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# LYAPUNOV CONTROL OF SCHRÖDINGER EQUATIONS: BEYOND THE DIPOLE APPROXIMATION

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## ABSTRACT

We analyse in this paper the Lyapunov trajectory tracking of the Schrödinger equation for a second order coupling operator. We present a theoretical convergence result; for situations not covered by the theoretical result we propose a numerical approach that is tested and works well in practice.

## KEY WORDS

Quantum control, Control Lyapunov function, Numerical simulations, Stabilization.

## 1 Introduction

Controllability of a finite dimensional quantum system,  $i\frac{d}{dt}\Psi(t) = (H_0 + u(t)H_1 + u^2(t)H_2)\Psi(t)$ , where  $H_0, H_1$  and  $H_2$  are  $n \times n$  Hermitian matrices with complex coefficients and  $u(t) \in \mathbb{R}$  is the control, can be studied via the general accessibility criteria proposed in [2, 17] and based on Lie brackets; more specific results can be found in [18]. However, such characterization does not provide in general a simple and efficient way for open-loop trajectory generation. Optimal control techniques (see, e.g., [11] and [15] and the references therein) provide a first set of methods. Another set consists in using feedback to generate trajectories and open-loop steering control. The original references on such feedback strategy to find open-loop controls are [3, 7, 10]. More recent results can be found in [13] for decoupling techniques, in [5, 6, 16, 19, 20] for Lyapunov-based techniques and in [1, 4, 14] for factorizations techniques of the unitary group.

In order to study systems with Hamiltonian  $H = H_0 + uH_1 + u^2H_2$  we adapt the corresponding analysis initially proposed for bilinear quantum systems i.e  $H = H_0 + uH_1$  (see [8, 12]). We use here a fictitious control  $\omega$  (see [12]) to take into account the physically meaningless global phase and to simplify convergence analysis. Our method is valid to track any eigen-state trajectory of a Schrödinger equation for a second order coupling operator.

The balance of the paper is as follows: in Section 2 we introduce the main notations and the Lyapunov tracking feedback for a particular case. Section 3 contains a convergence analysis followed in Section 4 by numerical results

and the presentation of a new type of feedback for all types of second order coupling operators.

## 2 Tracking feedback design

### 2.1 Dynamics and global phase

We consider a  $n$ -level quantum system ( $\hbar = 1$ ) evolving under the equation:

$$i\frac{d}{dt}\Psi(t) = (H_0 + u(t)H_1 + u^2(t)H_2)\Psi(t), \quad (1)$$

where  $H_0, H_1$  and  $H_2$  are  $n \times n$  Hermitian matrices with complex coefficients and  $u(t) \in \mathbb{R}$  is the control. The matrix  $H_0$  is the internal Hamiltonian,  $H_1$  and  $H_2$  are operators that couple the system with the laser field  $u$ . The wave function  $\Psi = (\Psi_i)_{i=1}^n$  is a vector in  $\mathbb{C}^n$ , verifying  $\sum_{i=1}^n |\Psi_i|^2 = 1$  thus it lives on the unit sphere of  $\mathbb{C}^n$ ,  $\Psi \in \mathbb{S}^{2n-1}$ . Physically,  $\Psi$  and  $e^{i\theta(t)}\Psi$  describe the same physical state for any global phase  $t \mapsto \theta(t) \in \mathbb{R}$ , i.e  $\Psi_1$  and  $\Psi_2$  are identified when exists  $\theta \in \mathbb{R}$  such that  $\Psi_1 = \exp(i\theta)\Psi_2$ . To take into account such non trivial geometry we add a second control  $\omega$  corresponding to  $\dot{\theta}$  (see also [12]). Thus we consider the following control system

$$i\frac{d}{dt}\Psi(t) = (H_0 + u(t)H_1 + u^2(t)H_2 + \omega(t))\Psi(t), \quad (2)$$

where  $\omega \in \mathbb{R}$  is a new control playing the role of a gauge degree of freedom. We can choose it arbitrarily without changing the physical quantities attached to  $\Psi$ . With such additional fictitious control  $\omega$ , we will assume in the sequel that the state space is  $\mathbb{S}^{2n-1}$  and the dynamics given by (2) admits two independent controls  $u$  and  $\omega$ .

