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Brief paper

Lyapunov control of bilinear Schrödinger equations☆

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Abstract

A Lyapunov-based approach for trajectory tracking of the Schrödinger equation is proposed. In the finite dimensional case, convergence is precisely analyzed. Connection between the controllability of the linearized system around the reference trajectory and asymptotic tracking is studied. When the linearized system is controllable, such a feedback ensures almost global asymptotic convergence. When the linearized system is not controllable, the stability of the closed-loop system is not asymptotic. To overcome such lack of convergence, we propose, when the reference trajectory is an eigenstate, a modification based on adiabatic invariance. Simulations illustrate the simplicity and also the interest for trajectory generation.

Keywords: Quantum systems; Stabilization; Control Lyapunov function; Adiabatic invariant; Tracking; Trajectory generation

1. Introduction

Controllability of a finite dimensional quantum system, $\imath\dot{\Psi} = (H_0 + u(t)H_1)\Psi$, where H_0 and H_1 are $n \times n$ Hermitian matrices with coefficients in $\mathbb{C}$, can be studied via the general accessibility criteria proposed in Brockett (1973), Sussmann and Jurdjevic (1972) and based on Lie brackets. More specific results might be found in e.g. Albertini and D'Alessandro (2003), Altafini (2002), Ramakrishna, Salapaka, Dahleh, and Rabitz (1995), Turinici and Rabitz (2003). However, such a characterization does not provide, in general, a simple and efficient way for open-loop trajectory generation. Optimal control techniques (see, e.g., Maday & Turinici, 2003; Shi, Woody, & Rabitz, 1988, and the references herein) provide the 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 control are Chen, Gross, Ramakrishna, Rabitz, and Mease (1995), Gross, Singh, Rabit, Mease, and Huang (1993), Kosloff, Rice, Gaspard, Tersigni, and Tannor (1989). More recent results can be found in Rabitz and anf Zhu (2003) for decoupling techniques, in Grivopoulos and Bamieh (2003), Ferrante, Pavon, and Raccanelli (2002), Sugawara (2003), Vaidya, D'Alessandro, and Mezic (2003), Vettori (2002) for Lyapunov-based techniques and in Altafini (2002), Constantinescu and Ramakrishna (2003), Ramakrishna, Ober, Flores, and Rabitz (2002) for factorizations techniques of the unitary group.

This paper is devoted to Lyapunov-based techniques. Since measurement and feedback in quantum systems lead to much more complicated models and dynamics than the simple Schrödinger equation, the design techniques developed in this work can be used only for generation of open-loop control laws. Nevertheless, the method presented here can be useful to elucidate issues regarding the state space and as a first step to more realistic designs that include real measurement and feedback. We show that controllability of the first variation around the reference trajectory is a necessary condition for asymptotic convergence. The

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analysis is based on an adaptation to bilinear quantum systems of the general method proposed in Jurdjevic and Quinn (1978) (see also, Gauthier, 1984). Moreover, we propose here to add a fictitious control ω (see (1)) to take into account the physically meaningless global phase and to improve convergence. Contrarily to other Lyapounov-based techniques, our method is valid to track any trajectory and admits a precise convergence analysis for two kind of trajectories (eigenstate and adiabatic). This method can be directly applied to several examples of physical interest including the O–H bond modeled via a Morse potential (Rabitz & anf Zhu, 2003) and examples considered as difficult in the chemistry literature since highly degenerate and for which the adiabatic method works directly (see the four-states system in Gross, Neuhauser, & Rabitz, 1991; Phan & Rabitz, 1997, 1999; Turinici & Rabitz, 2001 and the five-states system in Tersigni, Gaspard, & Rice, 1990; Ramakrishna et al., 1995).

The paper contains two convergence analyses. They are given in Theorem 1 when the reference trajectory is an eigenstate and in Theorem 3 when the reference trajectory is adiabatic. In Section 2, we introduce the additional fictitious phase control ω, we present the Lyapunov-based tracking feedback and we discuss three simulations that illustrate Theorems 1 and 3. This section is tutorial and technicalities are reduced to a strict minimum. The two remaining sections are more technical and formal; Section 3 (resp. 4) is devoted to Theorem 1 (resp. 3). In conclusion, we suggest extensions to the multi-input and infinite-dimensional cases. Preliminary versions of these results can be found in Mirrahimi and Rouchon,(2004a,b). Connected but different results can also be found in Mirrahimi, Turinici, and Rouchon (2005) where Lyapunov design is developed for the density operator ρ instead of the probability amplitudes Ψ, and also in Beauchard, Coron, Mirrahimi, and Rouchon (2004) that studies the stabilization around degenerate eigenstate where the linearized system is not controllable. The authors thank Claudio Altafini, Jean-Michel Coron and Laurent Praly for interesting discussions and comments.

