Proceedings of the 40th IEEE
Conference on Decision and Control
Orlando, Florida USA, December 2001

Non-reachable target states for pure-state controllable and non-controllable quantum systems

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Abstract

We consider the problem of identifying non-reachable target states for N-level quantum systems that are not completely controllable.

1 Introduction

The problem of controllability of quantum systems has received considerable attention recently and general criteria for various types of controllability for quantum systems with both discrete and continuous spectra have been derived [1, 2, 3, 4]. Many N-level quantum systems with a discrete spectrum have been shown to be completely controllable [4] and therefore density matrix and observable controllable [5, 6]. However, there nevertheless exist quantum systems of physical interest that are either only pure-state controllable or not controllable at all [6]. In this short paper we consider the problem of identifying non-reachable states for these systems.

2 Model description

We restrict our attention here to N-level quantum systems whose state is represented by a density operator $\hat{\rho}_0$ with a spectral representation

$$\hat{\rho}_0 = \sum_{n=1}^{N} w_n |\Psi_n\rangle\langle\Psi_n|, \tag{1}$$

where $\{|\Psi_n\rangle : 1 \le n \le N\}$ forms a complete orthonormal set in a Hilbert space $\mathcal{H}$ and the eigenvalues w_n satisfy $0 \le w_n \le 1$ and sum to one. If $\hat{\rho}_0$ has rank one, i.e., there is only a single non-zero eigenvalue with multiplicity one, then it is said to represent a *pure* state, otherwise it represents a *mixed* state of the system. The time evolution of $\hat{\rho}_0$ is governed by

$$\hat{\rho}(t) = \hat{U}(t)\hat{\rho}_0\hat{U}(t)^\dagger, \tag{2}$$

where $\hat{U}(t)$ is the unitary evolution operator of the system, which satisfies the Schrodinger equation

$$i\hbar\frac{\partial}{\partial t}\hat{U}(t) = \hat{H}\hat{U}(t) \tag{3}$$

with initial condition $\hat{U}(0) = \hat{I}$, where $\hat{I}$ is the identity operator. $\hat{H}$ in the equation above is the total Hamiltonian of the system. For a quantum system subject to external control, $\hat{H}$ is typically of the form

$$\hat{H} = \hat{H}_0 + \sum_{m=1}^{M} f_m(t)\hat{H}_m, \tag{4}$$

where $\hat{H}_0$ is the internal Hamiltonian of the unperturbed system and $\hat{H}_m$ are interaction terms governing the interaction of the system with an external field f_m. Note that the operators $\hat{H}_m$, $0 \le m \le M$, in (4) are Hermitian and their skew-Hermitian counterparts $i\hat{H}_m$ generate a Lie algebra $\mathcal{L}$ known as the dynamical Lie algebra of the control system. The corresponding dynamical Lie group S of the system is given by all unitary operators of the form $\exp(\hat{x})$, where $\hat{x}$ is an element in the dynamical Lie algebra $\mathcal{L}$.

3 Non-reachable states

The kinematical constraint of unitary evolution partitions the set of density matrices into equivalence classes. Two quantum states $\hat{\rho}_0$ and $\hat{\rho}_1$ are *kinematically equivalent* if there exists a unitary operator $\hat{U}$ such that $\hat{\rho}_1 = \hat{U}\hat{\rho}_0\hat{U}^\dagger$. The dynamical Lie group S of a quantum control system is said to act transitively on an equivalence class E of density matrices if any two states $\hat{\rho}_0, \hat{\rho}_1$ in E are dynamically accessible from each other. It is easy to see that $SU(N)$ and $U(N)$ act transitively on *every* equivalence class of states. Moreover, since the equivalence class of completely random ensembles consists only of the state $\hat{\rho} = \frac{1}{N}\hat{I}_N$, *every* group acts transitively on this equivalence class. By contrast, the only dynamical Lie groups that act transitively on the equivalence class of pure states besides $U(N)$ and $SU(N)$ are $Sp(\ell)$ and $Sp(\ell) \times U(1)$ if $N = 2\ell$ [5].

