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Implicit Lyapunov control for Schrödinger equations with dipole and polarizability term

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Abstract— **We analyze in this paper finite dimensional closed quantum systems in interaction with a laser field. The characteristic of the problem is that the interaction laser-system is modeled by a first order term (dipole coupling) and a second order term (polarisability coupling), that appear in the Hamiltonian of the Schrödinger equation. In order to determine the control, an implicit Lyapunov trajectory tracking procedure is applied when there is no direct coupling between the target state and the eigenvectors of the internal hamiltonian. The method is applied for the difficult case of degenerate systems too. The controlled Lyapunov function is defined by an implicit equation and its existence is shown by a fix point theorem. The convergence is analysed using the LaSalle invariance principle. The performance of the feedbacks is illustrated by numerical simulations.**

I. INTRODUCTION

The control of molecules dynamics at the quantum level is a core issue for numerous applications. This is why quantum control constitutes today a very active research field, both from the theoretical and experimental point of view ([2], [5], [17], [38] etc.). Before presenting the issues addressed in this paper, we first introduce the time-dependent Schrödinger equation, which models the time-evolution of a finite dimensional closed quantum system under the influence of a laser field:

$$i\frac{d}{dt}\Psi(t) = (H_0 + \epsilon(t)\mu_1 + \epsilon^2(t)\mu_2)\Psi(t), \qquad (1)$$

where H_0, μ_1 and μ_2 are $N \times N$ Hermitian matrices with complex entries. The wavefunction Ψ is a vector in $\mathbb{C}^N$, satisfying $\sum_{j=1}^{N} |\Psi_j|^2 = 1$, thus it lives on the unit sphere $\mathcal{S}^N(0,1)$ of $\mathbb{C}^N$ and $\epsilon(t) \in \mathbb{R}$ is the control (for example the laser intensity).

The term $H(t) = H_0 + \epsilon(t)\mu_1 + \epsilon^2(t)\mu_2$ is the Hamiltonian of the system and H_0 is the internal Hamiltonian. This last one characterizes the system in the absence of the laser. The matrices μ_1 and μ_2 describe the interaction of the quantum system with the laser field. This type of model is used when the first order term, $\epsilon(t)\mu_1$, also called dipole coupling [26] does not have enough influence on the system to reach the control goal; the goal may become accessible only after adding the polarizability term $\epsilon^2(t)\mu_2$ (see e.g. [9], [10] and related works).

One of the problems that must be clarified for the non-linear control equation (1) is to find if a final time T and a laser pulse $\epsilon(t)$ exist such that $\epsilon(t)$ is able to steer the system from an initial state Ψ_0 to some arbitrary predefined target $\Psi(t = T) = \Psi_{target}$. If the answer to this question is positive the systems is called controllable. Positive results of controllability are obtained by applying the Lie algebra criteria [4], [33] and especially the specific result in [36]. This study is detailed in [8].

The theoretical results of controllability do not offer automatically a method to determine the laser field. Very often this task is formulated as a cost functional to be minimized. Several techniques have been developed in this direction: iterative critical point methods (e.g. monotonic algorithms [16], [23], [24], [25], [19], [34], [29], [30], [39]), iterative stochastic techniques (e.g., genetic algorithms [37]), trajectory tracking methods or local control procedures [6], [12], [15], [18], [31], [22], [32], [21], [3], [20].

For control quantum systems evolving according to equation (1), Lyapunov trajectory tracking techniques [1], [7], [27] have been applied. One of the advantages of these approaches is that an explicit formula for the laser field is obtained. The method consists in defining a function V, which is nonnegative and vanishes when $\Psi = \Psi_{target}$:

$$V(\Psi, t) = \langle \Psi - \Psi_{target} | \Psi - \Psi_{target} \rangle = \|\Psi - \Psi_{target}\|^2, \qquad (2)$$

where $\langle .|. \rangle$ denotes the Hermitian product and Ψ_{target} a reference trajectory of (1). Imposing the condition $dV/dt \leqslant 0$, V has the properties of a Lyapunov function and we obtain an explicit formula for the control.

In order to make sure that the target Ψ_{target} will be reached using the laser thus obtained a convergence analysis must be provided. An initial positive result of asymptotic stability has been proved in [11] under the hypothesis:

$\mathcal{H}_1$: H_0 is non degenerate i.e.: $\lambda^i \neq \lambda^j$, $\forall\, i, j \in \{1, ..., N\}$ with $i \neq j$; $(\lambda^i)_{i=1,2,...,N}$ are the eigenvalues of H_0

$\mathcal{H}_2$: direct coupling, through μ_1, between the target state ϕ (first eigenvector of H_0 associated to the eigenvalue $\lambda \in \mathbb{R}$; $H_0\phi = \lambda\phi$) and **all** other eigenvectors i.e.: $\langle \mu_1 \phi^j | \phi \rangle \neq 0$, for every $j \in \{2, .., N\}$; $\phi, \phi_2, ..., \phi_N$ form an orthonormal system of eigenvectors of H_0, corresponding to the eigenvalues $(\lambda^i)_{i=1,2,...,N}$

