ .

Denote by  $\mathcal{H}_0^{G_2}$  the element of  $Lie(G_2)$  that is constructed from  $\mathcal{H}_0$  (and the same for  $\mathcal{H}_1$  and  $\mathcal{L}$ ). We associate to the evolution equation (4.2) the following evolution equation on the group  $G_2$ :

$$\begin{aligned} \frac{d}{dt}X(t) &= \left( \mathcal{H}_0^{G_2} + \epsilon(t)\mathcal{H}_1^{G_2} + \gamma(t)\mathcal{L}^{G_2} \right) X(t), \\ X(t=0) &= X_0. \end{aligned} \quad (4.14)$$

We will also write  $X(t; \epsilon, \gamma; X_0)$  when we will need to make explicit the dependence on the parameters; of course  $X(t; \epsilon, \gamma; X_0)$  belongs to the Lie group  $G_2$ . Then by definition  $\bar{\rho}(t) = X(t; \epsilon, \gamma; e)\bar{\rho}(0)$ .

**THEOREM 4.3.** *If the Lie algebra  $Lie\{\mathcal{H}_0^{G_2}, \mathcal{H}_1^{G_2}, \mathcal{L}^{G_2}\}$  generated by  $\{\mathcal{H}_0^{G_2}, \mathcal{H}_1^{G_2}, \mathcal{L}^{G_2}\}$  has dimension  $(N^2 - 1)N^2$  (as a vector space over the real numbers) then the system (4.2) is density matrix controllable.*

*Proof.* Without loss of generality we can suppose that  $\operatorname{tr}(H_0) = 0$  and  $\operatorname{tr}(H_1) = 0$ . We did not yet prove that  $G_2$  is indeed a Lie group: this results from Cartan's theorem that states that any closed subgroup of a Lie group is a Lie subgroup (we include  $G_2$  in the group of one-to-one transformations on  $\mathcal{H}_N$ ). We will use the same line of proof as in Theorem 4.2 and invoke Theorem 3.1 (this time without any change of variables) for  $G = G_2$ . Then  $\mathbb{L} = Lie\{i\mathcal{H}_0^{G_2}, i\mathcal{H}_1^{G_2}, \mathcal{L}^{G_2}\}$  is the Lie algebra generated by  $\mathcal{H}_0^{G_2}$ ,  $\mathcal{H}_1^{G_2}$  and  $\mathcal{L}^{G_2}$ .

Since  $\dim_{\mathbb{R}}(Lie(G_2)) = (N^2 - 1)N^2$  (dimension as vector space over  $\mathbb{R}$ ) the higher possible dimension for  $\mathbb{L}$  is  $(N^2 - 1)N^2$  (again over the real numbers) because  $\mathbb{L} \subset Lie(G_2)$ ; by hypothesis  $\dim_{\mathbb{R}}(\mathbb{L}) = (N^2 - 1)N^2$ , thus both have the same dimension  $(N^2 - 1)N^2$  and  $\mathbb{L} = Lie(G_2)$  and  $\mathbb{S} = G_2$ . Take now  $\epsilon = 0, \gamma = 0$ , then equation (4.14) becomes:

$$\begin{aligned} \frac{d}{dt}X(t) &= \mathcal{H}_0^{G_2} X(t), \\ X(t=0) &= e, \end{aligned} \quad (4.15)$$

with solution  $X(t) = e^{t\mathcal{H}_0^{G_2}}$ ; take a sequence of positive numbers  $\{t_n\}$  with  $t_n > 0$ ; we need to prove that

$$\lim_{n \rightarrow \infty} e^{t_n \mathcal{H}_0^{G_2}} \in \bar{\mathbb{S}}. \quad (4.16)$$

But  $\mathcal{H}_0^{G_2}$  is a skew-Hermitian map which means that  $e^{t_n \mathcal{H}_0^{G_2}}$  belongs to the group of orthogonal transformations of  $\mathcal{H}_N$  (isomorphic to the unitary matrix group  $U(N^2)$ ) which is a subgroup of  $G_2$ . Since the orthogonal group is compact it implies that up to extracting a subsequence  $\lim_{n \rightarrow \infty} e^{t_n \mathcal{H}_0^{G_2}}$  exists and is orthogonal. All orthogonal transformations  $e^{t_n \mathcal{H}_0^{G_2}}$  preserve the trace thus  $\lim_{n \rightarrow \infty} e^{t_n \mathcal{H}_0^{G_2}}$  exists, is orthogonal and trace preserving and hence an element of  $\mathbb{S}$ . Therefore  $\mathcal{R}(e) = \mathbb{S}$ . In particular  $X$  can reach any trace preserving orthogonal transformation from  $\mathcal{H}_N$  to itself. For any  $\rho_i$  and  $\rho_f$  with  $\text{tr}(\rho_i) = \text{tr}(\rho_f)$  we can find a trace preserving orthogonal transformation to map  $\rho_i \in \mathcal{H}_N$  to  $\rho_f \in \mathcal{H}_N$  i.e. we have controllability for  $\rho$ .  $\square$

