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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 herein) 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 ω (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, Ψ and $e^{i\theta(t)}\Psi$ describe the same physical state for any global phase $t \mapsto \theta(t) \in \mathbb{R}$, i.e Ψ_1 and Ψ_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 ω 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 Ψ . With such additional fictitious control ω , 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 ω .

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 Ψ 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 ϕ 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 λ_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 λ . 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 Ω -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 Φ_{α} is any eigenvector of H_0 not co-linear to ϕ such that $\langle \Phi_{\alpha} | H_1 | \phi \rangle = 0$.
2. If H_0 is not degenerate and $E = \mathbb{R}\phi$, the Ω -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 ω 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 $v \frac{d}{dt} \Psi = H_0\Psi$, $\frac{d}{dt} \Im(\langle H_1\Psi | \phi \rangle) = 0$ 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: $Re(\langle H_1 H_0 \Psi | \phi \rangle) = 0$ 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:

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

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

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

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

- Note first that in any case the Ω -limit set contains ϕ 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 Ω -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 ϕ_1 works when all states ϕ_2, \dots, ϕ_n are coupled to ϕ_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:

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

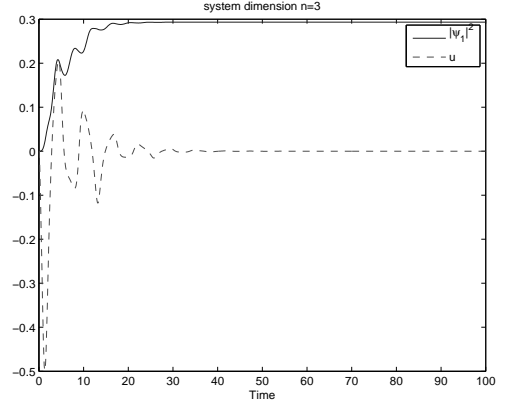


Figure 1. Population $|\Psi_1|^2$ (solid line) and control u (dashed line); initial condition $\Psi(t=0) = (0, 1/\sqrt{2}, 1/\sqrt{2})$; system defined by (9) with feedback (6). The feedback (6) fails to reach the target (quality is only 30%).

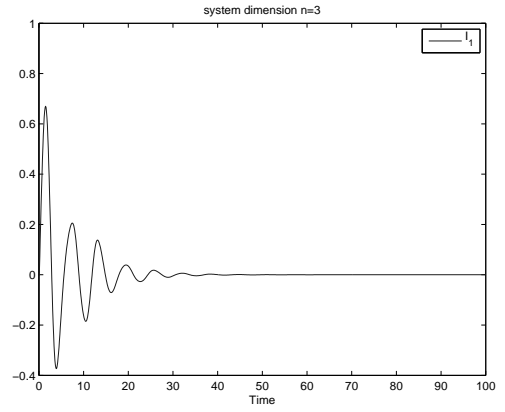


Figure 2. Time evolution of I_1 ; system defined by (9) with feedback (6). We note that I_1 converges to zero.

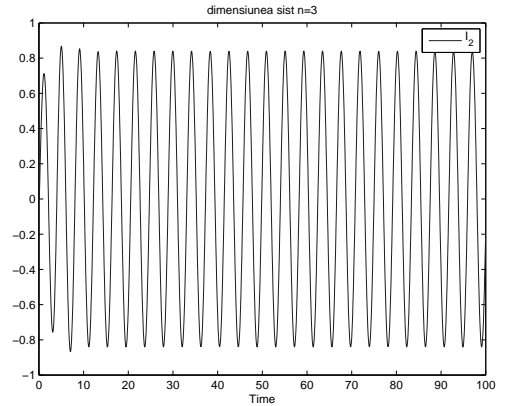


Figure 3. Time evolution of I_2 ; system defined by (9) with feedback (6). Contrary to I_1 , I_2 does not converge to zero.

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 Ψ . 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 ϕ only with the state Ψ_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.

