



HAL
open science

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

Andreea Grigoriu

► **To cite this version:**

Andreea Grigoriu. Stability analysis of discontinuous quantum control systems with dipole and polarizability coupling. 2010. hal-00578341v1

HAL Id: hal-00578341

<https://hal.science/hal-00578341v1>

Preprint submitted on 19 Mar 2011 (v1), last revised 4 Jul 2012 (v2)

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

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

Andreea Grigoriu ^a

^a Princeton University, Department of Chemistry, Princeton, 08540, USA

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 been recently proposed to control these type of systems. 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 LaSalle invariance principle for differential inclusions. Numerical simulations are included to illustrate the efficiency of the discontinuous control.

Key words: Quantum systems, Stabilization, Control Lyapunov function, Tracking, Differential inclusions

1 Introduction

Control of quantum systems using laser fields has been subject to significant developments in the last two decades ([1,5,14,16,18,33] etc.). The increasing interest on 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 obtained at the beginning of the 90s [1,14] many applications of this method have been developed: designing logical gates in future quantum computers, investigations of imaging by nuclear magnetic resonance - NMR, study of protein dynamics, molecular detection, molecular orientation and alignment, construction of ultra-short laser etc..

From the beginning, the complexity of chemical phenomena that arise during the interaction laser-quantum system has required the introduction of theoretical methods as an important step to 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, that models the evolution of

a quantum system:

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

where $H(t)$ is an Hermitian operator, called the Hamiltonian and Ψ 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 [23]. Thus, we recover a bilinear form of the Schrödinger equation, formally written:

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

In this case $H(t) = H_0 + \epsilon(t)\mu_1$, where H_0 is the internal Hamiltonian operator, that 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 where 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 e.g. [8,9] and related works).

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

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

Email address: aglachap@princeton.edu (Andreea Grigoriu).

For numerical reasons a finite dimensional setting is considered. The operators will be restrained to a linear space spanned by a 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 notations, i.e. we denote by H_0 , μ_1 and μ_2 , $N \times N$ Hermitian matrices with complex coefficients and by Ψ a N dimensional complex vector. One important problem is to determine efficient laser fields to control quantum systems whose Hamiltonian are defined by (3). For this purpose an analysis of the controllability has to be pursued, i.e. ask if any admissible quantum state can be attained with some admissible laser field. This can be studied via the general accessibility criteria [4,28] based on Lie brackets; more specific results can be found in [31]. A detailed presentation has been made in [7].

Even if positive results of controllability of systems (4) 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, that 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) [19], iterative critical point methods (monotonic algorithms) [20,25,29,34], trajectory tracking or local control procedures [3,6,10,13,17,21,22,24,27,32]. One advantage of this class of methods is that we obtain explicit control fields. Another one 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 [15,21], that 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 [7] for more details): discontinuous feedback and time varying feedback.

Only approximative asymptotic stability results have been proved for this last two situations. This paper focuses on the case of discontinuous feedback obtained for Hamiltonian (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 balance of the paper is as follows: in Section 2 we introduce the main notations, the Lyapunov tracking procedure followed by the presentation of the discontinuous feedback. Then, we study the existence of solutions in the Filippov sense. In Section 3 we analyze the stability. More precisely we prove a LaSalle invariance principle for differential inclusions and an asymptotic stability result for our problem. The last two sections are dedicated to numerical simulations and conclusions.

2 Lyapunov trajectory tracking

2.1 Lyapunov function

We consider equation (1), introduced in the above section, describing the evolution of a N -level quantum system submitted to an external action, with Hamiltonian $H(t)$ given by (3):

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

where the wave function $\Psi = (\Psi_j)_{j=1}^n$ 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 wave functions 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 into account the property we add a fictitious control ω (see also [21]). Hence we will replace the evolution equation (4) by:

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

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 the sequel that the state space is $\mathcal{S}^N(0, 1)$ and the dynamic given by (5) admit two independent controls u 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 $V(\Psi(t))$:

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

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 trajectories of (5).

$$\frac{dV}{dt} = 2u \text{Im}(\langle \mu_1 \Psi(t) | \phi \rangle) + 2u^2 \text{Im}(\langle \mu_2 \Psi(t) | \phi \rangle) + 2(\omega + \lambda) \text{Im}(\langle \Psi(t) | \phi \rangle), \quad (7)$$

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

Then note that if, for example, one takes

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

with k and c strictly positive parameters, one gets

$$dV/dt = -2k(I_1/(1+kI_2))^2 - 2c(\text{Im}(\langle \Psi(t) | \phi \rangle))^2 \leq 0,$$

and thus V is nonincreasing.

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

2.2 Discontinuous feedback

It has been proved that the use of controls defined by (8) is efficient for a particular type of systems. The theoretical result (see Theorem 2.1 in [12]) shows that tracking to ϕ works well when all eigenstates of H_0 , ϕ_2, \dots, ϕ_n , other than ϕ are coupled to ϕ by μ_1 , i.e. $\langle \phi_k, \mu_1 \phi \rangle \neq 0, k = 2, \dots, n$. For the important case when some of the coupling are realized by μ_2 instead and formulas (8) are ineffective. Discontinuous and time varying feedback have been proposed to stabilize the system (see [7]).