### 2.2 Lyapunov control design

Take a reference trajectory  $t \mapsto (\Psi_r(t), u_r(t), \omega_r(t))$ , i.e., a smooth solution of (2):

$$i\frac{d}{dt}\Psi_r = (H_0 + u_r H_1 + u_r^2 H_2 + \omega_r)\Psi_r.$$

Take the following time varying function  $V(\Psi, t)$ :

$$V(\Psi, t) = \langle \Psi - \Psi_r | \Psi - \Psi_r \rangle \quad (3)$$

where  $\langle \cdot | \cdot \rangle$  denotes the Hermitian product. The function  $V$  is positive for all  $t > 0$  and all  $\Psi \in \mathbb{S}^{2n-1}$  and vanishes when  $\Psi = \Psi_r$ . Simple computations show that  $V$  is a control Lyapunov function when  $\Psi$  satisfies (2). The derivative of  $V$  is given by:

$$\begin{aligned} \frac{dV}{dt} = & 2(u - u_r)Im(\langle H_1\Psi(t) | \Psi_r \rangle) + \\ & 2(u^2 - u_r^2)Im(\langle H_2\Psi(t) | \Psi_r \rangle) + \\ & 2(\omega - \omega_r)Im(\langle \Psi(t) | \Psi_r \rangle) \end{aligned} \quad (4)$$

where  $Im$  denotes the imaginary part.

For simplicity reasons we note:  $I_1 = Im(\langle H_1\Psi(t) | \Psi_r \rangle)$  and  $\tilde{I}_2 = Im(\langle H_2\Psi(t) | \Psi_r \rangle)$ . When for instance we take:

$$\begin{aligned} u &= u_r(t) - k(I_1 + 2u_r\tilde{I}_2)/(1 + k\tilde{I}_2) \\ \omega &= \omega_r(t) - cIm(\langle \Psi(t) | \Psi_r \rangle), \end{aligned} \quad (5)$$

with  $k$  and  $c$  strictly positive parameters, we ensure  $dV/dt \leq 0$ , i.e.  $V$  is decreasing.

Let us focus on the important case when the reference trajectory corresponds to an equilibrium:  $u_r = 0$ ,  $\omega_r = -\lambda$  and  $\Psi_r = \phi$  where  $\phi$  is an eigen-vector of  $H_0$  associated to the eigenvalue  $\lambda \in \mathbb{R}$  ( $H_0\phi = \lambda\phi$ ,  $\|\phi\| = 1$ ). We note:  $I_1 = Im(\langle H_1\Psi(t) | \phi \rangle)$  and  $I_2 = Im(\langle H_2\Psi(t) | \phi \rangle)$ . Then (5) becomes a static-state feedback:

$$\begin{aligned} u &= -kI_1/(1 + kI_2) \\ \omega &= -\lambda - cIm(\langle \Psi(t) | \phi \rangle). \end{aligned} \quad (6)$$

### 3 Convergence analysis

The goal of this section is to prove a convergence result for the feedback in equation (6). We denote by  $\lambda_i$ , with  $i = 1, \dots, N$  the eigenvalues of the matrix  $H_0$ . We say that  $H_0$  has non degenerate spectrum if for all  $(i, j)$ , with  $i \neq j$ ,  $i, j = 1, \dots, N$ ,  $\lambda_i \neq \lambda_j$ .

**Theorem 3.1** Consider (2) with  $\Psi \in \mathbb{S}^{2n-1}$  and an eigenstate  $\phi \in \mathbb{S}^{2n-1}$  of  $H_0$  associated to the eigenvalue  $\lambda$ . Take the static feedback (6) with  $c, k > 0$ . Then the two following propositions are true:

1. If the spectrum of  $H_0$  is not degenerate, the  $\Omega$ -limit set of the closed loop system is the intersection of  $\mathbb{S}^{2n-1}$  with the vector space  $E = \mathbb{R}\phi \cup_{\alpha} \mathbb{C}\Phi_{\alpha}$  where  $\Phi_{\alpha}$  is any eigenvector of  $H_0$  not co-linear to  $\phi$  such that  $\langle \Phi_{\alpha} | H_1 | \phi \rangle = 0$ .
2. If  $H_0$  is not degenerate and  $E = \mathbb{R}\phi$ , the  $\Omega$ -limit set reduces to  $\{\phi, -\phi\}$ .