3.1 Pure-state controllable systems

If $N = 2\ell$ and the dynamical Lie group $S \simeq Sp(\ell)$ [or $Sp(\ell)\times U(1)$] then the system is pure-state controllable. However, the action of $Sp(\frac{N}{2})$ on the equivalence class of pure states is *not* two-point transitive and it can be shown that $Sp(\ell)$ [or $Sp(\ell)\times U(1)$] acts transitively only

0-7803-7061-9/01/$10.00 © 2001 IEEE

on equivalence classes of density matrices with eigenvalues $w_1 \neq w_2 = \ldots = w_N$ and the equivalence class of completely random ensembles. Thus, there exist non-reachable target states for almost any equivalence class of mixed states.

Given a system with Hamiltonian (4) and dynamical Lie group $S \simeq Sp(\ell)$ there exists a $\hat{J}$ unitarily equivalent to

$$\left(\begin{array}{c|c} 0 & \hat{I}_\ell \\ \hline -\hat{I}_\ell & 0 \end{array}\right),$$

such that $\hat{x}_m^T \hat{J} + \hat{J}\hat{x}_m = 0$ for $0 \leq m \leq M$ and $\hat{x}_m = i\hat{H}_m - \frac{i}{N}\mathrm{Tr}(\hat{H}_m)\hat{I}_N$. To decide if two kinematically equivalent states $\hat{\rho}_0$, $\hat{\rho}_1$ are dynamically accessible from each other via a $\hat{U} \in S$ we note that any $\hat{U} \in S$ must satisfy $\hat{U}^T \hat{J} \hat{U} = \hat{J}$. Thus, two kinematically equivalent states $\hat{\rho}_0$, $\hat{\rho}_1$ are dynamically accessible from each other via a $\hat{U} \in S$ if and only if there exists a unitary $\hat{U}$ such that $\hat{\rho}_1 = \hat{U}\hat{\rho}_0\hat{U}^\dagger$ and $\tilde{\rho}_1 = \hat{U}\tilde{\rho}_0\hat{U}^\dagger$ where $\tilde{\rho} = (\hat{J}\hat{\rho}\hat{J}^\dagger)^*$.

Example 1 *If $S = Sp(2)$ with $\hat{J}$ as above then $\hat{\rho}_0 = diag(a,b,b,a)$ and $\hat{\rho}_1 = diag(a,b,a,b)$ are not dynamically accessible from each other unless $b = a$ since $\tilde{\rho}_1 = (\hat{J}\hat{\rho}_1\hat{J}^\dagger)^* = \hat{\rho}_1$ but $\tilde{\rho}_0 = (\hat{J}\hat{\rho}_0\hat{J}^\dagger)^* \neq \hat{\rho}_0$ and there cannot be a unitary operator such that $\hat{\rho}_1 = \hat{U}\hat{\rho}_0\hat{U}^\dagger = \hat{U}\tilde{\rho}_0\hat{U}^\dagger$ if $\hat{\rho}_0 \neq \tilde{\rho}_0$.*

3.2 Non-controllable systems

We shall explicitly consider the case of finding non-reachable pure states for a quantum system with Hamiltonian (4) whose dynamical Lie algebra $\mathcal{L}$ is a representation of $so(N)$ in terms of skew-Hermitian matrices. Let $\mathcal{B}_1 = \{|n\rangle : 1 \leq n \leq N\}$ be the basis of energy eigenstates satisfying $\hat{H}_0|n\rangle = E_n|n\rangle$, in which the operators $i\hat{H}_m$ are represented by skew-Hermitian matrices. Let B be a unitary transformation that maps the old basis $\mathcal{B}_1$ onto a new basis $\mathcal{B}_2 = \{|\tilde{n}\rangle : 1 \leq n \leq N\}$ with $|\tilde{n}\rangle = B|n\rangle$ such that $\tilde{H}_m = B(\mathrm{i}\hat{H}_m)B^\dagger$ are real anti-symmetic matrices and the Lie algebra $\tilde{\mathcal{L}}$ generated by $\tilde{H}_m$ is a representation of $so(N)$ or in terms of real anti-symmetric matrices.