The introduction of discontinuous feedback laws is motivated by the formula of the derivative of V with respect to time. We remark that dV/dt reads as the sum of $2(\omega + \lambda) \text{Im}(\langle \Psi(t) | \phi \rangle)$ and a function $U(\epsilon)$:

$$\frac{dV}{dt} = 2U(\epsilon) + 2(\omega + \lambda) \text{Im}(\langle \Psi(t) | \phi \rangle), \quad (9)$$

Here $U(\epsilon) = \epsilon^2 I_2 + \epsilon I_1$ is a second order function of ϵ , with coefficients depending on I_1 and I_2 . Consequently, the condition $dV/dt \leq 0$ depends on the sign of a second order function. Thus, the idea is to divide the space defined by I_1 and I_2 into disjoint regions. To each region we assign different formulas for the control $\epsilon(I_1, I_2)$ so that in any point (I_1, I_2) we have $U(\epsilon) \leq 0$.

To this goal we consider the regions (see Fig. 1):

$$\begin{aligned} A &= \{\Psi \mid I_2(\Psi) < -\sqrt{|I_1|}\}, \\ B &= \{\Psi \mid I_2(\Psi) > \sqrt{|I_1|}\}, \\ C &= \{\Psi \mid -\sqrt{|I_1|} \leq I_2(\Psi) \leq \sqrt{|I_1|}\} \end{aligned} \quad (10)$$

and for $k_1, k_2, c, \delta > 0$ we define the control as follows:

$$\epsilon(I_1(\Psi), I_2(\Psi)) = \begin{cases} k_1 I_2, & \text{in A} \\ 0, & \text{in B} \\ -k_2 I_1/(1+k_2 I_2), & \text{in C} \end{cases} \quad (11)$$

$$\omega = -\lambda - c \text{Im}(\langle \Psi(t) | \phi \rangle).$$

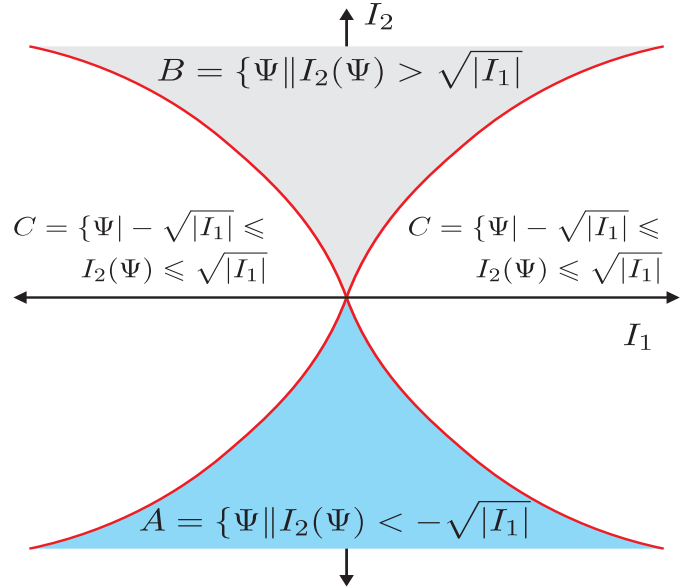


Fig. 1. Schematic view of the regions A, B, C. We consider arbitrary units for I_1 and I_2 .

Remark 2.1 Under some restrictions for k_1 and k_2 that will be introduced later one, the condition $U(\epsilon) \leq 0$ is fulfilled on the region A and C. On region B we have $U(\epsilon) = 0$.

Remark 2.2 In order to guarantee $1 + k_2 I_2 > 0$ in Eqn. (11), one notes that $|I_2| \leq |\langle \mu_2 \Psi(t) | \Psi_T \rangle| \leq \|\mu_2\|$; therefore $1 + k_2 I_2 > 0$ as soon as $k_2 < \frac{1}{\|\mu_2\|}$. From now on, unless otherwise specified, this condition will be supposed satisfied.

We replace the feedback (11) into equation (5) and we obtain a discontinuous right side equation:

$$i \frac{d}{dt} \Psi(t) = \begin{cases} \left(H_0 + k_1 I_2 \mu_1 + (k_1 I_2)^2 \mu_2 - \lambda - c \text{Im}(\langle \Psi(t) | \phi \rangle) \right) \Psi, & \text{in A} \\ (H_0 - \lambda I) \Psi, & \text{in B} \\ \left(H_0 - k_2 \frac{I_1}{1+k_2 I_2} \mu_1 + (k_2 \frac{I_1}{1+k_2 I_2})^2 \mu_2 - \lambda - c \text{Im}(\langle \Psi(t) | \phi \rangle) \right) \Psi, & \text{in C} \end{cases} \quad (12)$$

2.3 Existence of solutions in Filippov sense

For this type of cases before we can discuss the stability we have to study the existence of solutions of the equation (12). One idea is to consider solution in the Filippov sense.

Definition 2.1 Let us consider the equation

$$\dot{x}(t) = f(x(t)) \quad (13)$$

with piecewise discontinuous function $f : D \rightarrow \mathbb{R}^d$, where d is the dimension of the space and $D \subseteq \mathbb{R}^d$ a compact set. We recall that a solution in the Filippov sense of (13) is an locally absolutely continuous map such that:

$$\dot{x} \in \mathcal{F}(x(t)) \quad (14)$$

with

$$\mathcal{F} := \bigcap_{\delta > 0} \bigcap_{\mu(S)=0} \overline{\text{conv}}(f(x + \delta \mathcal{B}) \setminus N) \quad (15)$$

where μ is the Lebesgue measure, S is a arbitrary set of measure zero, $\overline{\text{conv}}(\mathcal{A})$ is the smallest closed convex set containing \mathcal{A} , \mathcal{B} is the unit ball of \mathbb{R}^d and f is a discontinuous function.