The explicit formula for the control, that proves to be efficient for the above cases is

$$\epsilon = -kI_1/(1 + kI_2) \qquad (3)$$

with k a constant that belongs to $]0, \frac{1}{\|\mu_2\|}[$, $\mathrm{I}_1 = \mathrm{Im}\langle \mu_1 \Psi | \phi \rangle$

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and $\mathrm{I}_2 = \mathrm{Im}\langle\mu_2\Psi|\phi\rangle$ (see [11], [8]). When some of the (direct) coupling is realized by μ_2 instead of μ_1 i.e:

$\mathcal{H}_3$: $\langle\mu_1\phi^j|\phi\rangle \neq 0$ or $\langle\mu_2\phi^j|\phi\rangle \neq 0$, for every $j \in \{2,..,N\}$

the previous feedback (3) is not efficient anymore. Numerical tests in [11], [8] show that the target it is not reached, the systems gets trapped into an unknown state. In order to take into consideration the problems that appear, two alternatives have been proposed: discontinuous feedback and time varying feedback (see [8] for more details). These allow to approximately asymptotically stabilize the system around the target ϕ.

There are systems for which the target ϕ is not directly connected by μ_1 or μ_2 with all the other eigenvectors and we are not longer in the hypothesis $\mathcal{H}_2$ or $\mathcal{H}_3$. An example is provided by the following 5-level quantum system [35] with the matrices H_0, μ_1 and μ_2 defined by:

$$H_0 = \begin{pmatrix} 1.0 & 0 & 0 & 0 & 0 \\ 0 & 1.2 & 0 & 0 & 0 \\ 0 & 0 & 1.3 & 0 & 0 \\ 0 & 0 & 0 & 1.4 & 0 \\ 0 & 0 & 0 & 0 & 2.15 \end{pmatrix},$$

$$\mu_1 = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{pmatrix}, \mu_2 = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \end{pmatrix}. \quad (4)$$

In Fig. 1, we represent the diagram of the coupling achieved by μ_1 and μ_2 between the eigenvectors of the internal Hamiltonian H_0 of the system (4). One can note that the first eigenvector $\phi_1 = \phi = (1, 0, ..., 0)$ is directly coupled only with ϕ_4 and ϕ_5 ($\langle\mu_1\phi|\phi_4\rangle \neq 0, \langle\mu_1\phi|\phi_5\rangle \neq 0$). There is no direct coupling by μ_1 or μ_2 with ϕ_2 and ϕ_3. In this case the target is $\phi = (1, 0, 0, 0, 0)$.

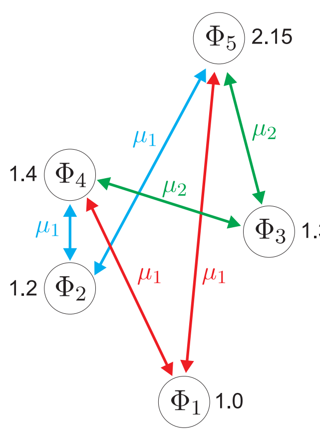

Fig. 1. Schematic view of the coupling realized by the matrices μ_1 and μ_2 defined by (4) between the first eigenvector ϕ of the internal Hamiltonian H_0 and all the other eigenvectors $\phi_2, ..., \phi_5$. The eigenvectors are represented by circles and next to each of them the corresponding energy level $(H_0)_{ii}$, $i = 1, ..., 5$ are written. The coupling are represented by edges, each of them being labelled with the corresponding matrix that achieves the coupling.

Another category of systems is the one with degenerate internal Hamiltonian (hypothesis $\mathcal{H}_1$ is not fulfilled). The common characteristic of all these systems is that there are still controllable and this constitutes a very strong motivation to their study. In this context the main goal of this paper is to introduce a Lyapunov trajectory tracking technique that permits to determine efficient laser fields for this cases too. To this end we will adapt the implicit Lyapunov method introduced in [3] for bilinear cases $H(t) = H_0 + \epsilon(t)\mu_1$.

The general idea is to track a mobile target ϕ_β, instead of a fixed target ϕ, where β implicitly depends on the state of the system Ψ. As we impose a slow convergence of ϕ_β to ϕ, we stabilize faster the state of the system around the vector ϕ_β applying a Lyapunov method as the one described by relation (2). This should guarantee that the system is stabilized around ϕ (see Fig. 2) and it does not get trapped into another unknown state.

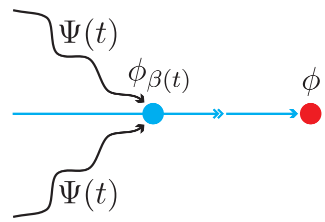

Fig. 2. Schematic view of the slow convergence of ϕ_β toward the target ϕ and a faster convergence of Ψ towards the mobile target ϕ_β.