#### Proof of Theorem 3.1

The proof follows the same ideas as in [12] and needs only a small adaptation to take into account this second order control situation. We give however for completeness the full proof below.

1. Up to a shift on  $\omega$  and  $H_0$ , we can assume that  $\lambda = 0$ . LaSalle's principle (see, e.g., theorem 3.4, page 115 of [9]) says that the trajectories of the closed-loop system converge to the largest invariant set contained in  $dV/dt = 0$  where  $V$  is defined by (3). The equation  $dV/dt = 0$  means that

$$I_1 = Im(\langle H_1\Psi | \phi \rangle) = Im(\langle \Psi | \phi \rangle) = 0,$$

Thus  $u = 0$  and  $\omega = 0$ . Invariance implies that  $\frac{d}{dt}\Psi = H_0\Psi$ ,  $\frac{d}{dt}Im(\langle H_1\Psi | \phi \rangle) = 0$  and  $\frac{d}{dt}Im(\langle \Psi | \phi \rangle) = 0$ . Clearly  $\frac{d}{dt}Im(\langle \Psi | \phi \rangle) = 0$  does not give any additional information since  $H_0\phi = 0$ . Only  $\frac{d}{dt}Im(\langle H_1\Psi | \phi \rangle) = 0$  provides a new independent equation:  $Re(\langle H_1H_0\Psi | \phi \rangle) = 0$  that reads

$$Re(\langle [H_0, H_1]\Psi | \phi \rangle) = 0,$$

where  $Re$  denotes the real part. Similarly  $\frac{d}{dt}Re(\langle [H_0, H_1]\Psi | \phi \rangle) = 0$  implies:

$$Im(\langle [H_0, [H_0, H_1]]\Psi | \phi \rangle) = 0.$$

And so on. Finally, the largest invariant set is characterized by  $Im(\langle \Psi | \phi \rangle) = 0$  with the following conditions:

$$\begin{aligned} Im(\langle H_1\Psi | \phi \rangle) &= 0 \\ Re(\langle [H_0, H_1]\Psi | \phi \rangle) &= 0 \\ Im(\langle [H_0, [H_0, H_1]]\Psi | \phi \rangle) &= 0, \\ &\dots \end{aligned}$$

that corresponds to the “ad-conditions” obtained in [8]. At each step, we have the Lie bracket of the Hamiltonian  $H_0$  with the Hamiltonian of the last step.

We can always assume that  $H_0$  is diagonal. Then we can easily compute the commutator  $[H_0, B]$ , where  $B = (B_{ij})$  is a  $n$  dimensional matrix. With  $H_0 = \text{diag}(\lambda_1, \dots, \lambda_n)$ , we have

$$[H_0, B]_{i,j} = (\lambda_i - \lambda_j)B_{ij}.$$

Let us take  $B = H_1$  in order to simplify the notations. We obtain the following system:

$$\begin{aligned} [H_0, B] &= ((\lambda_i - \lambda_j)B_{ij}), \\ [H_0, [H_0, B]] &= ((\lambda_i - \lambda_j)^2 B_{ij}), \\ &\vdots \\ \underbrace{[H_0, \dots, [H_0, B]]}_{k \text{ times}} &= ((\lambda_i - \lambda_j)^k B_{ij}), \end{aligned} \quad (7)$$