In our case a solution in the Filippov sense, Ψ of (12) is locally absolutely continuous map such that:

$$\frac{d}{dt} \Psi \in \mathcal{F}(\Psi(t)) \quad (16)$$

with \mathcal{F} defined by (15) and f given by

$$f(\Psi) = \begin{cases} -i \left(H_0 + k_1 I_2 \mu_1 + (k_1 I_2)^2 \mu_2 - \lambda - c \text{Im}(\langle \Psi(t) | \phi \rangle) \right) \Psi, & \text{in A} \\ -i (H_0 - \lambda I) \Psi, & \text{in B} \\ -i \left(H_0 - k_2 \frac{I_1}{1+k_2 I_2} \mu_1 + (k_2 \frac{I_1}{1+k_2 I_2})^2 \mu_2 - \lambda - c \text{Im}(\langle \Psi(t) | \phi \rangle) \right) \Psi, & \text{in C} \end{cases} \quad (17)$$

The way $\mathcal{F}(\Psi)$ is defined implies that is a nonempty, bounded, closed, convex set and an upper semicontinuous in Ψ as a function. Thus, we are in the hypothesis of Theorem 1 (page 70) in [11]) and the existence of an absolutely continuous function solution of (16) is assured.

3 Stability analysis

3.1 A first stability result

Before we can analyze the stability, it is necessary to define several notions:

Definition 3.1 A solution $\bar{\Psi}$ of the differential inclusion (16) is stable if for each $\epsilon > 0$, there is $\delta = \delta(\epsilon)$ such that if $|\Psi(0) - \bar{\Psi}| < \delta$ then

$$|\Psi(t) - \bar{\Psi}| < \delta, \quad \text{for every } t \geq 0. \quad (18)$$

Definition 3.2 A solution $\bar{\Psi}$ of the differential inclusion (16) is asymptotically stable if is stable and δ can be chosen such that if $|\Psi(0) - \bar{\Psi}| < \delta$ then

$$\lim_{t \rightarrow \infty} (\Psi(t) - \bar{\Psi}) = 0. \quad (19)$$

We can give now a first stability result:

Theorem 3.1 Consider (12) with $\Psi \in \mathcal{S}^N(0, 1)$ a solution in the Filippov sense and an eigenstate $\phi \in \mathcal{S}^N(0, 1)$ of H_0 associated to the eigenvalue λ . Take the constants $k_1 > 1$, $k_2 < \frac{1}{\|\mu_2\|}$ and $c > 0$. The solution $\Psi = \phi$ of the inclusion (16) is stable.

Proof 3.1 Up to a shift on ω and H_0 , we can assume that $\lambda = 0$. Since the function $V(\Psi)$ is C^1 with respect to Ψ , we can define the upper derivate by:

$$\dot{V}^* = \left(\frac{dV}{dt} \right)^* = \sup_{y \in F(\Psi)} (\nabla V \cdot y). \quad (20)$$

For almost all t the derivative $\dot{\Psi}$ exists and satisfies the differential inclusion (16). For these t there exists:

$$\dot{V} = \frac{d}{dt} V(\Psi(t)) = \nabla V \cdot \dot{\Psi}. \quad (21)$$

Theorem 1, page 153 in [11] says that if the condition $\dot{V}^* \leq 0$ is fulfilled then ϕ is a stable point. In order to check the fulfillment of the conditions of the theorem it suffices to make sure that $dV/dt = \partial V \cdot f \leq 0$ only

on the domains of continuity of the function f . In this domains $\mathcal{F}(\Psi) = f(\Psi)$. On the discontinuity points of the function f the set \mathcal{F} is defined as the closure of a convex set. This operation does not increase the upper boundary of the expression $\nabla V \cdot f$ (see [11] for more details). On the interior of the region $B = \{\Psi | I_2(\Psi) > \sqrt{|I_1|}\}$ the control $\epsilon(t)$ is zero, this implies

$$\frac{dV}{dt} = -2c(\text{Im}(\langle \Psi(t) | \phi \rangle))^2 \leq 0. \quad (22)$$

We have the same property on the interior of the region $C = \{\Psi | -\sqrt{|I_1|} \leq I_2(\Psi) \leq \sqrt{|I_1|}\}$, since the control $\epsilon(t)$, is chosen such that:

$$\begin{aligned} \frac{dV}{dt} &= 2 \frac{-k_2 I_1}{1 + k I_2} I_1 + 2 \frac{k_2^2 I_1^2}{(1 + k I_2)^2} I_2 - 2c(\text{Im}(\langle \Psi(t) | \phi \rangle))^2 \\ &= -2k_2 \frac{I_1^2}{(1 + k_2 I_2)^2} - 2c(\text{Im}(\langle \Psi(t) | \phi \rangle))^2 \leq 0, \end{aligned} \quad (23)$$

same conclusion on the interior of the region $A = \{\Psi | I_2(\Psi) < -\sqrt{|I_1|}\}$ since by hypothesis $k_1 > 1$:

$$\begin{aligned} \frac{dV}{dt} &= k_1 I_2 I_1 + k_1^2 I_2^2 I_2 < -k_1 I_1 \sqrt{|I_1|} - k_1 I_2^2 \sqrt{|I_1|} \\ &= -k_1 \sqrt{|I_1|} (I_1 + k_1 I_2^2) \leq 0 \end{aligned} \quad (24)$$

The condition $\dot{V}^* \leq 0$ is fulfilled, thus we can apply here Theorem 1, page 153 in [11], and the conclusion follows.

