CONTROLLABILITY OF QUANTUM SYSTEMS

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Abstract: An overview and synthesis of results and criteria for open-loop controllability of Hamiltonian quantum systems obtained using dynamical Lie group and algebra techniques is presented. Negative results for open-loop controllability of dissipative systems are discussed, and the superiority of closed-loop (feedback) control for quantum systems is established.

1. INTRODUCTION

Controlling the dynamics of quantum systems has been a long-standing goal of quantum physicists and chemists, which has received renewed attention recently driven by the desire to build quantum information processing devices. A central problem one faces when attempting to control quantum systems, is the question to which extent it is possible to control the dynamics of the system such as to achieve a certain aim or control objective.

In the following we first provide a synthesis of recent results on controllability of finite-dimensional closed quantum systems subject to open-loop coherent control, i.e., coherent control without measurements and feedback. The results show that for these systems open-loop control is sufficient for controllability in most cases. For open systems, i.e., systems subject to dissipative effects due to uncontrollable interactions with their environment, however, it has been shown that open-loop control is generally not sufficient for controllability, even in finite dimension. We discuss the negative controllability results in this case. Finally, we present a brief overview of recent results using closed-loop control of quantum systems, i.e., control involving measurements and feedback, which indicate its superiority over open-loop control in various settings.

2. MATHEMATICAL MODEL

We consider the problem of control of quantum systems whose state space is a Hilbert space $\mathcal{H}$ of dimension $N$. The state of such a system can be described by a density operator $\hat{\rho}$.

Definition 1. A density operator is a positive operator on $\mathcal{H}$ with unit trace. If it has rank one it is said to represent a pure state, otherwise it represents a mixed state.

A density operator representing a pure state is simply a projector onto a one-dimensional subspace of the Hilbert space $\mathcal{H}$, i.e., using Dirac notation we can write $\hat{\rho} = |\Psi\rangle\langle\Psi|$, where $|\Psi\rangle$ is an element in $\mathcal{H}$ called a wavefunction. Thus, the special case of a pure state can also represented by a wavefunction $|\psi\rangle \in \mathcal{H}$.
In general the operator $\dot{\rho}$ satisfies the quantum Liouville equation

$$i\hbar \frac{d}{dt} \rho(t) = [\hat{H}(t), \rho(t)] + i\hbar \mathcal{L}_D[\rho(t)], \quad (1)$$

where the commutator determines the Hamiltonian part of the evolution, and the second term represents the non-Hamiltonian part due to dissipative effects, which may include certain measurements that weakly perturb the system. The operator $\hat{H}(t)$ is the total Hamiltonian of the system subject to the control fields $\mathbf{f}(t)$. For the purpose of controllability studies the control Hamiltonian is usually assumed to be control-linear, i.e.,

$$\hat{H}[\mathbf{f}(t)] = \hat{H}_0 + \sum_{m=1}^{M} f_m(t) \hat{H}_m, \quad (2)$$

where $\hat{H}_0$ is the internal system Hamiltonian and $\hat{H}_m$, $m > 0$, are the interaction terms. This assumption is generally reasonable as long as the control fields are sufficiently weak compared, e.g., to relevant intra-atomic or molecular forces.

In the absence of dissipative effects, i.e., when $\mathcal{L}_D = 0$, the evolution of the system is Hamiltonian and the density operator satisfies the dynamical evolution equation

$$\dot{\rho}(t) = \hat{U}(t, t_0) \rho_0 \hat{U}(t, t_0)\dagger, \quad (3)$$

where $\hat{U}(t, t_0)$ is the Hilbert space evolution operator that satisfies the Schrodinger equation

$$i\hbar \frac{d}{dt} \hat{U}(t, t_0) = \hat{H}[\mathbf{f}(t)] \hat{U}(t, t_0), \quad (4)$$

and is hence restricted to the unitary group $U(N)$, $N$ being the dimension of the Hilbert space $\mathcal{H}$.