2. Tracking feedback design

2.1. Dynamics and global phase

Take $\imath(\mathrm{d}/\mathrm{d}t)\Psi = (H_0 + u(t)H_1)\Psi$, a n-states quantum system ($\hbar = 1$) where H_0 and H_1 are $n \times n$ Hermitian matrices with coefficients in $\mathbb{C}$ and $u(t) \in \mathbb{R}$ is the control. 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, the probability amplitudes Ψ and $e^{\imath\theta(t)}\Psi$ describe the same physical state for any global phase $t \mapsto \theta(t) \in \mathbb{R}$. This point has important consequences on the geometry of the physical state space: two probability amplitudes Ψ_1 and Ψ_2 are identified when $\theta \in \mathbb{R}$ exists such that $\Psi_1 = \exp(\imath\theta)\Psi_2$. To take into account such non-trivial geometry, we add a second control ω corresponding to $\dot{\theta}$. Thus, we consider the following control system:

$$\imath\frac{\mathrm{d}}{\mathrm{d}t}\Psi = (H_0 + uH_1 + \omega)\Psi, \tag{1}$$

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 (1) admit 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 (1); $\imath(\mathrm{d}/\mathrm{d}t)\Psi_r = (H_0 + u_r H_1 + \omega_r)\Psi_r$. Take the following time varying function $V(\Psi, t)$:

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

where $\langle .|. \rangle$ denotes the Hermitian product. 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 (1)

$$\frac{\mathrm{d}V}{\mathrm{d}t} = 2(u - u_r)\Im(\langle H_1\Psi(t)|\Psi_r\rangle) + 2(\omega - \omega_r)\Im(\langle \Psi(t)|\Psi_r\rangle),$$

where $\Im$ denotes the imaginary part. With, e.g.,

$$u = u_r(t) - a\Im(\langle H_1\Psi(t)|\Psi_r(t)\rangle),$$
$$\omega = \omega_r(t) - b\Im(\langle \Psi(t)|\Psi_r(t)\rangle), \tag{3}$$

($a > 0$ and $b > 0$ parameters), we ensure $\mathrm{d}V/\mathrm{d}t \leqslant 0$. Let us detail 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 eigenvector of H_0 associated to the eigenvalue $\lambda \in \mathbb{R}$ ($H_0\phi = \lambda\phi$, $\|\phi\| = 1$). Then (3) becomes a static-state feedback

$$u = -a\Im(\langle H_1\Psi|\phi\rangle), \quad \omega = -\lambda - b\Im(\langle \Psi|\phi\rangle). \tag{4}$$

2.3. Tutorial examples and simulations

Take $n = 3$, $\Psi = (\Psi_1, \Psi_2, \Psi_3)^T$ and

$$H_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{3}{2} \end{pmatrix}, \quad H_1 = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}. \tag{5}$$

Let us use the previous Lyapunov control in order to trap our system in the first eigenstate $\phi = (1, 0, 0)$ of energy $\lambda = 0$. We take (4) with $a = b = \frac{1}{2}$ ($\star$ means complex conjugate)

$$u = -\tfrac{1}{2}\Im(\Psi_2^\star + \Psi_3^\star), \quad \omega = -\tfrac{1}{2}\Im(\Psi_1^\star). \tag{6}$$

Simulations of Fig. 1 describe the trajectory with $\Psi^0 = (0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ as initial state. Other simulations indicate that the trajectories always converge to ϕ. It appears that such Lyapunov-based techniques is quite efficient for system (5).