3.2 Asymptotic stability analysis

In the following in order to prove an asymptotic stability result around the target ϕ we need to introduce first a LaSalle theorem for differential inclusions (14) defined on closed bounded domain $D \subseteq \mathbb{R}^d$. This result is largely inspired by the ones in [2,26]. In [26] Shevitz and Paden prove a LaSalle invariance principle for a class of nonsmooth Lipschitz continuous Lyapunov functions, under the main hypothesis that the solutions of the differential inclusion are uniques. The result in [2] of Bacciotti and Ceragioli is introduced for locally Lipschitz continuous Lyapunov functions $V : \mathbb{R}^d \rightarrow \mathbb{R}$. The statement of the theorem is more general since no assumption about the uniqueness of solutions is required, instead they suppose that the connected component L_l of level sets $\{x \in \mathbb{R}^d : V(x) \leq l\}$, such that $0 \in L_l$, is bounded. Since our differential inclusion is defined on compact domains and the Lyapunov function is continuously differentiable, some of the above hypothesis can be eliminated and we can state a theorem adapted to our context.

Before we can analyze the asymptotic stability, it is necessary to define several notions. Let x be a solution of (14). A point p is called ω limit of $x(t)$ if there exist

a sequence t_n converging to ∞ as $n \rightarrow \infty$, such that $x(t_n) \rightarrow p$ as $n \rightarrow \infty$. The set of all ω -limit points of a solution x of the differential inclusion 14 is called ω -limit set of x and is denoted by $\Omega(x)$.

Definition 3.3 A set M is weekly invariant if though each point $x_0 \in M$ passes a trajectory $x(t)$ of (14) contained in M .

Lemma 3.1 If the set $\mathcal{F}(x)$ is nonempty, bounded, closed, convex and the function F is upper semicontinuous in x , then the ω -limit set $\Omega(x)$ is nonempty, closed, convex and weekly invariant. Moreover if $x(t)$ is contained in a bounded domain $\Omega(x)$ is bounded and $\text{dist}(x, \Omega(x))$ converges to zero as $t \rightarrow \infty$.

Proof 3.2 see [11] page 129.

Now we can give a proof of LaSalle theorem for differential inclusions defined on a compact domain $D \subseteq \mathbb{R}^d$.

Theorem 3.2 We consider the differential inclusion (14) on a compact domain $D \subseteq \mathbb{R}^d$, where the set $\mathcal{F}(x)$ is nonempty, bounded, closed, convex and the function F is upper semicontinuous in x . Let us take $V : D \rightarrow \mathbb{R}$ a continuously differentiable function such that $v \leq 0$ for all $v \in \dot{V}$, where $\dot{V}(x) = \{\nabla V(x) \cdot u, u \in \mathcal{F}(x)\}$, a set $E = \{x \in D | 0 \in \dot{V}\}$ and M be the largest weekly invariant set in \bar{E} . Then every solution of (14) approaches M as $t \rightarrow \infty$ (in the sense of Lemma 3.1).

Proof 3.3 The proof follows the same steps as in Theorem 3.2 and Theorem 3 in [26,2] with a small adaptation, but for convenience we present the whole proof. The properties of F imply the existence of an absolutely continuous functions x , solutions of equation (14). Since V is absolutely continuous, $\frac{d}{dt} V(x(t))$ exists almost everywhere and $\frac{d}{dt} V(x(t)) \in \dot{V}(x)$ almost everywhere. Let us consider $\Omega(x)$ the ω -limit set of x .

Let us first prove that V is constant on $\Omega(x)$. Since the function $V(x(t))$ is absolutely continuous, \dot{V} is bounded from below and V is bounded above zero, $V(x)$ tend to a constant c , as $t \rightarrow \infty$. Let us take $p \in \Omega$, a ω -limit point of $x(t)$, then there exists a sequence t_n tending to ∞ as $n \rightarrow \infty$, such that $x(t_n) \rightarrow p$ as $n \rightarrow \infty$. By continuity of V we have $V(p) = c$.

Let us take now $p \in \Omega(x)$ and φ a solution of (14) lying in $\Omega(x)$ such that $\varphi(0) = p$. Since $V(\varphi(t)) = c$ for all t , $\frac{d}{dt} V(\varphi) = 0$. Therefore $0 \in \dot{V}$ almost everywhere, namely $p \in E$ almost everywhere.

Let $\{t_i\}$, $t_i \rightarrow 0$ be a sequence such that $\varphi(t_i) \in E$ for all i . The function φ is continuous, therefore $\lim_{i \rightarrow \infty} \varphi(t_i) = \varphi(0) = p \in \bar{E}$.

Moreover, since $x(t)$ is contained in a bounded domain we are in the hypothesis of the Lemma (3.1) this implies that $\Omega(x)$ is weakly invariant and $\text{dist}(x, \Omega(x)) \rightarrow 0$, thus $\Omega(x)$ is included in M , and every solution approaches M as $t \rightarrow \infty$.

Example 3.1 Let us consider the differential equation (13), with $f : [-10, 10] \rightarrow \mathbb{R}$ defined by (see Fig. 2):

$$f(x) = \begin{cases} 1, & \text{if } x \in [-10, 0[\\ -1, & \text{if } x \in]0, 10] \end{cases} \quad (25)$$

We want to apply Theorem 3.2 to prove that $x = 0$ is an asymptotically stable point for (13) with f given by (25). Let us consider the solutions in the Filippov sense, i.e. construct the differential inclusion (14) with \mathcal{F} defined by (15) By simple computations we obtain an explicit formula for \mathcal{F} (see Fig. 3):

$$\mathcal{F}(x) = \begin{cases} 1, & \text{if } x \in [-10, 0[\\ [-1, 1], & \text{if } x = 0 \\ -1, & \text{if } x \in]0, 10] \end{cases} \quad (26)$$

We consider the function $V : [-10, 10] \rightarrow \mathbb{R}$ with $V(x) = x^2$. For this example we have:

$$\dot{\bar{V}}(x) = \begin{cases} -x, & \text{if } x \in (0, 10] \\ [-x, x], & \text{if } x = 0 \\ x, & \text{if } x \in [-10, 0] \end{cases} \quad (27)$$

We can easily conclude that the set $E = \{x \in [-10, 10] | 0 \in \bar{V}\}$ contains only $x = 0$, therefore $x = 0$ is asymptotically stable.