The balance of the paper is as follows: in section II, we present the implicit Lyapunov technique. An existence result for the implicit Lyapunov function is proved followed by the convergence of the stabilization technique. Section III addresses the case of a degenerate target state. Finally, in section IV, we perform some numerical simulations for a five-dimensional test case followed by conclusions.

II. Implicit Lyapunov trajectory tracking

A. Lyapunov function

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 fictitiouss control ω (see also [21]). Hence we replace the evolution equation (1) by:

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

where $\omega \in \mathbb{R}$ is a new control . We can choose it arbitrarily without changing the physical quantities attached to Ψ.

In the following, for a given $\beta \in \mathbb{R}$, we denote by $(\lambda_\beta^j)_{1\leqslant j\leqslant N}$ the eigenvalues of the matrix $H(\beta) = H_0 + \beta\mu_1 + \beta^2\mu_2$, and by $(\phi_\beta^j)_{1\leqslant j\leqslant N}$ the associated normalized eigenvectors:

$$(H_0 + \beta\mu_1 + \beta^2\mu_2)\phi_\beta^j = \lambda_\beta^j\phi_\beta^j. \quad (6)$$

For simplicity we denote $\phi_\beta = \phi_\beta^1$ and $\lambda_\beta = \lambda_\beta^1$

We introduce the function $V(\Psi)$ defined by (2) with $\Psi_{target} = \phi_{\beta(\Psi)}$:

$$V(\Psi, t) = \langle\Psi - \phi_{\beta(\Psi)}|\Psi - \phi_{\beta(\Psi)}\rangle = \|\Psi - \phi_{\beta(\Psi)}\|^2 \quad (7)$$

where the function $\Psi \to \beta(\Psi)$ is implicitly defined as below:

$$\beta(\Psi) = \Gamma(\|\Psi - \phi_{\beta(\Psi)}\|^2). \tag{8}$$

The properties of the function Γ are formulated in the following lemma in order to assure the existence of function β.

Lemma 2.1: Suppose that hypothesis $\mathcal{H}_1$ holds and consider a continuously differentiable function $\Gamma : \mathbb{R}^+ \to [0, \beta^*]$ satisfying :

$$\begin{aligned} \Gamma(0) &= 0,\ \Gamma(s) > 0 \text{ for every s} > 0 \\ \|\Gamma'\|_\infty &< \frac{1}{8C}, \end{aligned} \tag{9}$$

with

$$C = 1 + \max\left\{ \left\| \left(\frac{d\phi_\beta}{d\beta}\right)\Big|_{\beta=\beta_0} \right\|;\ \beta_0 \in [0, \beta^*] \right\}, \tag{10}$$

where ϕ_β is the first eigenvector of the matrix $H(\beta)$ and $\left(\frac{d\phi_\beta}{d\beta}\right)\Big|_{\beta=\beta_0}$ is the derivative of ϕ_β at the point $\beta = \beta_0$.

Then there exists a unique map $\beta \in C^\infty(\mathcal{S}^N(0,1); [0, \beta^*])$, such that for every $\Psi \in \mathcal{S}^N(0,1)$:

$$\beta(\Psi) = \Gamma(\|\Psi - \phi_{\beta(\Psi)}\|^2) \text{ with } \beta(\phi) = 0. \tag{11}$$

Proof: The proof follows the ideas of [3] but needs a minor adaptation to take into account the second order control term $\epsilon^2(t)\mu_2$ and the different definition of the Lyapunov function (2). For completeness we give however the full proof below.

Since we made the assumption that all the eigenvalues of the internal Hamiltonian H_0 are different, we are in the settings of Theorem XII.1 and Theorem XII.4 of [28]. This implies that the eigenvalue and the eigenvectors of the matrix $H(\beta)$ are analytic functions of β and

$$\mathcal{H}_4 :\quad \lambda_\beta^j \neq \lambda_\beta^l \text{ for j} \neq \text{l},\ \text{j}, \text{l} = 1, ..., \text{N}. \tag{12}$$

in the interval $[0, \beta^*]$. Since ϕ_β is analytic the derivative $\frac{d\phi_\beta}{d\beta}$ exists for every point $\beta_0 \in [0, \beta^*]$, and is bounded on $[0, \beta^*]$. This implies:

$$C = 1 + \max\left\{ \left\| \left(\frac{d\phi_\beta}{d\beta}\right)\Big|_{\beta=\beta_0} \right\|,\ \beta_0 \in [0, \beta^*] \right\} < \infty. \tag{13}$$

- Uniqueness of function β.