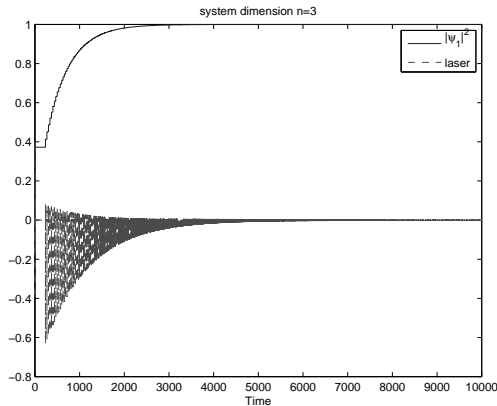


Figure 4. Population $|\Psi_1|^2$ (solid line) and control u (dashed line); initial condition: $\Psi(t = 0) = (0, 1/\sqrt{2}, 1/\sqrt{2})$; system defined by (9) with feedback (11).

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 ϕ . 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.

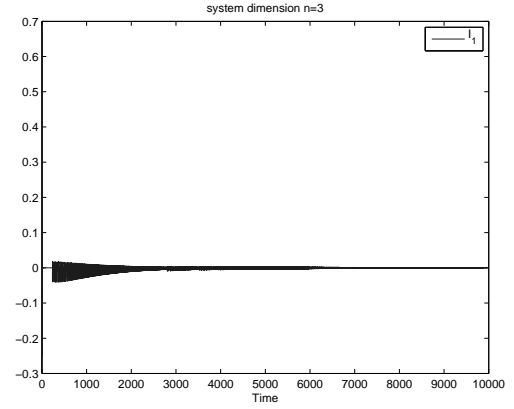


Figure 5. Time evolution of I_1 ; system defined by (9) with feedback (11); I_1 oscillates and its absolute value converges to zero.

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.

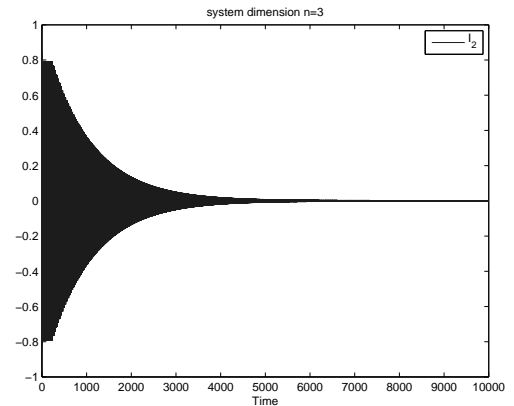


Figure 6. Time evolution of I_2 ; system defined by (9) with feedback (11); I_2 oscillates and its absolute values converges to zero.

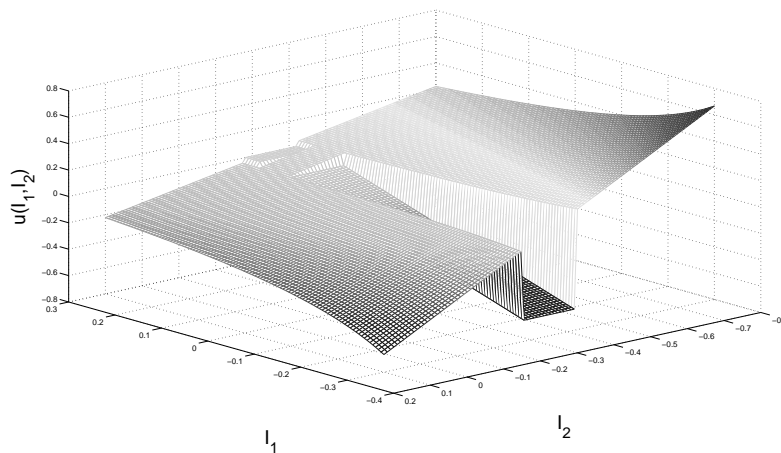


Figure 7. $u(I_1, I_2)$, u defined by (11), for $\delta = 0.5$.

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