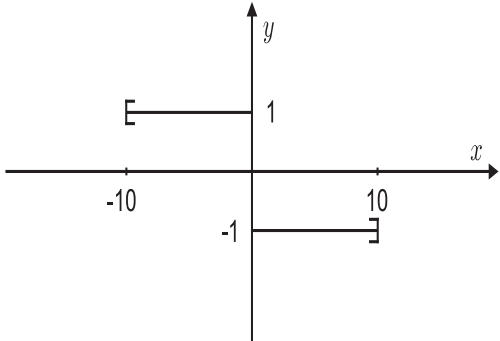


Fig. 2. The function f defined by (25).

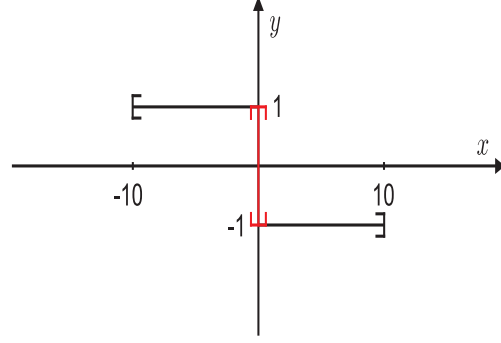


Fig. 3. The inclusion \mathcal{F} defined by (15) associated to the differential equation (14), with f defined by (25)

Remark 3.1 In order to use the previous Lemma (3.1) for the asymptotic stability analysis for the system defined by (12), we need to consider $\Psi = \Psi_R + i\Psi_I$, where Ψ_R is the real part and Ψ_I the imaginary part of Ψ . Therefore in the following by Ψ we understand $\Psi = \begin{pmatrix} \Psi_R \\ \Psi_I \end{pmatrix}$.

Theorem 3.3 Consider (12) with $\Psi \in \mathcal{S}^N(0, 1)$ a solution in the Filippov sense and an eigenstate $\phi \in \mathcal{S}^n(0, 1)$ of H_0 associated to the eigenvalue λ . Take the feedback (11) with $k_1 > 1$, $k_2 < \frac{1}{\|\mu_2\|}$ and $c > 0$. Under the hypothesis:

- (1) $\lambda_j \neq \lambda_l$ for $j \neq l$,
- (2) for any $j = 2, \dots, N$: $\langle \mu_1 \phi_j | \phi \rangle \neq 0$ or $\langle \mu_2 \phi_j | \phi \rangle \neq 0$, where ϕ_1, \dots, ϕ_N is an orthogonal system of eigenvectors of H_0 corresponding to the eigenvalues $(\lambda_i)_{i=1, \dots, N}$,

the ω limit set of $\Psi(t)$ reduces to $\pm\phi$.

Proof 3.4 Up to a shift in ω and H_0 , we may assume that $\lambda = 0$. Theorem (3.2) says that the trajectories of the system (16) converge to the largest weakly invariant set contained in $E = \{\Psi \in D | 0 \in \bar{V}\}$, with V defined by (6).

Let us first compute the differential inclusion \mathcal{F} defined by (15) for the discontinuous function f defined by (12): if $I_2(\Psi) > \sqrt{|I_1|}$ the function f is continuous then

$$\mathcal{F} = -i(H_0 - \lambda I)\Psi. \quad (28)$$

if $-\sqrt{|I_1|} < I_2(\Psi) < \sqrt{|I_1|}$ the function f is continuous thus

$$\mathcal{F} = -i \left(H_0 - k_2 \frac{I_1}{1 + k_2 I_2} \mu_1 + \left(k_2 \frac{I_1}{1 + k_2 I_2} \right)^2 \mu_2 - \lambda - c \text{Im}(\langle \Psi(t) | \phi \rangle) \right) \Psi. \quad (29)$$

if $I_2(\Psi) < -\sqrt{|I_1|}$ the function f is continuous this im-

plies

$$\mathcal{F} = -i \left(H_0 + k_1 I_2 \mu_1 + (k_1 I_2)^2 \mu_2 - \lambda - c \operatorname{Im}(\langle \Psi(t) | \phi \rangle) \right) \Psi. \quad (30)$$

On the contrary on the set $\{\Psi | I_2(\Psi) = \sqrt{|I_1(\Psi)|}\}$ the function f is discontinuous, hence

$$\mathcal{F}(\Psi) = \begin{cases} [b, c], & \text{if } b \leq c \\ [c, b], & \text{if } c \leq b \end{cases} \quad (31)$$

Same property on the set $\{\Psi | I_2(\Psi) = -\sqrt{|I_1(\Psi)|}\}$:

$$\mathcal{F}(\Psi) = \begin{cases} [a, c], & \text{if } a \leq c \\ [c, a], & \text{if } c \leq a, \end{cases} \quad (32)$$

where we have denoted:

$$\begin{aligned} a &= -i \left(H_0 + k_1 I_2 \mu_1 + (k_1 I_2)^2 \mu_2 - \lambda - c \operatorname{Im}(\langle \Psi(t) | \phi \rangle) \right) \Psi, \\ b &= -i(H_0 - \lambda I) \Psi \\ c &= -i \left(H_0 - k_2 \frac{I_1}{1 + k_2 I_2} \mu_1 + (k_2 \frac{I_1}{1 + k_2 I_2})^2 \mu_2 - \lambda - c \operatorname{Im}(\langle \Psi(t) | \phi \rangle) \right) \Psi. \end{aligned} \quad (33)$$