In order to prove the uniqueness of the function β let us consider the function Γ defined by:

$$\beta \longmapsto \Gamma(\|\Psi - \phi_{\beta(\Psi)}\|^2)$$

with $\beta \in [0, \beta^*]$. For every β_1 and β_2 from $[0, \beta^*]$, there exists $\overline{\beta} \in]\beta_1, \beta_2[$ such that:

$$\begin{aligned} &\Gamma(\|\Psi - \phi_{\beta_1(\Psi)}\|^2) - \Gamma(\|\Psi - \phi_{\beta_2(\Psi)}\|^2) = \\ &\left(\frac{d}{d\beta}\Gamma(\|\Psi - \phi_{\beta(\Psi)}\|^2)\right)\Big|_{\beta=\overline{\beta}}\Big(\beta_1 - \beta_2\Big). \end{aligned} \tag{14}$$

Since

$$\begin{aligned} &\frac{d}{d\beta}\Gamma(\|\Psi - \phi_{\beta(\Psi)}\|^2) = \\ &-2\Gamma'(\|\Psi - \phi_{\beta_1(\Psi)}\|^2) Re\Big(\langle \frac{d\phi_\beta}{d\beta} | \Psi - \phi_\beta \rangle\Big) \end{aligned} \tag{15}$$

and $|Re(\langle \frac{d\phi_\beta}{d\beta} | \Psi \rangle)| \leq |\langle \frac{d\phi_\beta}{d\beta} | \Psi \rangle| \leq \|(\frac{d\phi_\beta}{d\beta})|_{\beta=\beta_0}\|$, together with $\|\Gamma'\| < \frac{1}{8C}$ we obtain that the function $\Gamma(\|\Psi - \phi_{\beta(\Psi)}\|^2)$ is contracting for fixed $\Psi \in \mathcal{S}^N(0,1)$. Thus, for any fixed $\Psi \in \mathcal{S}^N(0,1)$ there exists a unique $\beta(\Psi) \in [0, \beta^*]$ that verifies (8).

- Existence of function β.

In order to prove the existence of β, let us consider:

$$F(\Psi, \beta) = \beta - \Gamma(\|\Psi - \phi_{\beta(\Psi)}\|^2). \tag{16}$$

This application is C^∞ with respect to Ψ and β, and for fixed $\Psi \in \mathcal{S}^N(0,1)$ we have:

$$F(\Psi, \beta(\Psi)) = 0. \tag{17}$$

Moreover from relation (15) we have:

$$\frac{d}{d\beta}F(\beta, \Psi) = 1 + 2\Gamma'(\|\Psi - \phi_{\beta(\Psi)}\|^2) Re\Big(\langle \frac{d\phi_\beta}{d\beta} | \Psi - \phi_\beta \rangle\Big), \tag{18}$$

which is non zero since $\|\Gamma'\| < \frac{1}{8C}$, with C defined by (10) on the interval $[0, \beta^*]$. We are in the hypothesis of the implicit function theorem, this implies the existence of the application $\Psi \to \beta(\Psi)$ that belongs to $C^\infty(\mathcal{S}^N(0,1); [0, \beta^*])$. ■

Now, we can focus on finding feedback controls such that V is a Lyapunov function. To this end we compute the derivative of V along trajectories of (5) and impose the condition $dV/dt \leq 0$. We have:

$$\begin{aligned} \frac{dV}{dt} &= 2(\epsilon - \beta)\mathrm{Im}(\langle \mu_1 \Psi(\mathrm{t}) | \phi_\beta \rangle) + \\ &\quad 2(\epsilon^2 - \beta^2)\mathrm{Im}(\langle \mu_2 \Psi(\mathrm{t}) | \phi_\beta \rangle) + \\ &\quad 2(\omega + \lambda_\beta)\mathrm{Im}(\langle \Psi(\mathrm{t}) | \phi_\beta \rangle) - \\ &\quad 2\dot{\beta}\mathrm{Re}\Big(\langle \frac{\mathrm{d}\phi_\beta}{\mathrm{d}\beta} | \Psi - \phi_\beta \rangle\Big), \end{aligned} \tag{19}$$

where Im denotes the imaginary part and Re the real part. For convenience we denote: $\mathrm{I}_1^\beta = \mathrm{Im}(\langle \mu_1 \Psi(\mathrm{t}) | \phi_\beta \rangle)$ and $\mathrm{I}_2^\beta = \mathrm{Im}(\langle \mu_2 \Psi(\mathrm{t}) | \phi_\beta \rangle)$.