The constraint of unitary evolution for Hamiltonian systems imposes restrictions on the quantum states that can be reached from a given initial state. Since the former limitations are independent of the control fields and their type of interaction with the system, we shall refer to them as kinematical constraints, to distinguish them from dynamical constraints arising from constraints on the control fields or the interaction with those fields. Precisely, given an initial state $\rho_0$ and a target state $\rho_1$, the target state is kinematically admissible if and only if there exists a unitary operator $\hat{U}$ such that $\rho_1 = \hat{U} \rho_0 \hat{U}^{-1}. This equation defines an equivalence relation that partitions the set of density operators into kinematical equivalence classes. Two density matrices $\rho_1, \rho_2$ are kinematically equivalent if they are unitarily equivalent, i.e., if $\rho_2 = \hat{U} \rho_1 \hat{U}^{-1}$ for some unitary operator $\hat{U}$. It follows immediately that any density matrices are kinematically equivalent if and only if they have the same eigenvalues. Hence, the set of pure states forms one such equivalence class of states.

3. DEGREES OF CONTROLLABILITY FOR CLOSED SYSTEMS

Closed quantum systems, i.e., systems that are decoupled from their environment except for (controlled) interactions with coherent control fields, exhibit Hamiltonian dynamics if they are subjected to open-loop coherent control. Various notions of controllability exist for such systems. Depending on the application, one may be interested in complete controllability, observable or operator controllability, and mixed-state or pure-state controllability [Albertini and D’Alessandro (2001); Schirmer et al. (2002a)].

Definition 2. A quantum system subject to Hamiltonian dynamics is completely controllable if any unitary evolution is dynamically realizable, i.e., if for any unitary operator $\hat{U}$, there exists an admissible control-trajectory pair $(\mathbf{f}(t), \hat{U}(t, t_0))$ defined for $t_0 \leq t \leq t_F$ (for some $t_F < \infty$) such that $\hat{U} = \hat{U}(t_F, t_0)$.

Definition 3. A quantum system subject to Hamiltonian dynamics is density matrix controllable if for any pair of kinematically equivalent density matrices $\rho_0$ and $\rho_1$, there exists an admissible control-trajectory pair $(\mathbf{f}(t), \hat{U}(t, t_0))$ defined for $t_0 \leq t \leq t_F$ (for some $t_F < \infty$) such that $\rho_1 = \hat{U}(t_F, t_0) \rho_0 \hat{U}(t_F, t_0)\dagger$.

Definition 4. A quantum system subject to Hamiltonian dynamics is pure-state controllable if for any two pure states given by the (normalized) wavefunctions $|\Psi_0\rangle, |\Psi_1\rangle$, there exists an admissible control-trajectory pair $(\mathbf{f}(t), \hat{U}(t, t_0))$ defined for $t_0 \leq t \leq t_F$ (for some $t_F < \infty$) such that $|\Psi_1\rangle = \hat{U}(t_F, t_0) |\Psi_0\rangle$.

Definition 5. A quantum system subject to Hamiltonian dynamics is observable controllable if for any observable $\hat{A}$ and initial state $\rho_0$ of the system, there exists an admissible control-trajectory pair $(\mathbf{f}(t), \hat{U}(t, t_0))$ defined for $t_0 \leq t \leq t_F$ (for some $t_F < \infty$) such that the ensemble average $\text{Tr}[\rho(t)\hat{A}]$ of $\hat{A}$ assumes any kinematically admissible value [Girardeau et al. (1998)].

4. LIE-ALGEBRAIC CRITERIA FOR CONTROLLABILITY

The notions of controllability for closed quantum systems subject to open-loop coherent control defined in the previous section can be related to the dynamical Lie group and Lie algebra of the control system.

Definition 6. The dynamical Lie algebra of a quantum system with Hamiltonian (2) is the Lie
algebra \( \mathcal{L} \) generated by the skew-Hermitian operators \( i\hat{H}_m \) by taking all linear combinations and iterated commutators.