After simple computations the system (7) reads:

$$\begin{aligned}
\operatorname{Im}(\Sigma_j B_{1j} \Psi_j) &= 0, \\
\operatorname{Re}(\Sigma_j (\lambda_1 - \lambda_j) B_{1j} \Psi_j) &= 0, \\
&\vdots \\
\operatorname{Im}(\Sigma_j (\lambda_1 - \lambda_j)^{2k} B_{1j} \Psi_j) &= 0, \\
\operatorname{Re}(\Sigma_j (\lambda_1 - \lambda_j)^{2k+1} B_{1j} \Psi_j) &= 0, \\
&\dots
\end{aligned} \tag{8}$$

Using the Vandermonde structure and the property of non-degenerate spectrum of  $H_0$ , we obtain that the wave function  $\Psi$  is in the  $\Omega$ -limit set if and only if

$$B_{1j} \Psi_j = 0, \forall j \in \{2, \dots, n\},$$

and  $\operatorname{Im}(\Psi_1) = 0$ .

- Note first that in any case the  $\Omega$ -limit set contains  $\phi$  and  $-\phi$ , because both are stationary points.

If  $H_0$  has a non-degenerate spectrum and  $E = \mathbb{R}\phi$  then proposition (1) implies that the  $\Omega$ -limit set contains the states  $\lambda\phi$  with  $\lambda \in \mathbb{R}$  and  $\|\lambda\phi\|_{L^2} = 1$  which reduces to  $\{\pm\phi\}$ .

**Remark 3.1** The theorem above shows that tracking e.g to  $\phi_1$  works when all states  $\phi_2, \dots, \phi_n$  are coupled to  $\phi_1$  by  $H_1$ . However we do not know what happens when some of the coupling are realized by  $H_2$  instead (the theorem does not apply but the system is still controllable cf. [18]). We analyze such a case in section 4.

## 4 Examples and Simulations

Numerical simulations have been performed for a three-dimensional test system with  $H_0$ ,  $H_1$  and  $H_2$  given by:

$$\begin{aligned}
H_0 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{3}{2} \end{pmatrix}, \quad H_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
H_2 &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}.
\end{aligned} \tag{9}$$

In this case the wave function is  $\Psi = (\Psi_1, \Psi_2, \Psi_3)^T$ . We use the previous Lyapunov control in order to reach the first eigen-state  $\phi = (1, 0, 0)$  of energy  $\lambda = 0$ , at the final time  $T$ .

The equation (2) is solved with the numerical scheme:

$$\begin{aligned}
\psi((m+1)\Delta t) &= \exp(-i\Delta t(H_0 + u(m\Delta t)H_1 \\
&\quad + u^2(m\Delta t)H_2))\psi(m\Delta t), \tag{10}
\end{aligned}$$

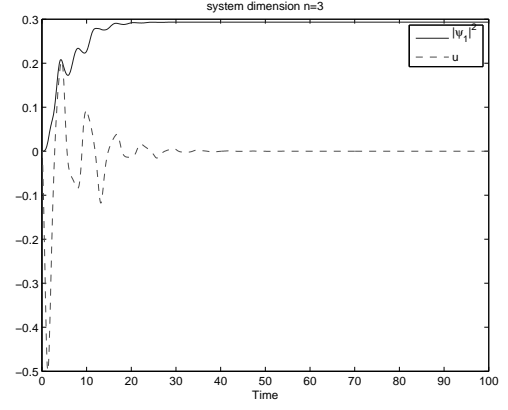


Figure 1. Population  $|\Psi_1|^2$  (solid line) and control  $u$  (dashed line); initial condition  $\Psi(t=0) = (0, 1/\sqrt{2}, 1/\sqrt{2})$ ; system defined by (9) with feedback (6). The feedback (6) fails to reach the target (quality is only 30%).

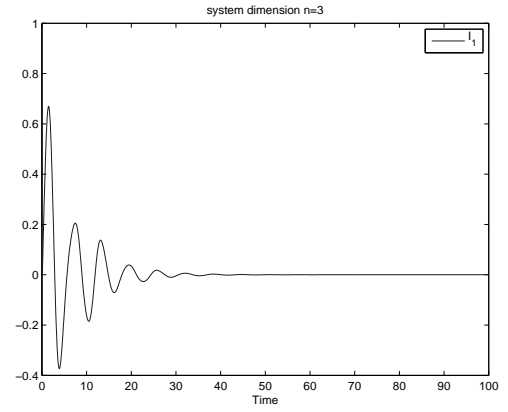


Figure 2. Time evolution of  $I_1$ ; system defined by (9) with feedback (6). We note that  $I_1$  converges to zero.