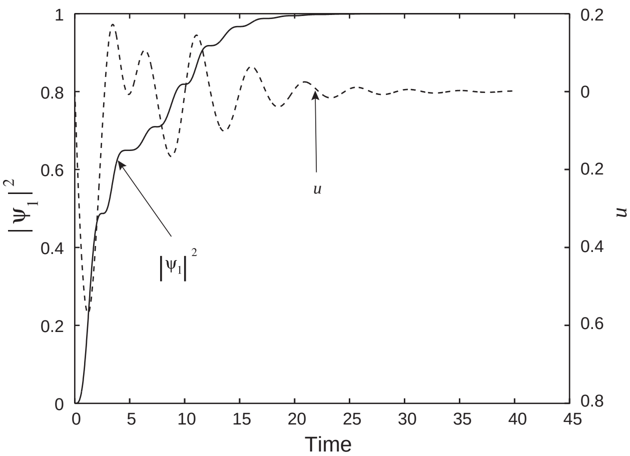

Fig. 1. Population $|\Psi_1|^2$ and control u; initial condition $(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$; system defined by (5) with feedback (6).

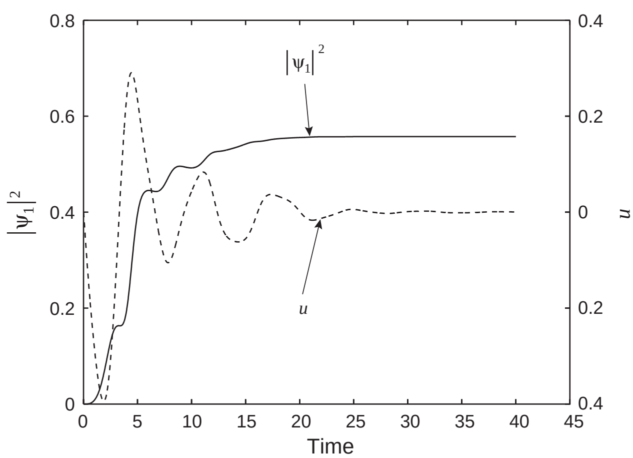

Fig. 2. Population $|\Psi_1|^2$ and control u; initial condition $(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$; H_0 defined by (5), H_1 by (7) and u, ω by (8).

In Theorem 1, it is shown that almost global convergence is equivalent to the controllability of the linearized system around ϕ.

Let us consider another example that clearly illustrates the limitation of such Lyapunov-based technique: H_0 and the goal state ϕ remain unchanged but H_1 becomes

$$H_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{7}$$

The feedback becomes

$$u = -\frac{\Im(\Psi_2^\star)}{2}, \quad \omega = -\frac{\Im(\Psi_1^\star)}{2}. \tag{8}$$

Simulations of Fig. 2 start with $(0, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ as initial condition for Ψ. We clearly realize that such a feedback reduces the distance to the first state but does not ensure its convergence to 0. This is not due to a lack of controllability.

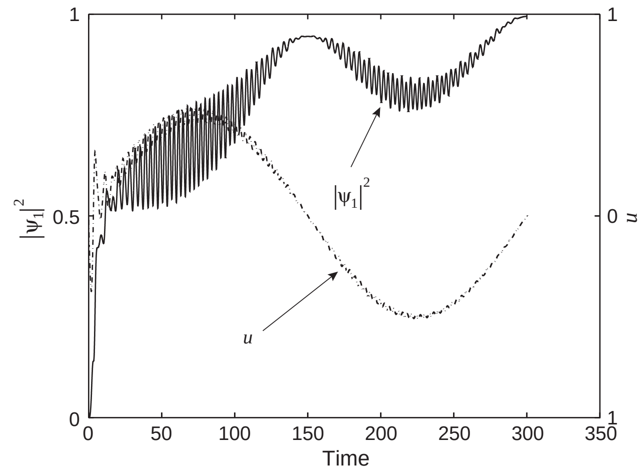

Fig. 3. System and initial conditions identical to Fig. 2; adiabatic trajectory (9) tracking via the feedback (10).

This system is controllable since the Lie algebra spanned by $H_0/\imath$ and $H_1/\imath$ coincides with $u(3)$ (Ramakrishna et al., 1995). As explained in Theorem 1, such convergence deficiency comes form the fact that the linearized system around ϕ is not controllable.