Suppose we have a pure initial state $\tilde{\rho}_0$, given by $\mathrm{diag}(1,0,0,\ldots)$ with respect to the basis $\mathcal{B}_2$, as well as a unitary transformation $\hat{U}$ that maps $\tilde{\rho}_0$ onto a state $\tilde{\rho}_1$ whose matrix representation with respect to the basis $\mathcal{B}_2$ has complex entries. Then $\tilde{\rho}_1$ cannot be reached by a map of the form $\exp(x)$, where x is an element of the Lie algebra $\tilde{\mathcal{L}}$, since $\tilde{\mathcal{L}}$ consists only of real anti-symmetric matrices and hence $\exp(x)$ is real and orthogonal. A real orthogonal transformation cannot map a matrix with real entries onto a matrix with non-real entries. Thus, noting that $\tilde{\rho}_0 = |\tilde{1}\rangle\langle\tilde{1}| = B\hat{\rho}_0 B^\dagger$ or equivalently $\hat{\rho}_0 = B^\dagger|\tilde{1}\rangle\langle\tilde{1}|B$ we can conclude that $\hat{\rho}_1 \equiv B^\dagger\tilde{\rho}_1 B$ cannot be reached from $\hat{\rho}_0$ by a transformation $B^\dagger \exp(x) B$, i.e., a transformation in the exponential image of the original Lie algebra $\mathcal{L}$.

Example 2 *Consider a three-level system with $i\hat{H}_0 = i\mu(-\hat{e}_{11} + \hat{e}_{33})$ and $i\hat{H}_1 = d(\hat{y}_{12} + \hat{y}_{23})$, where $\hat{e}_{mn}$ is a 3×3 matrix whose mth row and nth column entry is one and all other entries are zero, $\hat{x}_{mn} = \hat{e}_{mn} - \hat{e}_{nm}$ and $\hat{y}_{mn} = \mathrm{i}(\hat{e}_{mn} + \hat{e}_{nm})$. The Lie algebra generated by $i\hat{H}_0$ and $i\hat{H}_1$ is spanned by $\hat{x} \equiv \hat{x}_{12} + \hat{x}_{23}$, $\hat{y} \equiv \hat{y}_{12} + \hat{y}_{23}$ and $\hat{z} \equiv \mathrm{i}(-\hat{e}_{11} + \hat{e}_{33})$ and isomorphic to $so(3)$.*

$$\hat{B} = \exp\left[\frac{\pi}{2\sqrt{2}}(\hat{y}_{12} - \hat{y}_{23})\right]$$

is a unitary transformation that maps $i\hat{H}_0 = \mu\hat{z}$ and $i\hat{H}_1 = d\hat{y}$ onto $\tilde{H}_0 = (-\hat{x}_{12} + \hat{x}_{23})/\sqrt{2}$ and $\tilde{H}_1 = -\sqrt{2}\hat{x}_{13}$. Since the $\hat{x}_{mn}$ are real and anti-symmetric, so are $\tilde{H}_0$, $\tilde{H}_1$. Observe that the pure state $\hat{\rho}_0 = \frac{1}{2}(|1\rangle + |3\rangle)(\langle 1| + \langle 3|)$ is invariant under the basis change above, i.e., $\tilde{\rho}_0 = \hat{\rho}_0$, while the state $\hat{\rho}_1 = |1\rangle\langle 1|$ transforms into a matrix with complex entries. Thus, we can conclude that the pure energy eigenstate $|1\rangle$ is not dynamically reachable if the system is initially in the superposition state $(|1\rangle + |3\rangle)/\sqrt{2}$ and vice versa. It can be shown that the observable $\hat{A} = i\hat{x}$ is non-optimizable for certain initial states to the extent that its expectation value remains zero independent of the controls applied.

4 Conclusion

We have provided a brief summary of results about the action of various dynamical Lie groups on the equivalence classes of states for quantum control systems as well as criteria for reachability of states and examples of non-reachable states for pure-state controllable systems and non-controllable systems of Lie type $so(N)$.

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