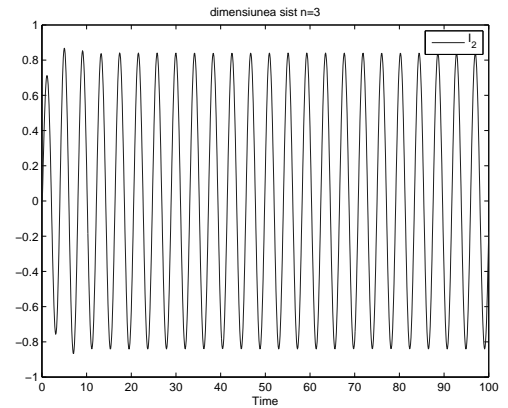


Figure 3. Time evolution of  $I_2$ ; system defined by (9) with feedback (6). Contrary to  $I_1$ ,  $I_2$  does not converge to zero.

where  $m$  is the index of the time step and  $\Delta t = T/m$  is the discretization time step. The control  $u$  is defined by (6) with  $k = c = 1/2$ .

Simulations of Figure 1 start with  $(0, 1/\sqrt{2}, 1/\sqrt{2})$  as initial condition for  $\Psi$ . We clearly see that such a feedback reduces the distance to the first state but does not ensure its convergence to  $\phi = (1, 0, 0)$ . This is not due to a lack of controllability. This system is controllable since the Lie algebra spanned by  $(H_0)/i$ ,  $H_1/i$  and  $H_2/i$  coincides with  $u(3)$ , (see [12]). As explained in Remark 3.1, such convergence deficiency comes from the fact that operator  $H_1$  couples  $\phi$  only with the state  $\Psi_2$ . We plot the evolution of  $|\Psi_1|^2$ ,  $I_1$  and  $I_2$ , corresponding to system defined by (9) with feedback (6), in Figure 1, Figure 2 and Figure 3.

In order to overcome the lack of convergence for cases similar to that presented above, we consider the feedback:

$$u(I_1, I_2) = \begin{cases} kI_2, & \text{if } |I_1| < \delta \text{ and } I_2 < -\delta \\ 0, & \text{if } |I_1| < \delta \text{ and } I_2 > \delta \\ -kI_1/(1 + kI_2), & \text{in any other case.} \end{cases}$$

$$\omega = -\lambda - cIm(\langle \Psi(t) | \phi \rangle). \quad (11)$$

We plot in Figure 7 the function  $u(I_1, I_2)$  for  $\delta = 0.5$ . Note that with  $c > 0$ ,  $k > 0$  and  $\delta > 0$  we ensure:  $dV/dt \leq 0$ , i.e  $V$  is decreasing.

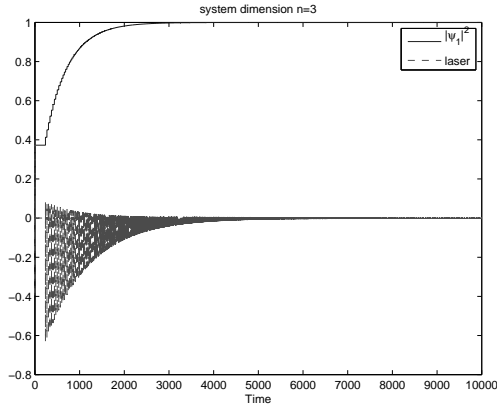


Figure 4. Population  $|\Psi_1|^2$  (solid line) and control  $u$  (dashed line); initial condition:  $\Psi(t = 0) = (0, 1/\sqrt{2}, 1/\sqrt{2})$ ; system defined by (9) with feedback (11).