A simple computation leads to:

$$\begin{aligned} \dot{\beta} &= \Gamma'(V)\Big\{ 2(\epsilon - \beta)\mathrm{I}_1^\beta + 2(\epsilon^2 - \beta^2)\mathrm{I}_2^\beta + \\ &\quad 2(\omega + \lambda_\beta)\mathrm{Im}(\langle \Psi(\mathrm{t}) | \phi_\beta \rangle) - \\ &\quad 2\dot{\beta}\mathrm{Re}\Big(\langle \frac{\mathrm{d}\phi_\beta}{\mathrm{d}\beta} | \Psi - \phi_\beta \rangle\Big)\Big\}. \end{aligned} \tag{20}$$

It follows that:

$$\begin{aligned} \dot{\beta} &= \frac{\Gamma'(V)((\epsilon - \beta)\mathrm{I}_1^\beta + (\epsilon^2 - \beta^2)\mathrm{I}_2^\beta}{1 + 2\Gamma'(V)\mathrm{Re}\Big(\langle \frac{\mathrm{d}\phi_\beta}{\mathrm{d}\beta} | \Psi - \phi_\beta \rangle\Big)} + \\ &\quad \frac{2(\omega + \lambda_\beta)\mathrm{Im}(\langle \Psi(\mathrm{t}) | \phi_\beta \rangle))}{1 + 2\Gamma'(V)\mathrm{Re}\Big(\langle \frac{\mathrm{d}\phi_\beta}{\mathrm{d}\beta} | \Psi - \phi_\beta \rangle\Big)}. \end{aligned} \tag{21}$$

Remark 2.1: Since $\Gamma'(V) < 1/(8C^*)$ with C^* defined by (10) we have:

$$1 + 2\Gamma'(V)\mathrm{Re}\Big(\langle \frac{\mathrm{d}\phi_\beta}{\mathrm{d}\beta} | \Psi - \phi_\beta \rangle \neq 0, \tag{22}$$

moreover

$$\|2\Gamma'(V)\mathrm{Re}\Big(\langle\frac{\mathrm{d}\phi_\beta}{\mathrm{d}\beta}|\Psi-\phi_\beta\rangle\|\Big)<\frac{1}{2}. \qquad (23)$$

If we replace relation (20) in (19) we obtain:

$$\begin{aligned}\frac{dV}{dt} &= 2((\epsilon-\beta)\mathrm{I}_1^\beta+(\epsilon^2-\beta^2)\mathrm{I}_2^\beta+\\ &\quad 2(\omega+\lambda_\beta)\mathrm{Im}(\langle\Psi(\mathrm{t})|\phi_\beta\rangle))\times\Big(1-\frac{\mathrm{g(t)}}{1+\mathrm{g(t)}}\Big)\end{aligned} \qquad (24)$$

with

$$g(t)=2\Gamma'(V)\mathrm{Re}\Big(\langle\frac{\mathrm{d}\phi_\beta}{\mathrm{d}\beta}|\Psi-\phi_\beta\rangle\Big). \qquad (25)$$

From Remark 2.1 we have $1-\frac{g(t)}{1+g(t)}\geqslant 0$. If we denote $v=\epsilon-\beta$ and we take:

$$\begin{cases} v=-k(\mathrm{I}_1^\beta+2\beta\mathrm{I}_2^\beta)/(1+\mathrm{k}\mathrm{I}_2^\beta)\\ \omega=-\lambda_\beta-c\mathrm{Im}(\langle\Psi(\mathrm{t})\mid\phi_\beta\rangle),\end{cases} \qquad (26)$$

with k and c strictly positive parameters, one gets $dV/dt\leq 0$, i.e. V is nonincreasing. Thus we obtain the following feedback control:

$$\begin{aligned}\epsilon &= \beta-k(\mathrm{I}_1^\beta+2\beta\mathrm{I}_2^\beta)/(1+\mathrm{k}\mathrm{I}_2^\beta)\\ \omega &= -\lambda_\beta-c\mathrm{Im}(\langle\Psi(\mathrm{t})\mid\phi_\beta\rangle).\end{aligned} \qquad (27)$$

Remark 2.2: To guarantee that the denominator $1+k\mathrm{I}_2^\beta>0$, one notes that $|\mathrm{I}_2^\beta|\leq|\langle\mu_2\Psi(\mathrm{t})|\Psi_\beta\rangle|\leq\|\mu_2\|$; therefore $1+k\mathrm{I}_2^\beta>0$ as soon as $k<\frac{1}{\|\mu_2\|}$. From now on, unless otherwise specified, this condition will be assumed.

B. Convergence analysis

In the following we prove the convergence of the trajectories Ψ of the system (5) toward the target ϕ. The idea is to use that the feedback presented previously (27) for Hamiltonian $H(t)=H_0+\beta\mu_1+\beta^2\mu_2$ assures the convergence towards the set $\mathcal{Z}_\beta=\{\phi_\beta\}$ for every $\beta\in]0,\beta^*]$. So we let β tending to zero and by construction the convergence towards $\mathcal{Z}_\beta$ must be faster than the convergence of β towards zero.