The associated dynamical Lie group \( G \) is formed by the elements \( \exp(\hat{x}) \) where \( \hat{x} \) is an element of \( \mathcal{L} \). Knowledge of the dynamical Lie group of the system is fundamental to understanding the dynamics of the system and especially limitations on its control since the dynamical evolution operator \( \hat{U}(t,t_0) \) of the system is constrained to this Lie group for all times, independent of the control fields applied, and the set of reachable states and dynamically realizable bounds on the expectation values of observables depend on this dynamical Lie group.

For Hamiltonian quantum systems it is obvious from the definition that only a system with dynamical Lie group \( U(N) \), where \( N \) is the dimension of the Hilbert space \( \mathcal{H} \), can be completely controllable. Density matrix controllability requires that the dynamical Lie group act transitively on all equivalence classes of density matrices, while pure-state controllability requires only transitive action of the dynamical Lie group on the equivalence class of pure states. Since the latter can be represented by normalized wavefunctions or unit vectors in \( \mathbb{C}^N \), pure-state controllability requires only transitive action of the dynamical Lie group on the unit sphere in \( \mathbb{C}^N \).

It can furthermore be shown that density matrix controllability is both necessary and sufficient for observable controllability as defined above [Schirmer et al. (2002a)]. Based on these observations, the degree of controllability of a Hamiltonian quantum system with control-linear Hamiltonian (2) can be characterized in terms of its dynamical Lie algebra:

**Theorem 7.** [Albertini and D’Alessandro (2001); Schirmer et al. (2002a)] A Hamiltonian quantum system with control-linear Hamiltonian is

- completely controllable if and only if \( \mathcal{L} \simeq u(N) \).
- density matrix controllable if and only if \( \mathcal{L} \simeq su(N) \) or \( \mathcal{L} \simeq u(N) \).
- pure-state controllable if and only if \( \mathcal{L} \) is isomorphic to either \( u(N), su(N) \), or (when \( N = 2\ell \)) \( sp(\ell), sp(\ell) \oplus u(1) \).

Complete controllability thus implies density matrix and observable controllability and the latter guarantees pure-state controllability. According to our definition complete controllability is strictly speaking a slightly stronger requirement than density matrix or observable controllability but the difference is essentially only a phase factor, which is not important for most applications.

**Definition 8.** For simplicity we shall therefore call a system controllable if it is density matrix and observable controllable.

An interesting consequence of the previous result is that pure-state controllability is equivalent to mixed-state controllability if the dimension of \( \mathcal{H} \) is odd, but it is a weaker requirement if the dimension of \( \mathcal{H} \) is even, i.e., there exist even-dimensional quantum systems that are pure-state controllable but not mixed-state controllable.

For a system that is not controllable there exist initial states for which the set of dynamically accessible target states does not comprise the entire kinematical equivalence class, i.e., at least some of the kinematical equivalence classes are partitioned into disjoint subsets of dynamically equivalent states. If the system fails to be pure-state controllable then there exists such a partition for the equivalence class of pure states [Schirmer and Solomon (2001); Schirmer et al. (2002c)]. However, lack of controllability does not necessarily imply that the dynamical Lie group of the system does not act transitively on any kinematical equivalence class. For instance, every dynamical Lie group clearly acts transitively on the equivalence class of completely random ensembles, which consists of the single element \( \hat{\rho}_R = \frac{1}{N}\hat{I}_N \), where \( \hat{I}_N \) is the identity matrix of dimension \( N \).

5. **GRAPH-CONNECTIVITY CRITERIA FOR CONTROLLABILITY**

Although a characterization of the degree of controllability in terms of the dynamical Lie algebra is useful, it can be quite time-consuming to compute the Lie algebra of a system for large \( N \). It is therefore desirable to have criteria for controllability that are easier to verify.

For strongly regular Hamiltonian control systems with a control Hamiltonian of the form

\[
\hat{H}[f(t)] = \hat{H}_0 + f(t)\hat{H}_1,
\]

it has been shown that controllability can be related to the transition graph determined by the interaction Hamiltonian \( \hat{H}_1 \).