To overcome such lack of convergence observed with simulations on Fig. 2, we will use (3) with an adiabatic reference trajectory

$$\imath \frac{\mathrm{d}}{\mathrm{d}t} \Psi_\mathrm{r} = (H_0 + u_\mathrm{r}(t) H_1) \Psi_\mathrm{r}, \quad \Psi_\mathrm{r}(0) = (1, 0, 0), \tag{9}$$

where $u_\mathrm{r} = \frac{1}{2}\sin(2\pi t/T)$ with a period $T = 300$, large compared with the natural periods of H_0 to ensure that u_r is a slowly varying time function. Take the following tracking feedback:

$$u = u_\mathrm{r} - \frac{\Im(\langle H_1 \Psi | \Psi_\mathrm{r}(t) \rangle)}{2}, \quad \omega = -\frac{\Im(\langle \Psi | \Psi_\mathrm{r}(t) \rangle)}{2}. \tag{10}$$

Since u_r varies slowly, adiabatic theory ensures that Ψ_r will follow closely the first eigenstate of $H_0 + u_\mathrm{r} H_1$ (Messiah, 1962). So when u_r returns to 0, Ψ_r will almost return to the first eigenspace spanned by $(1, 0, 0)$: we have $\Psi_\mathrm{r}(T) \approx (\exp(\imath\theta), 0, 0)$ for some phase shift θ. If during this slow motion, the reference trajectory Ψ_r is in the neighborhood of an eigen-state of $H_0 + u_\mathrm{r} H_1$, where the linearized system is controllable, this will strongly improve convergence. This is effectively the case as shown in Fig. 3 that illustrates the efficiency of combining Lyapunov design and adiabatic invariance. See also Beauchard et al. (2004) for a different method based on an implicitly defined control-Lyapunov function that ensures local convergence when the linearized system around ϕ is not controllable.

3. Convergence analysis

The goal of this section is to prove the following theorem that underlies simulations of Figs. 1 and 2:

Take $\lambda \in \mathbb{R}$. The spectrum $\{\lambda_\alpha\}_{1 \leqslant \alpha \leqslant n}$ of H_0 is said to be λ-degenerate when exist α and β in $\{1, \ldots, n\}$ such that $\alpha \neq \beta$ and $|\lambda_\alpha - \lambda| = |\lambda_\beta - \lambda|$.

Theorem 1. *Consider* (1) *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* (4) *with* $a, b > 0$. *Then the two following propositions are true*:

(1) *If the spectrum of* H_0 *is not* λ*-degenerate* (*all eigenvalues are distinct*), *the* Ω*-limit set of the closed-loop system is the intersection of* $\mathbb{S}^{2n-1}$ *with the vector space* $E = \mathbb{R}\phi \bigcup_\alpha \mathbb{C}\Phi_\alpha$ *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) *The* Ω*-limit set reduces to* $\{\phi, -\phi\}$ *if and only if* H_0 *is not* λ*-degenerate and* $E = \mathbb{R}\phi$. *In this case: the equilibrium* ϕ *is exponentially stable* (*on* $\mathbb{S}^{2n-1}$); *the equilibrium* $-\phi$ *is unstable*; *the attractor set of* ϕ *is exactly* $\mathbb{S}^{2n-1}/\{-\phi\}$. *This case corresponds to the controllability of the linearized system at* ϕ, *a time-invariant linear system that lives on the* $2n-1$ *plane tangent to* $\mathbb{S}^{2n-1}$ *at* ϕ.

For example in Fig. 1, it becomes clear that $E = \mathbb{R}\phi$ since H_0 is not λ-degenerate and $\phi = (1, 0, 0)$ is almost globally asymptotically stable. Note the condition $E = \mathbb{R}\phi$ says that, physically, the target-state ϕ is connected to all other eigenstates via mono-photonic transitions (see, e.g., Messiah, 1962).

For example in Fig. 2, elements of E are of the form $(x, 0, z)$ with $x \in \mathbb{R}$ and $z \in \mathbb{C}$; we observe effectively that the Ω-limit set contains elements of the form $(x, 0, r\exp(\imath\theta))$ with x, r and θ in $\mathbb{R}$ such that $x^2 + r^2 = 1$. Physically, the transition between ϕ and state of energy $\frac{3}{2}$ necessitates at least two photons: the feedback (8) cannot find such multi-photonic processes.

The proof of Theorem 1 mainly relies on the characterization of the Ω-limit set via LaSalle invariance principle. It provides here a complete description of the invariant subset via the linear system (11). Such description becomes very simple when H_0 is not degenerate.