Theorem 2.1: Assume that the hypothesis $\mathcal{H}_1$ and $\mathcal{H}_5$ hold, where

$$\begin{aligned}\mathcal{H}_5: \quad & \text{denote } \mathrm{J}_1=\{\mathrm{j}|\mathrm{j}\neq 1,\langle\mu_1\phi_\beta^\mathrm{j}|\phi_\beta\rangle)\neq 0\}\\ & \text{and } \mathrm{J}_2=\{\mathrm{j}|\mathrm{j}\neq 1,\langle\mu_2\phi_\beta^\mathrm{j}|\phi_\beta\rangle)\neq 0\},\\ & J_1\cup J_2=\{2,3,\ldots,n\} \text{ and } \mathrm{J}_1\cap\mathrm{J}_2=\emptyset \text{ on } [0,\beta^*].\end{aligned}$$

Consider (5) with $\Psi\in\mathcal{S}^N(0,1)$ and an eigenvector $\phi\in\mathcal{S}^N(0,1)$ of H_0 associated to the eigenvalue λ. If we take the feedback (27) with $k<\frac{1}{\|\mu_2\|}$ and $c>0$, then the limit set of $\Psi(t)$ is reduced to $\pm\phi$.

Proof: Up to a shift on ω and H_0, we may assume that $\lambda=0$. Since hypothesis $\mathcal{H}_1$ holds we can apply Theorem XII.1 of [28]. This implies that hypothesis $\mathcal{H}_5$ is fulfilled.

LaSalle's principle (see, e.g., [14, Theorem 3.4, page 115]) guarantees that the trajectories of the system (5) converge to the largest invariant set contained in $dV/dt=0$, this implies that V is constant, i.e. $V(\Psi)=\widetilde{V}$. Since by definition $\beta=\Gamma(V)$, $\beta(\Psi)$ is constant i.e. $\beta=\beta_c$.

The equation $dV/dt=0$ means that:

$$\mathrm{I}_1^\beta+2\beta_\mathrm{c}\mathrm{I}_2^\beta=0,\ \mathrm{Im}(\langle\Psi(\mathrm{t})|\phi_{\beta_\mathrm{c}}\rangle)=0, \qquad (28)$$

Since the Ω-limit set is also invariant under the flow generated by (5) it follows, taking into account (28), that this set consists in fact of trajectories of the system:

$$i\frac{d}{dt}\Psi=(H_0+\beta_c\mu_1+\beta_c^2\mu_2)\Psi. \qquad (29)$$

The solutions of (29) have the form:

$$\Psi=\sum_{j=1}^N b_j e^{-it\lambda_{\beta_c}^j}\phi_{\beta_c}^j. \qquad (30)$$

The eigenvectors $(\phi_{\beta_c}^j)_{j\in\{1,\ldots,N\}}$ of $H(\beta_c)=H_0+\beta_c\mu_1+\beta_c^2\mu_2$ can be chosen to form an orthonormal basis. Moreover, the orthonormal eigenvectors are holomorphic functions of β_c (see [13], page 121).

If $\beta_c=0$ we have $\Gamma(\widetilde{V})=0$ which implies $\widetilde{V}=0$. In this case the limit set of Ψ only contains ϕ.

If $\beta_c\neq 0$, on the contrary we substitute relation (30) into relation (28) and we obtain:

$$\begin{aligned}\mathrm{Im}(\langle\Psi(\mathrm{t})|\phi_{\beta_c}\rangle) &= \mathrm{Im}(\mathrm{b}_1)\langle\phi_{\beta_\mathrm{c}},\phi_{\beta_\mathrm{c}}\rangle+\\ &\quad \sum_{j=2}^N\mathrm{Im}(\mathrm{b_j}\langle\phi_{\beta_\mathrm{c}}^\mathrm{j},\phi_{\beta_\mathrm{c}}\rangle\mathrm{e}^{-\mathrm{it}\lambda_{\beta_\mathrm{c}}^\mathrm{j}}).\\ &= 0.\end{aligned} \qquad (31)$$

and

$$\begin{aligned}\mathrm{I}_1^\beta+2\beta_\mathrm{c}\mathrm{I}_2^\beta &= \mathrm{Im}(\mathrm{b}_1)\langle\mu_1\phi_{\beta_\mathrm{c}},\phi_{\beta_\mathrm{c}}\rangle+\\ &\quad \sum_{j\in J_1}\mathrm{Im}(\mathrm{b_j}\langle\mu_1\phi_{\beta_\mathrm{c}}^\mathrm{j},\phi_{\beta_\mathrm{c}}\rangle\mathrm{e}^{-\mathrm{it}\lambda_{\beta_\mathrm{c}}^\mathrm{j}})\\ &\quad +2\beta_\mathrm{c}\Big(\mathrm{Im}(\mathrm{b}_1)\langle\mu_2\phi_{\beta_\mathrm{c}},\phi_{\beta_\mathrm{c}}\rangle+\\ &\quad \sum_{k\in J_2}\mathrm{Im}(\mathrm{b_j}\langle\mu_2\phi_{\beta_\mathrm{c}}^\mathrm{j},\phi_{\beta_\mathrm{c}}\rangle\mathrm{e}^{-\mathrm{it}\lambda_{\beta_\mathrm{c}}^\mathrm{j}})\Big)\\ &= 0.\end{aligned} \qquad (32)$$