**Definition 9.** The internal system Hamiltonian \( \hat{H}_0 \) is regular if it has unique eigenvalues, i.e., if each eigenvalue occurs with multiplicity one. \( \hat{H}_0 \) is strongly regular if in addition, the difference between any pair of eigenvalues is unique, i.e., \( E_i - E_j \neq E_m - E_n \) unless \( (i, j) = (m, n) \).

**Definition 10.** The transition graph of a quantum system subject to a single control field is obtained as follows: Choose a Hilbert space basis \( \lbrace |n\rangle : 1 \leq n \leq N \rbrace \) of the system's state space with the \( n \)-th basis element in the range of \( \hat{H}_0 \) and define a graph with vertices \( V \) and edges \( E \) such that \( (v_i, v_j) \in E \) if and only if \( |v_i - v_j| = 1 \) and \( \hat{H}_0 |v_i\rangle = E_i |v_i\rangle \) and \( \hat{H}_0 |v_j\rangle = E_j |v_j\rangle \). The graph is connected if and only if \( \hat{H}_0 \) is strongly regular.
6. OTHER CONTROLLABILITY RESULTS

Theorem 12 is very useful when applicable as it is much easier to verify than the general Lie algebraic criteria for various notions of controllability. Note, however, that the hypothesis of strong regularity of \( \hat{H}_0 \) is restrictive. Although this requirement can be relaxed slightly, e.g., transitions that occur with zero probability can be ignored, etc., it essentially restricts the applicability of the result to systems with non-degenerate energy levels and non-degenerate transition frequencies.

Nevertheless, there are positive controllability results for systems that do not satisfy the hypothesis of strong regularity, or even regularity of \( \hat{H}_0 \). For instance, in some cases the general Lie algebraic criteria (theorem 7) can be applied to derive conditions on the parameters of a model system that guarantee controllability.

**Theorem 13.** [Fu et al. (2001); Schirmer et al. (2001)] A quantum control system with Hamiltonian \( H = \hat{H}_0 + f(t)\hat{H}_1 \), where

\[
\hat{H}_0 = \sum_{n=1}^{N} E_n |n\rangle\langle n|,
\]

\[
\hat{H}_1 = \sum_{n=1}^{N-1} d_n (|n\rangle\langle n+1| + |n+1\rangle\langle n|)
\]

is controllable if \( d_n \neq 0 \) for \( 1 \leq n \leq N-1 \) and either

1. there exists \( p \) such that \( \omega_n \neq \omega_p \) for \( n \neq p \) where \( \omega_n = E_{n+1} - E_n \); or
2. \( \omega_n = \omega \) for all \( n \) but there exists \( p \) such that \( v_n \neq v_p \) for \( n \neq p \), where \( v_n \equiv 2\lambda^2 - d_n^2 - d_{n+1}^2 \).

If \( N = 2p \) then \( d_{p-k}^2 \neq d_{p+k}^2 \) for some \( k \neq 0 \) is required as well. If in addition \( \text{Tr}(\hat{H}_0) \neq 0 \) then the system is completely controllable.

Essentially, this theorem shows that a sequentially coupled Hamiltonian quantum system is controllable if there is a single unique transition frequency, and this is not the ‘middle’ transition in case of an even-dimensional system. If the unique transition frequency is the middle transition and the system dimension is even, then the degree of controllability depends on whether the system satisfies a symplectic symmetry relation, in which case we have only pure-state controllability, or not, in which case we have general controllability [Schirmer et al. (2002b)].

If there is no unique transition frequency then controllability depends on the values of the dipole moments, but even if all transition frequencies are the same, the system is still controllable for most choices of the dipole moments.
Furthermore, even for systems with no non-degenerate energy levels (i.e., completely non-regular $H_0$) such as electronic transitions in atomic or ionic systems, positive controllability results have been obtained in many cases using Lie algebraic techniques [Schirmer et al. (2002a)].