If we take in consideration the computations in the proof of Theorem 3.1 we have:

$$\dot{\mathcal{V}} = \begin{cases} -k_1 I_2 (I_1 + k_1 I_2^2), & \text{if } I_2 < -\sqrt{|I_1|} \\ -2k_2 \frac{I_1^2}{(1+k_2 I_2)^2} - 2c(\operatorname{Im}(\langle \Psi(t) | \phi \rangle))^2, & \text{if } -\sqrt{|I_1|} < I_2 < \sqrt{|I_1|} \\ -2c(\operatorname{Im}(\langle \Psi(t) | \phi \rangle))^2, & \text{if } I_2 > \sqrt{|I_1|} \end{cases} \quad (34)$$

On the contrary on the discontinuity set $\{\Psi | I_2(\Psi) = \sqrt{|I_1(\Psi)|}\}$ we use relation (31) and we obtain:

$$\dot{\mathcal{V}} = \begin{cases} [e, g], & \text{if } e \leq g \\ [g, e], & \text{if } g \leq e \end{cases} \quad (35)$$

In the same way, on the set $\{\Psi | I_2(\Psi) = -\sqrt{|I_1(\Psi)|}\}$,

considering relation (32) and we have:

$$\dot{\mathcal{V}} = \begin{cases} [f, g], & \text{if } f \leq g \\ [g, f], & \text{if } g \leq f, \end{cases} \quad (36)$$

where:

$$\begin{aligned} e &= -k_1 I_2 (I_1 + k_1 I_2^2), \\ f &= -2c(\operatorname{Im}(\langle \Psi(t) | \phi \rangle))^2 \\ g &= -2k_2 \frac{I_1^2}{(1+k_2 I_2)^2} - 2c(\operatorname{Im}(\langle \Psi(t) | \phi \rangle))^2. \end{aligned} \quad (37)$$

Since $(I_1 + k_1 I_2^2) > 0$, it follows that the limit set is characterized by:

$$I_1 = 0, \quad I_2 = 0, \quad \operatorname{Im}(\langle \Psi(t) | \phi \rangle) = 0, \quad (38)$$

and therefore $\epsilon = 0$.

This implies that the set E consists in fact of trajectories of the uncontrolled system:

$$i \frac{d}{dt} \Psi = H_0 \Psi. \quad (39)$$

with solutions having the form:

$$\Psi = \sum_{j=1}^n b_j e^{-i\lambda_j t} \phi_j. \quad (40)$$

We substitute (40) in (38) and we obtain:

$$\begin{aligned} \operatorname{Im}(\langle \Psi(t) | \phi \rangle) &= \operatorname{Im}(b_1) \langle \phi, \phi \rangle + \sum_{j=2}^n \operatorname{Im}(b_j \langle \phi_j, \phi \rangle) e^{-i\lambda_j t} \\ &= 0. \end{aligned} \quad (41)$$

$$\begin{aligned} I_1(\Psi) &= \operatorname{Im}(b_1) \langle \mu_1 \phi, \phi \rangle + \sum_{j \in J_1} \operatorname{Im}(b_j \langle \mu_1 \phi_j, \phi \rangle) e^{-i\lambda_j t} \\ &= 0. \end{aligned} \quad (42)$$

$$\begin{aligned} I_2(\Psi) &= \operatorname{Im}(b_1) \langle \mu_2 \phi, \phi \rangle + \sum_{k \in J_2} \operatorname{Im}(b_k \langle \mu_2 \phi_k, \phi \rangle) e^{-i\lambda_k t} \\ &= 0. \end{aligned} \quad (43)$$

Without loss of generality we take $\phi = \phi_1$. From equation (38) and (41), together with $\langle \phi_j, \phi \rangle = 0$ for all $j = 2, \dots, n$ we obtain $\operatorname{Im}(b_1) = 0$. Since along the trajectories Ψ in $\Omega(\Psi)$, $I_1(\Psi) \equiv 0$, we have

$\sum_{j \in J_1} \text{Im}(b_j \langle \mu_1 \phi_j, \phi \rangle e^{-i\lambda_j t}) = \sum_{j \in J_1} B'_j \sin(\lambda_j t + \theta_j) = 0$. The functions $\sin(\lambda_j t + \theta_j)$ are linearly independent as the λ_j are all different, hence the sum can only vanish if all coefficients B'_j vanish. Observe now that $B'_j = 0, j \in J_1$ if and only if $b_j = 0, j \in J_1$. Using $\text{Im}(b_1) = 0$ we have:

$$\begin{aligned} I_2(\Psi) &= \sum_{j \in J_2} \text{Im}(b_j \langle \mu_2 \phi_j, \phi \rangle e^{-i\lambda_j t}) \\ &= \sum_{j \in J_2} B_j \sin(\lambda_j t + \theta_j). \end{aligned} \quad (44)$$

Since $I_2(\Psi) = 0$, for every t , it follows from the same arguments as above that $b_j = 0$ for $j = 2, \dots, n$. Now considering the form of the limit trajectories (40) this leaves only $\Psi = b_1 e^{-i\lambda t} \phi = b_1 \phi$ (we assumed $\lambda = 0$). Since $\text{Im}(b_1) = 0$ the only case remained is $\Psi = \pm \phi$. This concludes the proof of Theorem 3.3.