From equation (31), together with $\langle\phi_{\beta_c}^j,\phi_{\beta_c}\rangle=0$ for all $j=2,...,N$ we obtain that $\mathrm{Im}(\mathrm{b}_1)=0$. Moreover, equation (32) becomes:

$$\begin{aligned}\mathrm{I}_1^\beta+2\beta_\mathrm{c}\mathrm{I}_2^\beta &= \sum_{j\in J_1}\mathrm{Im}(\mathrm{b_j}\langle\mu_1\phi_{\beta_\mathrm{c}}^\mathrm{j},\phi_{\beta_\mathrm{c}}\rangle\mathrm{e}^{-\mathrm{it}\lambda_{\beta_\mathrm{c}}^\mathrm{j}}),\\ &\quad +2\beta_c\sum_{k\in J_2}\mathrm{Im}(\mathrm{b_j}\langle\mu_2\phi_{\beta_\mathrm{c}}^\mathrm{j},\phi_{\beta_\mathrm{c}}\rangle\mathrm{e}^{-\mathrm{it}\lambda_{\beta_\mathrm{c}}^\mathrm{j}})\\ &= 0.\end{aligned} \qquad (33)$$

We use hypothesis $\mathcal{H}_5$ together with $\beta_c\neq 0$ and we obtain $b_j=0$ for every $j\in J$ (see [8] for more details). This implies that the limit set only contains $\pm\phi_{\beta_c}$. We let β_c tend to zero and conclusion follows.

■

III. Degenerate cases

For systems with degenerate internal Hamiltonian positive numerical tests have been performed using discontinuous and time varying controls obtained by applying "explicit" Lyapunov tracking techniques (see [8]). Under more restrictive hypothesis than for non degenerate cases convergence might be obtained. The advantage of applying an implicit Lyapunov technique is that adding a small perturbation of the form $\beta\mu_1 + \beta^2\mu_2$, with $\beta \in [0, \beta^*]$ the degeneracy of H_0 is withdrawn and a asymptotic stability result as the one in Theorem 2.1 is obtained. Moreover we conserve the same type of hypothesis as in the non-degenerate case.

Theorem 3.1: Assume that the hypothesis $\mathcal{H}_4$ and $\mathcal{H}_5$ hold. Consider (5) with $\Psi \in \mathcal{S}^N(0,1)$ and an eigenvector $\phi \in \mathcal{S}^N(0,1)$ of H_0 associated to the eigenvalue λ. If we take the feedback (27) with $k < \frac{1}{\|\mu_2\|}$ and $c > 0$, then the limit set of $\Psi(t)$ reduces $\pm\phi$.

Proof: It follows the same steps as in Theorem 2.1. ■

Before being able to apply Theorem 3.1, some details have to be discussed. In the above section the space generated by any eigenvector of the internal Hamiltonian H_0 is always of dimension one. Therefore we were tracking without loss of generality the first eigenvector ϕ of H_0. This is no longer the case for a degenerate situation. We may try to stabilize the system around an arbitrary eigenvector ϕ_k, which can generate a space of dimension larger than 1. As a consequence, first we need to recall a result from the perturbation theory for finite dimensional Hermitian operators ([13], page 121).

Lemma 3.1: Let us consider the $N \times N$ dimensional complex matrices H_0, μ_1, μ_2 and let us take

$$H(\beta) = H_0 + \beta\mu_1 + \beta^2\mu_2. \quad (34)$$

For each real β, there exists an orthonormal basis $(\phi_n(\beta))_{n\in\{1,\dots,N\}}$ of $\mathbb{C}^N$ consisting of eigenvectors of $H(\beta)$. Moreover, the orthonormal eigenvectors can be chosen as holomorphic functions of β.

In order to track any eigenvector ϕ^k of a degenerate matrix H_0 it is enough to consider $\Psi_{target} = \phi^k_\beta$ in definition (2) of the function V, where ϕ^k_β is defined in the above lemma. Since ϕ^k_β is continuously differentiable its derivative $d\phi^k_\beta/d\beta$ is bounded on the interval $[0, \beta^*]$ and the existence and uniqueness of $\beta(\Psi)$ is guaranteed.

IV. Numerical simulations

We consider next the five-dimensional system (see [35]) defined by (4). We use the Lyapunov control (27) in order to reach the first eigenvector $\phi = (1,0,0,0,0,0)$ of energy $\lambda = 1$, at the final time T. Note that $\|\mu_2\| = 1$.