3.1. Proof of proposition (1) of Theorem 1

Up to a shift on ω and H_0, we can assume that $\lambda = 0$. LaSalle's principle (see, e.g., Khalil, 1992, Theorem 3.4, p. 115) says that the trajectories of the closed-loop system converge to the largest invariant set contained in $\mathrm{d}V/\mathrm{d}t = 0$ where V is defined by (2). The equation $\mathrm{d}V/\mathrm{d}t = 0$ means that $\Im(\langle H_1\Psi|\phi\rangle) = \Im(\langle \Psi|\phi\rangle) = 0$. Thus $u = 0$ and $\omega = 0$. Invariance means that $\imath(\mathrm{d}/\mathrm{d}t)\Psi = H_0\Psi$, $(\mathrm{d}/\mathrm{d}t)\Im(\langle H_1\Psi|\phi\rangle) = 0$ and $(\mathrm{d}/\mathrm{d}t)\Im(\langle \Psi|\phi\rangle) = 0$. Clearly $(\mathrm{d}/\mathrm{d}t)\Im(\langle \Psi|\phi\rangle) = 0$ does not give any additional information since $H_0\phi = 0$. Only $(\mathrm{d}/\mathrm{d}t)\Im(\langle H_1\Psi|\phi\rangle) = 0$ provides a new independent equation: $\Re(\langle H_1 H_0\Psi|\phi\rangle) = 0$ that reads $\Re(\langle [H_0, H_1]\Psi|\phi\rangle) = 0$. Similarly $(\mathrm{d}/\mathrm{d}t)\Re(\langle [H_0, H_1]\Psi|\phi\rangle) = 0$ 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:

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

that corresponds to the "ad-conditions" obtained in Jurdjevic and Quinn (1978). 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 $n \times n$ matrix. With $H_0 = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$, we have $[H_0, A]_{i,j} = (\lambda_i - \lambda_j)B_{ij}$. Let take $B = H_1$ in order to simplify the notations. So

$$\begin{array}{rcl} [H_0, B] & = & ((\lambda_i - \lambda_j)B_{ij}), \\ [H_0, [H_0, B]] & = & ((\lambda_i - \lambda_j)^2 B_{ij}), \\ & \vdots & \\ \underbrace{[H_0, [H_0, \ldots, [H_0}_{k \quad times}, B]] \ldots] & = & ((\lambda_i - \lambda_j)^k B_{ij}). \end{array}$$

Thus the previous system reads

$$\begin{array}{rcl} \Im(\Sigma_j B_{1j}\Psi_j) & = & 0, \\ \Re(\Sigma_j(\lambda_1 - \lambda_j)B_{1j}\Psi_j) & = & 0, \\ & \vdots & \\ \Im(\Sigma_j(\lambda_1 - \lambda_j)^{2k}B_{1j}\Psi_j) & = & 0, \\ \Re(\Sigma_j(\lambda_1 - \lambda_j)^{2k+1}B_{1j}\Psi_j) & = & 0. \end{array} \tag{11}$$

Using the Vandermonde structure and the fact that H_0 has a non-λ-degenerate spectrum, $\Psi \in \mathbb{S}^{2n-1}$ is in the Ω-limit set if and only if $B_{1j}\Psi_j = 0, \forall j \in \{2, \ldots, n\}$. and $\Im(\Psi_1) = 0$.

3.2. Proof of proposition (2) of Theorem 1

Note first that in any case the Ω-limit set contains ϕ and $-\phi$. If H_0 has a non-λ-degenerate spectrum and $E = \mathbb{R}\phi$ then proposition (1) implies that the Ω-limit set is just $\{\pm\phi\}$. Now let us suppose that at least one of these two conditions is not fulfilled.

Assume that $E \neq \mathbb{R}\phi$. Thus exists an eigenvector Φ of H_0 not co-linear to ϕ such that $\langle H_1\Phi|\phi\rangle = 0$. With $\Psi(0) = \Phi$ as initial state, we have $u(t) = 0$ and $\omega(t) = -\lambda$ and $\Psi(t) = \Phi$ for all $t > 0$. The Ω-limit set contains Φ.

Assume $E = \mathbb{R}\phi$ but that H_0 has a λ-degenerate spectrum. We will consider two cases

(1) There exists an eigenvector ϕ_k with length 1 of H_0 orthogonal to ϕ but with the same eigenvalue λ. Since $E = \mathbb{R}\phi$, $B_{1k} = (\langle H_1\phi_k|\phi\rangle) \neq 0$. With $\Psi(0) = (B_{1k}/|B_{1k}|)\phi_k$ as initial state, we have $u(t) = 0$, $\omega = -\lambda$ and $\Psi(t) = (B_{1k}/|B_{1k}|)\phi_k$ belongs to the Ω-limit set.