The question arises whether the hypothesis of strong regularity in theorem 12 is necessary. Unfortunately, in spite of some encouraging results, the answer is yes. Regularity is not sufficient for controllability in general. For instance, the Lie algebra of a system with equally spaced but non-degenerate energy levels and uniform transition dipole moments has been shown to be $sp(N/2)$ if $N$ even, and $so(N)$ if $N$ odd [Schirmer et al. (2002b)]. Thus, the system is remains pure-state controllable if it is even-dimensional, but is not controllable in the odd-dimensional case. Note that this result does not violate theorem 13 since there is no unique transition frequency and the system does not satisfy hypothesis (b) of the theorem either.

7. CONTROLLABILITY OF OPEN SYSTEMS

While there are perhaps still some interesting open problems regarding the degree of controllability of closed quantum systems subject to Hamiltonian dynamics and open-loop coherent control, the results of the previous sections show that their controllability properties are quite well understood, and that they are controllable in most cases. The situation is quite different for open quantum systems, i.e., systems that interact (incoherently) with their environment in addition to any interaction with coherent control fields. Such incoherent interactions with the environment lead to a non-zero dissipative term $L_D$ in the quantum Liouville equation, and inevitably result in non-Hamiltonian dynamics.

It has been suggested that dissipative effects increase the amount of control since the dissipative term, being non-Hamiltonian, removes restrictions such as unitary evolution and tends to enlarge the dynamical Lie group of the system. However, this picture is only partially true. Indeed, dissipative effects usually enlarge the Lie algebra of the system [Solomon and Schirmer (2002)], and states not reachable from a given initial state via coherent control in the non-dissipative case may become reachable when dissipation is added. In fact, important applications such as optical pumping or laser cooling rely on the combined effect of dissipation and coherent control fields [Schirmer (2001); Schirmer and Solomon (2002)].

However, dissipative effects generally do not increase open-loop controllability of quantum systems. Before we discuss why, it should be noted that it does not make sense to distinguish between pure and mixed state controllability for open systems, since dissipative effects can convert pure states into mixed states and vice versa. Furthermore, since the kinematical equivalence classes of states that exist for closed systems (subject to Hamiltonian dynamics) are not preserved, the only sensible definition of (state) controllability for open systems appears to be the following.

**Definition 14.** An open (non-Hamiltonian) quantum system is (density matrix) controllable if any target state represented by a density operator $\hat{\rho}_1$ can be reached from any given initial state $\hat{\rho}_0$.

It can be shown that open quantum systems are virtually never open-loop controllable according to this definition [Solomon and Schirmer (2002); Altafini (2002b)]. The main reason for this is that dissipative effects are (a) generally not controllable — but rather constitute a non-Hamiltonian drift (or disturbance) term — and always lead to irreversible semi-group dynamics. This means that for open systems there always exist states that are not accessible (via open-loop control), and the set of such states may be large.

Nonetheless, non-Hamiltonian drift terms may render states not accessible from a given initial state by coherent control in the non-dissipative case, accessible via open-loop control. Thus, it appears that the more important issue for control of open systems is the study of the set of reachable states. For systems with sufficiently small non-Hamiltonian drift terms, it may be interesting to compare the set of reachable states with and without drift as a function of time and to consider the amount of overlap of these sets. Since dissipative systems tend to asymptotically converge to a stationary state (which may depend on the initial state) when no control fields are applied, and coherent control operations are unitary, it is to be expected that the set of reachable states from any initial state will contract with time for many systems. One question of interest in this regard is what states are asymptotically reachable for a given open system using open-loop control.

8. CLOSED-LOOP (FEEDBACK) CONTROL

The previous sections have focused exclusively on the extent to which it is possible to control a quantum system (Hamiltonian or otherwise) using open-loop coherent control. While there are many potential applications of open-loop control for quantum systems, this type of control clearly has its limitations. An alternative is to add measurements and condition the controls based on the result of these measurements. This type of control
is generally referred to as closed-loop or feedback control.

Feedback control can be difficult to realize for quantum systems since feedback requires measurements, which perturb the system and generally lead to nonlinear dynamics. Projective measurements give rise to discontinuous evolution and jumps in state space. Weak (non-projective) measurements can ameliorate the situation by eliminating discontinuities, but may be difficult to perform and still lead to non-linear dynamics.