The function β is defined by (8) with $\Gamma(x) = 0.75x$. Even if $\Gamma(x)$ doesn't satisfy the hypothesis $\|\Gamma'\|_\infty < \frac{1}{8C}$ of lemma 2.1, the convergence of β towards zero takes place (see Fig. 4, right image). This happens because the condition is much stronger than the one required by the numerical simulations. Simulations of Figure 3 describe the evolution of the population of the trajectory $\Psi = (\Psi_1, \Psi_2, \dots, \Psi_5)$, for the initial state $\Psi(t=0) = (1,1,1,1,1)/\sqrt{5}$. We take $c = 0.8$. Simulations of Fig. 4, left figure describe the evolution of the Lyapunov function defined by (7) and the right figure the evolution of the function β. The evolution of the control ϵ defined by (27) is described in Fig. 5.

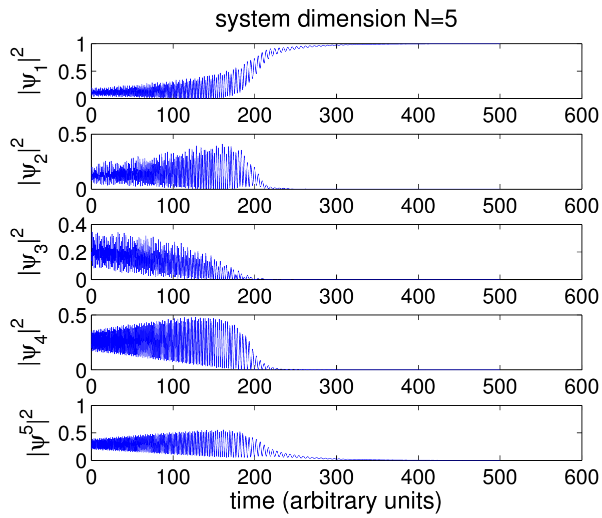

Fig. 3. The populations corresponding to system (4) with trajectory $\Psi = (\Psi_1, \Psi_2, \dots, \Psi_5)$; initial condition: $\Psi(t=0) = (1,1,1,1,1)\sqrt{5}$; the feedback is defined by (27)($c = 0.8$, $k = 0.02$)

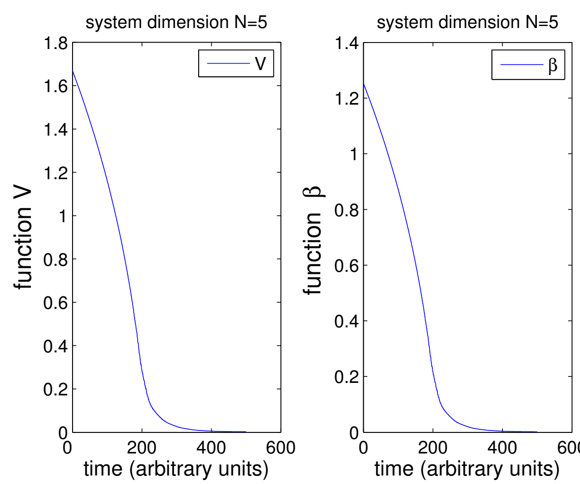

Fig. 4. Left: evolution of the Lyapunov function V; Right: evolution of the function β; initial condition: $\Psi(t=0) = (1,1,1,1,1)\sqrt{5}$; system defined by (4) with feedback (27)($c = 0.8$, $k = 0.02$).

V. Conclusions

In this paper we study implicit Lyapunov trajectory tracking procedures for closed quantum systems submitted to an external interaction, a laser field. The interaction between the system and the laser is described by a first order term $\epsilon(t)\mu_1$ and a second order term consisting in a polarizability term $\epsilon^2(t)\mu_2$. More precisely the hamiltonian of the Schrodinger equation that models the evolution is equal to $H_0 + \epsilon\mu_1 + \mu_2\epsilon^2$, with H_0 the internal Hamiltonian.

The goal is to determine efficient controls for two types of controllable systems. For the first type there is not direct

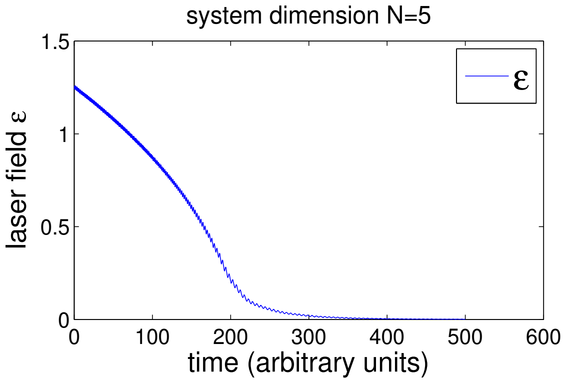

Fig. 5. Evolution of control ϵ ; initial condition: $\Psi(t=0) = (1,1,1,1,1)\sqrt{5}$; system defined by (4) with feedback (27)($c=0.8$,$k=0.02$).

coupling between the target state and all the eigenvectors on the internal hamiltonian H_0 This corresponds in the bilinear setting $H_0+\epsilon\mu_1$ with the non controllability of the linearized system. The second one is characterized by non degenerate internal Hamiltonian. A description of the method, a convergence result together with numerical simulations are presented.

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