(2) There exist two orthogonal eigenvectors ϕ_k and ϕ_l of H_0, with length one and admitting the eigenvalues $\mu \neq \lambda$. Since $E = \mathbb{R}\phi$, $B_{1k} = (\langle H_1\phi_k|\phi\rangle) \neq 0$ and $B_{1l} = (\langle H_1\phi_l|\phi\rangle) \neq 0$. With $\Psi(0) = (B_{1k}\phi_l - B_{1l}\phi_k)/\sqrt{|B_{1k}|^2 + |B_{1l}|^2}$, we have $u(t) = 0$, $\omega = -\lambda$ and

$$\Psi(t) = \mathrm{e}^{-\imath(\mu-\lambda)t}\Psi(0).$$

Thus the Ω-limit set contains $(\mathrm{e}^{\imath\alpha}\Psi(0))_{\alpha\in[0,2\pi]}$.

The proof of the first part of proposition (2) is thus done.

Let us prove now that ϕ is locally exponentially stable when H_0 is not λ-degenerate and $E = \mathbb{R}\phi$. We will prove that the linearized closed-loop system is asymptotically stable. This will automatically imply that the equilibrium ϕ is locally exponentially stable. Set $\Psi(t) = \phi + \Delta\Psi(t)$ with $\Delta\Psi$ small. Then up to second order terms we have

$$\imath\frac{\mathrm{d}}{\mathrm{d}t}\Delta\Psi = (H_0 - \lambda I)\Delta\Psi - a\Im(\langle H_1\Delta\Psi|\phi\rangle)H_1\phi - b\Im(\langle\Delta\Psi|\phi\rangle)\phi$$

and $\Re(\langle\Delta\Psi|\phi\rangle) = 0$ (definition of the tangent space at ϕ to the unit sphere $\mathbb{S}^{2n-1}$). Set $W(\Delta\Psi) = \frac{1}{2}\langle\Delta\Psi|\Delta\Psi\rangle$. Simple computations show that $\mathrm{d}W/\mathrm{d}t \leqslant 0$ and $E = \mathbb{R}\phi$ implies that the LaSalle's invariant set of this linearized system reduces to $\Delta\Psi = 0$ on the tangent space at ϕ to $\mathbb{S}^{2n-1}$.

The fact that $-\phi$ is unstable results from the fact that the Lyapunov function V reaches its maximum on $\mathbb{S}^{2n-1}$ only for $\Psi = -\phi$. Thus if $\Psi(0) \neq -\phi$, then necessary $\Psi(t)$ must converge to the other point of the Ω-limit set. Thus $\lim_{t\mapsto+\infty}\Psi(t) = \phi$; the equilibrium $-\phi$ is unstable, the attraction region of ϕ is $\mathbb{S}^{2n-1}/\{-\phi\}$.

Let us finally prove that H_0 non-λ-degenerate and $E = \mathbb{R}\phi$ is equivalent to the controllability of the linearized system at ϕ.

Set $\Psi(t) = \phi + \Delta\Psi(t)$ with $\Re(\langle\Delta\Psi|\phi\rangle) = 0$, $u = \Delta u$ and $\omega = -\lambda + \Delta\omega$ with $\Delta\Psi$, Δu and $\Delta\omega$ small. Then up to second order terms, (1) reads

$$\imath\frac{\mathrm{d}}{\mathrm{d}t}\Delta\Psi = (H_0 - \lambda I)\Delta\Psi + \Delta u H_1\phi + \Delta\omega\phi.$$

Take $(\phi_1, \ldots, \phi_n)$ an orthonormal eigen-basis of H_0 associated to $(\lambda_1, \ldots, \lambda_n)$ with $\phi_1 = \phi$ and $\lambda_1 = \lambda$. Set $(z_1, \ldots, z_n) \in \mathbb{C}^n$ the coordinates of $\Delta\Psi$ in this basis. Then $\Re(z_1) = 0$ and

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}(\Im(z_1)) &= -\Delta\omega - B_{11}\Delta u,\\
\imath\frac{\mathrm{d}}{\mathrm{d}t}z_2 &= (\lambda_2 - \lambda_1)z_2 + B_{12}\Delta u,\\
&\vdots\\
\imath\frac{\mathrm{d}}{\mathrm{d}t}z_n &= (\lambda_n - \lambda_1)z_n + B_{1n}\Delta u,
\end{aligned}$$

where $B_{ij} = \langle\phi_i|H_1\phi_j\rangle$. Controllability is then equivalent to the fact that $B_{1i} \neq 0$ and $|\lambda_i - \lambda| \neq |\lambda_j - \lambda|$ for $i \neq j$ (use, e.g., Kalman controllability matrix). This is clearly equivalent to H_0 non-λ-degenerate and $E = \mathbb{R}\phi$.