REMARK 4.2. *A straightforward extension is to consider the circumstance when several non-null controls  $\gamma_2, \dots$  are present; the theoretical results can be proved in the same manner.*

REMARK 4.3. *In this paper two controllability results are proved for  $\gamma(t) \in \mathbb{R}$  but not necessarily positive [5]. However physical considerations may impose  $\gamma$  to be positive (see [6] for more details). Previous controllability results cannot be used due to the loss of compactness. Therefore the controllability analysis of the system defined by (3.1), for  $\gamma(t) \geq 0$ , remains for now a conjecture and leads to the question: are Theorems 4.2 and 4.3 true if  $\gamma(t)$  takes only positive values ?*

**5. Application.** In the following we illustrate the theoretical results introduced in the above section. For this purpose consider two finite-dimensional systems defined by

$$H_0 = \begin{pmatrix} -4 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix}, H_1 = \begin{pmatrix} 0 & -2 & 0 \\ -2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, A = \begin{pmatrix} 2 & 1 & 3 \\ 1 & -1 & 0 \\ 3 & 0 & -1 \end{pmatrix}, \quad (5.1)$$

and

$$H_0 = \begin{pmatrix} -4 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 3 \end{pmatrix}, H_1 = \begin{pmatrix} 0 & -2 & 0 \\ -2 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, A = \begin{pmatrix} 2 & 1 & 1 \\ 1 & -1 & 0 \\ 3 & 0 & -1 \end{pmatrix}. \quad (5.2)$$

First note that the system defined by  $H_0$  and  $H_1$  alone (i.e., with  $A = 0$ ) is not controllable as the dimension of the Lie algebra generated by  $-iH_0$  and  $-iH_1$  is 4, short of  $3^2 - 1 = 8$  needed for controllability. Also note that for the system defined by (5.1)  $A$  is a symmetric matrix. We want to verify if systems (5.1) and (5.2) are controllable i.e., verify the hypotheses of Theorem 4.2 and Theorem 4.3.

To do so we choose a parameterization such that we can write (4.2) as a linear system

$$\frac{d}{dt} \tilde{\rho} = -i\tilde{\mathcal{H}}_0 \tilde{\rho} - i\epsilon(t)\tilde{\mathcal{H}}_1 \tilde{\rho} + \gamma(t)\tilde{\mathcal{L}} \tilde{\rho} \quad (5.3)$$

Numerically  $\tilde{\mathcal{H}}_0, \tilde{\mathcal{H}}_1, \tilde{\mathcal{L}}$  are  $N^2 \times N^2$  dimensional matrices and  $\tilde{\rho}$  is a  $N^2 \times 1$  vector. For the Hamiltonian part of the dynamics this is known as the Liouville equation in the adjoint representation.

In order to analyze the controllability we need to numerically compute the dimension of the Lie algebra (as subalgebra of  $N^2 \times N^2$  matrices) generated by  $\{i\tilde{\mathcal{H}}_0, i\tilde{\mathcal{H}}_1, \tilde{\mathcal{L}}\}$ , which we denote by  $\text{Lie}\{i\tilde{\mathcal{H}}_0, i\tilde{\mathcal{H}}_1, \tilde{\mathcal{L}}\}$  and verify for  $A$  a Hermitian  $N$ -dimensional matrix if  $\dim_{\mathbb{R}}(\text{Lie}\{i\tilde{\mathcal{H}}_0, i\tilde{\mathcal{H}}_1, \tilde{\mathcal{L}}\}) = (N^2 - 1)^2$  or when  $A$  is an arbitrary if  $\dim_{\mathbb{R}}(\text{Lie}\{i\tilde{\mathcal{H}}_0, i\tilde{\mathcal{H}}_1, \tilde{\mathcal{L}}\}) = (N^2 - 1)N^2$ . For the system in (5.1) numerical computations give the result

$$\dim_{\mathbb{R}}(\text{Lie}\{i\tilde{\mathcal{H}}_0, i\tilde{\mathcal{H}}_1, \tilde{\mathcal{L}}\}) = 64, \quad (5.4)$$

and for the system (5.2)

$$\dim_{\mathbb{R}}(\text{Lie}\{i\tilde{\mathcal{H}}_0, i\tilde{\mathcal{H}}_1, \tilde{\mathcal{L}}\}) = 72. \quad (5.5)$$

We conclude that both systems are controllable.



