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Brief paper

Stability analysis of discontinuous quantum control systems with dipole and polarizability coupling☆

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ABSTRACT

Closed quantum systems under the influence of a laser field, whose interaction is modeled by a Schrödinger equation, with a coupling control operator containing both a linear (dipole) and a quadratic (polarizability) term, are analyzed. Discontinuous feedbacks, obtained by a Lyapunov trajectory tracking procedure, have recently been proposed to control these types of system. The purpose of this paper is to study the asymptotic stability by considering the solutions in the Filippov sense. The analysis is developed by applying a variant of the LaSalle invariance principle for differential inclusions. Numerical simulations are included to illustrate the efficiency of the discontinuous control.

1. Introduction

Control of quantum systems using laser fields has been subject to significant developments in the last two decades (see, for example, (Assion et al., 1998; Brumer & Shapiro, 1989; Judson & Rabitz, 1992; Levis, Menkir, & Rabitz, 2001; Weinacht, Ahn, & Bucksbaum, 1999)). The increasing interest in this domain is motivated by the effects of the technique: we can create or break chemical bonds, each time with finesse far beyond the usual macroscopic means (temperature, pressure, etc.).

Since the first successful laboratory experiments at the beginning of the 1990s (Assion et al., 1998; Judson & Rabitz, 1992), many applications of this method have been developed: designing logical gates in future quantum computers, investigations of imaging by nuclear magnetic resonance (NMR), studies of protein dynamics, molecular detection, molecular orientation and alignment, construction of ultra-short lasers, etc.

From the beginning, the complexity of chemical phenomena that arise during the interaction between the laser and the quantum system has required the introduction of theoretical methods as an important step in the experimental phase. This type of analysis can reveal the set of objectives that can be achieved, and the nature of the laser pulse that can be used. In this context, we consider the time-dependent Schrödinger equation, which models the evolution of a quantum system:

$$i\frac{d}{dt}\Psi(t) = H(t)\Psi(t), \tag{1}$$

where $H(t)$ is an Hermitian operator called the Hamiltonian, and Ψ is a complex function called the wavefunction. When the system is controlled by selecting a convenient laser intensity $\epsilon(t)$, the interaction between the laser and the system is described by an operator μ_1, also called dipole coupling (Rabitz, Shi, & Woody, 1988). Thus, we recover a bilinear form of the Schrödinger equation, formally written as

$$i\frac{d}{dt}\Psi(t) = (H_0 + \epsilon(t)\mu_1)\Psi(t). \tag{2}$$

In this case, $H(t) = H_0 + \epsilon(t)\mu_1$, where H_0 is the internal Hamiltonian operator which characterizes the system when the laser is shut down ($\epsilon(t) = 0$). In the limit of small laser intensities, the first-order term $\epsilon(t)\mu_1$ may be enough to adequately describe the interaction; however, situations exist in which the dipole coupling does not have enough influence on the system to reach the control goal; the goal may become accessible only after taking into account terms of higher order in the expansion of $H(t)$, for example a polarizability term $\epsilon^2(t)\mu_2$ (see, for example, Dion et al. (1999); Dion, Keller, Atabek, and Bandrauk (1999)).

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In the following, we focus on the case when a second-order term is added in the expansion of the Hamiltonian:

$$H(t) = H_0 + \epsilon(t)\mu_1 + \epsilon^2(t)\mu_2. \tag{3}$$

For numerical reasons, a finite-dimensional setting is considered. The operators will be restrained to a linear space spanned by an N-dimensional set D. This set can contain for example the first N eigenvalues of the infinite-dimensional internal Hamiltonian H_0. For simplicity, we conserve the same notation, i.e., we denote by H_0, μ_1, and μ_2, $N \times N$ Hermitian matrices with complex coefficients and by Ψ an N-dimensional complex vector.

One important problem is to determine efficient laser fields to control quantum systems whose Hamiltonians are defined by (3). For this purpose, an analysis of the controllability has to be pursued, i.e., we ask if any admissible quantum state can be attained with some admissible laser field. This can be studied via the general accessibility criteria (Brockett, 1973; Sussmann & Jurdjevic, 1972) based on Lie brackets; more specific results can be found in Turinici (2007). A detailed presentation has been made in Coron, Grigoriu, Lefter, and Turinici (2009).

Even if positive results of controllability for systems, with the Hamiltonian defined by (3), have been obtained, finding efficient numerical algorithms to determine the control field remains a very difficult task. A solution is to present the problem as a minimization of a cost functional, which describes the goal to be achieved, and eventually some other constraints. This approach led to procedures such as stochastic iterative approaches (e.g., genetic algorithms) (Li, Turinici, Ramakhrishna, & Rabitz, 2002), iterative critical point methods (monotonic algorithms) (Maday & Turinici, 2003; Tannor, Kazakov, & Orlov, 1992; Zhu & Rabitz, 1998), trajectory tracking, or local control procedures ((Beauchard, Coron, Mirrahimi, & Rouchon, 2007; Chen, Gross, Ramakrishna, Rabitz, & Mease, 1995; Ferrante, Pavon, & Raccanelli, 2002; Grivopoulos & Bamieh, 2003; Mirrahimi, Rouchon, & Turinici, 2005; Rabitz & Zhu, 2003; Sugawara, 2003)). One advantage of this class of methods is that we obtain explicit control fields. Another is that few propagations in time are required to approach the solution of the time-dependent Schrödinger equation (TDSE). This is an important aspect when larger systems are considered.