Nevertheless, many different types of measurements and feedback are conceivable for quantum systems, and various schemes have recently been proposed. A detailed discussion of this topic is beyond the scope of a short paper such as this, but closed-loop control has been shown to be generally more powerful than open-loop control, especially for control of open system dynamics [Lloyd and Viola (2000)]. Feedback control using weak measurements has been proposed for tasks that are not possible via open-loop coherent control such as continuous quantum error correction [Ahn et al. (2003)]. Furthermore, the combination of measurements and coherent control allows the implementation of non-unitary dynamics even for otherwise closed systems [Lloyd and Viola (2002)]. Recent results even suggest that non-dissipative systems that are not open-loop controllable because the dynamical Lie group does not act transitively on the equivalence classes of states, may be controllable if certain measurements are possible [Mendes and Man’ko (2002)].

9. CONCLUSION

We have presented a concise summary of recent results on open-loop controllability of (closed) quantum systems subject to Hamiltonian dynamics, showing the importance of the dynamical Lie algebra and related Lie group in assessing the degree of controllability of the system. Negative (open-loop) controllability results of for open quantum systems with non-Hamiltonian drift terms have been discussed, and we have argued for the importance of studying the reachable sets in this case. Finally, we have presented a brief discussion of recent results on closed-loop control of quantum systems, indicating the challenges of implementing feedback control, and demonstrating its superiority over open-loop control.

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REFERENCES

C. Ahn, H. W. Wiseman, and G. J. Milburn. Quantum error correction for continuously detected errors. quant-ph/0302006, 2003.

F. Albertini and D. D’Alessandro. Notions of controllability for quantum-mechanical systems. quant-ph/0106128, 2001.

C. Altafini. Controllability of quantum mechanical systems by root space decompositions of su(n). J. Math. Phys., 43(5):2051–2062, 2002a.

Claudio Altafini. Controllability properties for finite dimensional quantum markovian master equations. quant-ph/0211094, 2002b.

H. Fu, S. G. Schirmer, and A. I. Solomon. Complete controllability of finite-level quantum systems. J. Phys. A, 34:1679, 2001.

M. D. Girardeau, S. G. Schirmer, J. V. Leahy, and R. M. Koch. Kinematical bounds on optimization of observables for quantum systems. Phys. Rev. A, 58:2684, 1998.

Seth Lloyd and Lorenza Viola. Control of open quantum system dynamics. quant-ph/0008101, 2000.

Seth Lloyd and Lorenza Viola. Engineering quantum dynamics. Phys. Rev. A, 65:010101, 2002.

R. V. Mendes and V. I. Man’ko. Quantum control and the Strocci map. quant-ph/0212006, 2002.

S. G. Schirmer. Laser cooling of internal molecular degrees of freedom for vibrationally hot molecules. Phys. Rev. A, 63(1):013407, 2001.

S. G. Schirmer, H. Fu, and A. I. Solomon. Complete controllability of quantum systems. Phys. Rev. A, 63:063410, 2001.

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, 2002a.

S. G. Schirmer, I. C. H. Pullen, and A. I. Solomon. Identification of dynamical lie algebras for finite-level quantum control systems. J. Phys. A, 35(9):2327, 2002b.

S. G. Schirmer and A. I. Solomon. Non-reachable target states for pure-state controllable and non-controllable quantum systems. In 40th IEEE CDC Proceedings (Omnipress, Madison, WI), pages 2605–2606, 2001.

S. G. Schirmer and A. I. Solomon. Quantum control of dissipative systems. In Proceedings of the MTNS 2002, available online at www.nd.edu/~mtns/papers/2178_4.pdf, 2002.

S. G. Schirmer, A. I. Solomon, and J. V. Leahy. Criteria for dynamical reachability of quantum states. J. Phys. A, 35:8551–8562, 2002c.

Allan I. Solomon and Sonia G. Schirmer. Dissipative groups and the bloch ball. quant-ph/0211027, 2002.

G. Turinici and H. Rabitz. Quantum wavefunction controllability. Chem. Phys., 267:1–9, 2001.