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#### REFERENCES

- [1] C. ALTAFINI, *Controllability of quantum mechanical systems by root space decomposition of  $su(n)$* , J. Math. Phys., 43 (2002), p. 2051.
- [2] C. ALTAFINI, *Controllability properties for finite dimensional quantum Markovian master equations*, Journal of Mathematical Physics, 44(6) (2003), pp. 2357–2372.
- [3] ———, *Controllability properties for finite dimensional quantum Markovian master equations*, Physical Review A, 70 (2004), p. 012106.
- [4] A. ASSION, T. BAUMERT, M. BERGT, T. BRIKNER, B. KIEFER, V. SEYFRIED, M. STREHLE, AND G. GERBER, *Control of chemical reactions by feedback-optimized phase-shaped femtosecond laser pulses*, Science, 282 (1998), pp. 919–922.
- [5] HEINZ-PETER BREUER, *Genuine quantum trajectories for non-Markovian processes*, Phys. Rev. A, 70 (2004), p. 012106.
- [6] H.-P. BREUER AND F. PETRUCCIONE, *The theory of open quantum systems*, Clarendon Press, Oxford, 2006.
- [7] P. BRUMER AND M. SHAPIRO, *Coherent chemistry: Controlling chemical reactions with lasers.*, Acc. Chem. Res., 22 (1989), p. 407.
- [8] I. L. CHUANG, R. LAFLAMME, P. W. SHOR, AND W. H. ZUREK, *Quantum computers, factoring, and decoherence*, Science, 270 (1995), pp. 1633–1635.
- [9] M. DAHLEH, H. RABITZ, V. RAMAKRISHNA, A. PIERCE, AND M. AND SALAPAKA, *Controllability of molecular systems*, Phys. Rev. A, 51 (2) (1995), pp. 960–966.
- [10] V. GORINI, A. FRIGERIO, M. VERRI, A. KOSSAKOWSKI, AND E. C. G. SUDARSHAN, *Properties of Quantum Markovian Equations*, Rep. Math. Phys., 13 (1978), p. 149.
- [11] V. GORINI, I. KOSSAKOWSKI, AND E. C. G. SUDARSHAN, *Completely positive dynamical semigroups of  $N$ -level systems*, J. Math. Phys, 17 (1976), p. 821.
- [12] R.S. JUDSON AND H. RABITZ, *Teaching lasers to control molecules*, Phys. Rev. Lett, (1992).
- [13] VELIMIR JURDJEVIC AND HECTOR J. SUSSMANN, *Control systems on Lie groups.*, J. Differ. Equations, 12 (1972), pp. 313–329.
- [14] R. J. LEVIS, G.M. MENKIR, AND H. RABITZ, *Selective bond dissociation and rearrangement with optimally tailored, strong-field laser pulses*, Science, 292 (2001), pp. 709–713.
- [15] A. PECHEN AND H. RABITZ, *Teaching the environment to control quantum systems*, Phys. Rev. A, 73 (2006), p. 062102.
- [16] H. RABITZ AND G. TURINICI, *Wavefunction controllability in quantum systems*, J. Phys.A., 36 (2003), pp. 2565–2576.
- [17] H. RABITZ, G. TURINICI, AND E. BROWN, *Control of quantum dynamics: Concepts, procedures and future prospects*, in Computational Chemistry, Special Volume (C. Le Bris Editor) of Handbook of Numerical Analysis, vol X, Ph. G. Ciarlet, ed., Elsevier Science B.V., 2003, pp. 833–887.
- [18] T.C. WEINACHT, J. AHN, AND P.H. BUCKSBAUM, *Controlling the shape of a quantum wavefunction*, Nature, 397 (1999), pp. 233–235.
- [19] R. WU, A. PECHEN, C. BRIF, AND H. RABITZ, *Controllability of open quantum systems with Kraus-map dynamics*, J. Phys. A, 40 (2007), p. 40 5681.