4 Numerical simulations

We consider next the five-dimensional system (see [30]) defined by:

$$\begin{aligned} H_0 &= \begin{pmatrix} 1.0 & 0 & 0 & 0 & 0 \\ 0 & 1.2 & 0 & 0 & 0 \\ 0 & 0 & 1.3 & 0 & 0 \\ 0 & 0 & 0 & 1.4 & 0 \\ 0 & 0 & 0 & 0 & 2.15 \end{pmatrix}, \\ \mu_1 &= \begin{pmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{pmatrix}, \mu_2 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}. \end{aligned} \quad (45)$$

In Fig. 4 simulations describe the evolution of the population of the trajectory $\Psi = (\Psi_1, \Psi_2, \dots, \Psi_5)$, for the initial state $\Psi(t=0) = (0, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4})$. We take $k_1 = 1.1, k_2 = c = 0.8$. We remark that the discontinuous laser field (11) is efficient to reach the first eigenstate $\phi = (1, 0, 0, 0, 0)$ of energy $\lambda = 1$, at the final time T . Note that here $\|\mu_2\| = 1$.

The Fig. 5 describe the evolution of the Lyapunov function defined by (6).

5 Conclusions

We study in this paper the control of Schrödinger equation. The particularity of the problem is that the interaction between the system and the laser is not described

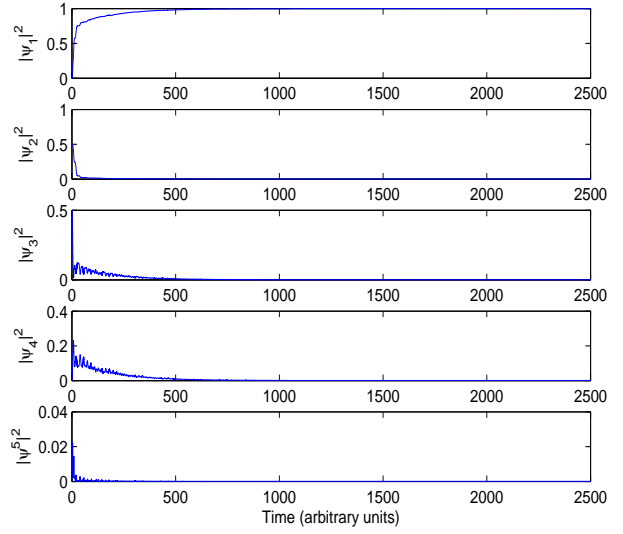


Fig. 4. The population of the system (45) with trajectory $\Psi = (\Psi_1, \Psi_2, \dots, \Psi_5)$; initial condition: $\Psi(t=0) = (0, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4})$; the feedback is defined by (11), with $k_1 = 1.1, k_2 = c = 0.8$.

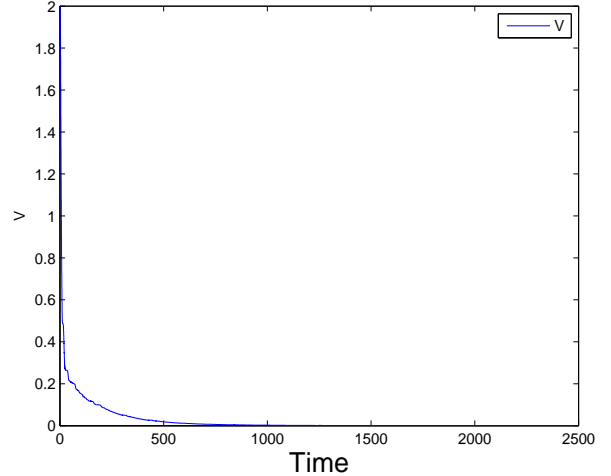


Fig. 5. Evolution of the Lyapunov function $V(\Psi)$ defined by (6); initial condition: $\Psi(t=0) = (0, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4})$; system defined by (45) with feedback (11). We take $k_1 = 1.1, k_2 = c = 0.8$.

just by a first order term $\epsilon(t)\mu_1$, but also by a second order, polarizability term $\epsilon^2(t)\mu_2$. In a previous work, in order to find a control field that exploits the polarizability coupling, two different solutions have been proposed. The first one is to use a discontinuous feedback with memory terms, the other is to use time-dependent (periodic) forcing. For both cases only approximative stability results have been proved. The present paper studies the discontinuous case and focuses on obtaining asymptotic stability. To this end solutions in the Filippov sense

are considered and a LaSalle type result is introduced for differential inclusions on closed, bounded sets. Related numerical simulations are also presented.