Simulations of Figure 4 describe the evolution of population  $|\Psi_1|^2$  for the initial state  $\Psi(t = 0) = (0, 1/\sqrt{2}, 1/\sqrt{2})$ . We take  $k = c = 0.8$  and  $\delta = e^{-t/b}$ , with  $b = 1000$ . We can observe that the trajectories converge to  $\phi$ . It appears that the new type of feedback is quite efficient for system (9). We present the evolution of  $I_1$  and  $I_2$  corresponding to system defined by (9) with feedback (11), in Figure 5 and Figure 6.

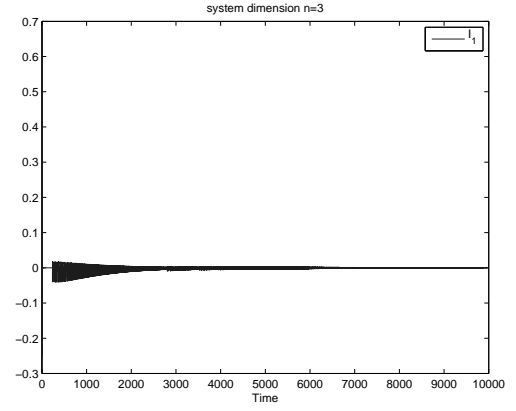


Figure 5. Time evolution of  $I_1$ ; system defined by (9) with feedback (11);  $I_1$  oscillates and its absolute value converges to zero.

## 5 Conclusions

We analyze in this paper the feedback control of a Schrödinger equation with Hamiltonian  $H = H_0 + uH_1 + u^2H_2$ . When the linearized system is controllable we prove a theoretical result concerning the convergence of a standard Lyapunov algorithm [12]. We show numerically that this algorithm does not converge when some couplings are realized by  $H_2$  instead of  $H_1$ . For these situations we propose a new algorithm that is tested numerically and gives good results.

We are currently working on a convergence proof for this situation too.

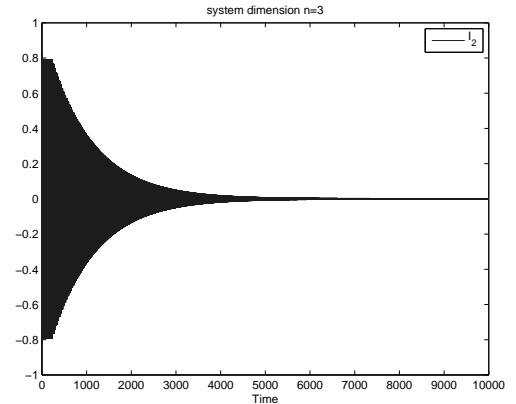


Figure 6. Time evolution of  $I_2$ ; system defined by (9) with feedback (11);  $I_2$  oscillates and its absolute values converges to zero.

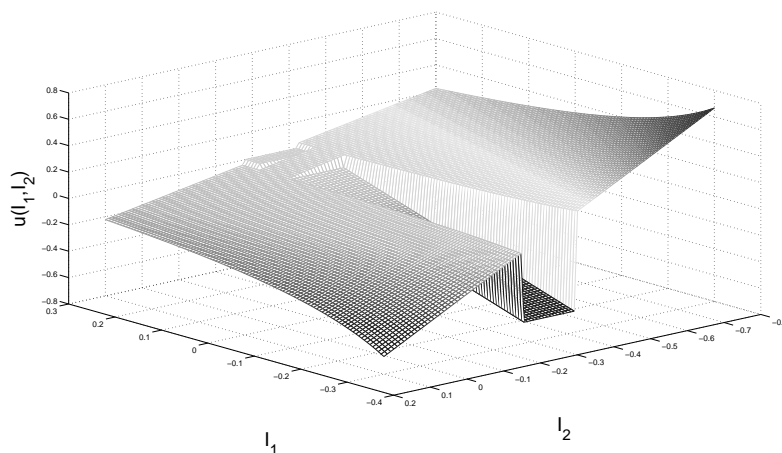


Figure 7.  $u(I_1, I_2)$ ,  $u$  defined by (11), for  $\delta = 0.5$ .

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