Lyapunov trajectory tracking techniques have been applied for systems with Hamiltonian (3) in order to determine the control ϵ. A first positive result has been obtained by adapting the analysis presented in Jurdjevic and Quinn (1978) and Mirrahimi et al. (2005), which deals with bilinear quantum systems $H_0 + \epsilon(t)\mu_1$. The success of the feedback control depends on whether there exists (non-zero) direct coupling, through μ_1, between the target state and *all* other eigenstates. When the same property holds for Hamiltonian $H(t) = H_0 + \epsilon(t)\mu_1 + \epsilon^2(t)\mu_2$, the same type of feedback formulas hold. When some of the (direct) coupling is realized through μ_2 instead of μ_1, the previous feedback formulas do not hold any more, and two alternatives have been proposed (see Coron et al. (2009) for more details): discontinuous feedback and time-varying feedback.

Only approximative asymptotic stability results have been proved for these last two situations. This paper focuses on the case of discontinuous feedback obtained for quantum systems with the Hamiltonian defined by (3). The goal is to prove stability results, and especially asymptotic stability considering the solutions of the quantum system (1), with Hamiltonian H given by (3), in the Filippov sense.

The rest of the paper is arranged as follows. In Section 2, we introduce the main notation and the Lyapunov tracking procedure, followed by the construction of the discontinuous feedback. Then, we study the existence of solutions in the Filippov sense. In Section 3, we prove a first stability result followed by an asymptotic stability result. Sections 4 and 5 are dedicated to numerical simulations and conclusions, respectively.

2. Lyapunov trajectory tracking

2.1. The Lyapunov function

We consider Eq. (1), with Hamiltonian $H(t)$ given by (3), which describes the evolution of an N-level quantum system submitted to an external action:

$$i\frac{d}{dt}\Psi(t) = (H_0 + \epsilon(t)\mu_1 + \epsilon^2(t)\mu_2)\Psi(t). \tag{4}$$

The wavefunction $\Psi = (\Psi_j)_{j=1}^N$ is a vector in $\mathbb{C}^N$, verifying $\sum_{j=1}^N |\Psi_j|^2 = 1$, i.e., Ψ belongs to the unit sphere $\mathcal{S}^N(0, 1)$ of $\mathbb{C}^N$. The function Ψ represents a complete physical description of the state of the quantum system at every instant t.

Recall that two wavefunctions Ψ_1 and Ψ_2 that differ by a phase $\theta(t) \in \mathbb{R}$, i.e., $\Psi_1 = \exp(i\theta(t))\Psi_2$, describe the same physical state. To take this property into account, we add a fictitious control ω (see also Mirrahimi et al. (2005)). Hence we will replace the evolution Eq. (4) by

$$i\frac{d}{dt}\Psi(t) = (H_0 + \epsilon(t)\mu_1 + \epsilon^2\mu_2 + \omega(t))\Psi(t), \tag{5}$$

where $\omega \in \mathbb{R}$ is a new control. We can choose it arbitrarily without changing the physical quantities attached to Ψ. We assume in what follows that the state space is $\mathcal{S}^N(0, 1)$ and that the dynamics given by (5) admits two independent controls, ϵ and ω.

In order to obtain an explicit formula for the laser field $\epsilon(t)$, we apply a Lyapunov trajectory tracking technique. The method consists in introducing a time-varying function $V(\Psi(t))$:

$$V(\Psi(t)) = \langle \Psi - \phi | \Psi - \phi \rangle = \|\Psi - \phi\|^2, \tag{6}$$

with Ψ a smooth solution of (5) and ϕ an eigenvector of H_0 associated to the eigenvalue λ.

The function V is nonnegative for all $t > 0$ and all $\Psi \in \mathcal{S}^N(0, 1)$, and vanishes when $\Psi = \phi$. We search for feedback controls such that V is a Lyapunov function. To do that, we compute formally the derivative of V along the trajectories of (5):

$$\begin{aligned}\frac{dV}{dt} &= 2\epsilon Im(\langle \mu_1\Psi(t)|\phi\rangle) + 2\epsilon^2 Im(\langle \mu_2\Psi(t)|\phi\rangle)\\ &\quad + 2(\omega + \lambda)Im(\langle \Psi(t) \mid \phi\rangle),\end{aligned} \tag{7}$$

where Im denotes the imaginary part. For convenience, we denote $I_1 = Im(\langle \mu_1\Psi(t)|\phi\rangle)$ and $I_2 = Im(\langle \mu_2\Psi(t)|\phi\rangle)$.

Then note that if, for example, one takes

$$\begin{cases}\epsilon(I_1, I_2) = -kI_1/(1 + kI_2)\\ \omega = -\lambda - cIm(\langle \Psi(t)|\phi\rangle),\end{cases} \tag{8}$$

with k and c strictly positive parameters, one gets

$$dV/dt = -2k(I_1/(1 + kI_2))^2 - 2c(Im(\langle \Psi(t) \mid \phi\rangle))^2 \le 0,$$

and thus V is nonincreasing.

However, even if the feedback is chosen such that is V monotonically decreasing, this does not automatically imply that the minimum value will be reached. A convergence analysis is required.

2.2. Discontinuous feedback

The theoretical result (see Theorem 2.1) in Grigoriu, Lefter, and Turinici (2009) shows that tracking to ϕ works well when all eigenstates of $H_0, \phi_2, \ldots, \phi_N$ other than ϕ, are coupled to ϕ by μ_1; i.e., $\langle \phi_j, \mu_1\phi\rangle \neq 0, j = 2, \ldots, N$. For the important case when some of the couplings are realized by μ_2 instead of μ_1, formulas (8) are ineffective. Discontinuous and time-varying feedbacks have been proposed to stabilize the system (see Coron et al. (2009)).