References

- [1] A. Assion, T. Baumert, M. Bergt, T. Brixner, B. Kiefer, V. Seyfried, M. Strehle, and G. Gerber. Control of chemical reactions by feedback-optimized phase-shaped femtosecond laser pulses. *Science*, 282:919–922, 1998.
- [2] A. Baciotti and F. Ceragioli. Stability and stabilization of discontinuous systems and nonsmooth Lyapunov functions. *ESIAM*, 4:361–376, 1999.
- [3] K. Beauchard, J.-M. Coron, M. Mirrahimi, and P. Rouchon. Implicit Lyapunov control of finite dimensional Schrödinger equations. *Systems Control Lett.*, 56(5):388–395, 2007.
- [4] R. Brockett. Lie theory and control systems defined on spheres. *SIAM J. Appl. Math.*, 25(2):213–225, 1973.
- [5] P. Brumer and M. Shapiro. Coherent chemistry: Controlling chemical reactions with lasers. *Acc. Chem. Res.*, 22:407, 1989.
- [6] Y. Chen, P. Gross, V. Ramakrishna, H. Rabitz, and K. Mease. Competitive tracking of molecular objectives described by quantum mechanics. *J. Chem. Phys.*, 102:8001–8010, 1995.
- [7] J.-M. Coron, A. Grigoriu, C. Lefter, and G. Turinici. Quantum control design by lyapunov trajectory tracking for dipole and polarizability coupling. *New Journal of Physics*, 11(10):105034 (22pp), 2009.
- [8] C.M. Dion, A.D. Bandrauk, O. Atabek, A. Keller, H. Umeda, and Y. Fujimura. Two-frequency IR laser orientation of polar molecules. Numerical simulations for HCN. *Chem. Phys. Lett.*, 302:215–223, 1999.
- [9] C.M. 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(2):1382, 1999.
- [10] A. Ferrante, M. Pavon, and G. Raccanelli. Control of quantum systems using model-based feedback strategies. In *Proc. of the International Symposium MTNS'2002*, 2002.
- [11] A. F. Filippov. *Differential Equations with Discontinuous Righthand Sides*. Kluwer Academic Publishers, 2009.
- [12] A. Grigoriu, C. Lefter, and G. Turinici. Lyapunov control of Schrödinger equations: beyond the dipole approximation. In *Proceedings of the 28th MIC IASTED Conference, Innsbruck, Austria, Feb. 16–18*, pages 119–123, 2009. retrieved August 10th 2009 from <http://hal.archives-ouvertes.fr/hal-00364966/>.
- [13] S. Grivopoulos and B. Bamieh. Lyapunov-based control of quantum systems. In *Proceedings of the 42nd IEEE Conference on Decision and Control*, volume 1, pages 434–438, 2003.
- [14] R.S. Judson and H. Rabitz. Teaching lasers to control molecules. *Phys. Rev. Lett.*, 1992.
- [15] V. Jurdjevic and J.P. Quinn. Controllability and stability. *J. Diff. Eq.*, 28:381–389, 1978.
- [16] K. Kompa, M. Motzkus, H. Rabitz, and R. de Vivie-Riedle. Whither the future of controlling quantum phenomena? *Science*, 288:824–828, 2000.
- [17] R. Kosloff, S.A. Rice, P. Gaspard, S. Tersigni, and D.J. Tannor. Wavepacket dancing: Achieving chemical selectivity by shaping light pulses. *Chem. Phys.*, 139:201–220, 1989.
- [18] R. J. Levis, G.M. Menkir, and H. Rabitz. Selective bond dissociation and rearrangement with optimally tailored, strong-field laser pulses. *Science*, 292:709–713, 2001.
- [19] B. Li, G. Turinici, V. Ramakrishna, and H. Rabitz. Optimal dynamic discrimination of similar molecules through quantum learning control. *J. Phys. Chem. A*, 106:8125–8131, 2002.
- [20] Y. Maday and G. Turinici. New formulations of monotonically convergent quantum control algorithms. *J. Chem. Phys.*, 118(18), 2003.
- [21] M. Mirrahimi, P. Rouchon, and G. Turinici. Lyapunov control of bilinear Schrödinger equations. *Automatica*, 41:1987–1994, 2005.
- [22] M. Mirrahimi, G. Turinici, and P. Rouchon. Reference trajectory tracking for locally designed coherent quantum controls. *J. Phys. Chem. A*, 109(11):2631–2637, 2005.
- [23] H. Rabitz, S. Shi, and A. Woody. Optimal control of selective vibrational excitation in harmonic linear chain molecules. *J. Chem. Phys.*, 88:6870–6883, 1988.
- [24] H. Rabitz and W. Zhu. Quantum control design via adaptive tracking. *J. Chem. Phys.*, 119(7), 2003.
- [25] S. Schirmer, M. Girardeau, and J. Leahy. Efficient algorithm for optimal control of mixed-state quantum systems. *Phys. Rev. A*, 61:012101, 2000.
- [26] D. Shevitz and B. Paden. Lyapunov stability theory of nonsmooth systems. *IEEE Transactions on Automatic Control*, 39(9):1910–1914, September 1994.
- [27] M. Sugawara. General formulation of locally designed coherent control theory for quantum systems. *J. Chem. Phys.*, 118(15):6784–6800, 2003.
- [28] H.J. Sussmann and V. Jurdjevic. Controllability of nonlinear systems. *J. Diff. Eq.*, 12:95–116, 1972.
- [29] D. Tannor, V. Kazakov, and V. Orlov. Control of photochemical branching: Novel procedures for finding optimal pulses and global upper bounds. In Broeckhove J. and Lathouwers L., editors, *Time Dependent Quantum Molecular Dynamics*, pages 347–360. Plenum, 1992.
- [30] S. H. Tersigni, P. Gaspard, and S.A. Rice. On using shaped light pulses to control the selectivity of product formation in a chemical reaction: An application to a multiple level system. *J. Chem. Phys.*, 93(3):1670–1680, 1990.
- [31] G. Turinici. Beyond bilinear controllability: applications to quantum control. In *Control of coupled partial differential equations*, volume 155 of *Internat. Ser. Numer. Math.*, pages 293–309. Birkhäuser, Basel, 2007. Retrieved August 10th 2009 from <http://hal.archives-ouvertes.fr/hal-00311267/>.
- [32] P. Vettori. On the convergence of a feedback control strategy for multilevel quantum systems. In *Proc. of the International Symposium MTNS'2002*, 2002.
- [33] T.C. Weinacht, J. Ahn, and P.H. Bucksbaum. Controlling the shape of a quantum wavefunction. *Nature*, 397:233–235, 1999.
- [34] W. Zhu and H. Rabitz. Uniform rapidly convergent algorithm for quantum optimal control of objectives with a positive semi-definite Hessian matrix. *Phys. Rev. A.*, 58:4741–4748, 1998.