3.3. A technical lemma

The following lemma will be used during the Proof of Theorem 3:

Lemma 2. *Consider* (1). *Take $\phi \in \mathbb{S}^{2n-1}$ an eigenvector of H_0 associated to the eigenvalue λ. Assume that H_0 is not λ-degenerate and the vector-space E defined in Theorem* 1 *coincides with $\mathbb{R}\phi$. Take $\theta \in \mathbb{R}$ and consider the following closed-loop system* $(a, b > 0)$:

$$(\Upsilon)\begin{cases}\imath(\mathrm{d}/\mathrm{d}t)\Psi &= (H_0 + uH_1 + \omega)\Psi,\\ u &= -a\Im(\langle H_1\Psi|\mathrm{e}^{\imath(\theta-\lambda t)}\phi\rangle),\\ \omega &= -b\Im(\langle\Psi|\mathrm{e}^{\imath(\theta-\lambda t)}\phi\rangle).\end{cases}$$

Then for all $\eta > 0$ and $\varepsilon > 0$, exists $T > 0$, such that for all $\theta \in \mathbb{R}$ and $\Psi^0 \in \mathbb{C}^n$ satisfying $\|\Psi^0 - \exp(\imath\theta)\phi\| \leqslant 2 - \eta$, we have $\forall t \geqslant T$, $\min_{\alpha\in[0,2\pi]}\|\Psi(t) - \exp(\imath\alpha)\phi\| \leqslant \varepsilon$ where Ψ is the solution of (Υ) with $\Psi(0) = \Psi^0$.

Note that T is independent of θ: this point will be crucial in the proof of Theorem 3. The detailed proof of this lemma is left to the reader. It relies on the following arguments:

- Up to a shift of $-\lambda$ on ω and H_0, and multiplying Ψ by $\mathrm{e}^{-\imath\theta}$, we can assume $\lambda = 0$ and $\theta = 0$; one recognizes feedback (4).
- $\|\Psi - \phi\|^2$ is a Lyapunov function that reaches its maximum value 2 only for $\Psi = -\phi$.
- Ψ lives on the compact $\mathbb{S}^{2n-1}$ and according to proposition (2) of Theorem 1, the Ω-limit set of (Υ) is made of two equilibrium $\{\phi, -\phi\}$ with ϕ exponentially stable with attraction region $\mathbb{S}^{2n-1}/\{-\phi\}$.
- The time taken by $\Psi(t)$ to enter the sphere of center ϕ and radius ε is a continuous function of $\Psi(0) \in \mathbb{S}^{2n-1}/\{-\phi\}$. It reaches its maximum on every compact subset of $\mathbb{S}^{2n-1}/\{-\phi\}$.

4. Lyapunov tracking of adiabatic trajectories

The goal of this section is to prove the following theorem that underlies simulations of Fig. 3:

Theorem 3. *Consider* (1) *and an analytic map $u \mapsto (\phi^u, \lambda^u)$ where ϕ^u is an eigenvector of $H_0 + u_1H_1$ of length* 1 *associated to the eigenvalue λ^u. Take a smooth map $f : [0, 1] \mapsto [0, 1]$ such that $f(0) = f(1) = 0$. For $T > 0$, denote by $[0, T] \ni t \mapsto \Psi_\mathrm{r}(t)$ the reference trajectory solution of*

$$(\Sigma_\mathrm{r})\begin{cases}\imath(\mathrm{d}/\mathrm{d}t)\Psi_\mathrm{r} &= (H_0 + u_\mathrm{r}(t)H_1)\Psi_\mathrm{r},\\ \Psi_\mathrm{r}(0) &= \phi^0,\\ u_\mathrm{r}(t) &= f(t/T).\end{cases}$$

and by $[0,T]\ni t\mapsto \Psi(t)$ *the trajectory of closed-loop system* (*see* (3), $a,b>0$ *constant*)

$$(\Sigma)\begin{cases} \imath(\mathrm{d}/\mathrm{d}t)\Psi &= (H_0+u(t)H_1+\omega)\Psi,\\ \Psi(0) &= \Psi^0,\\ u &= u_{\mathrm{r}}(t)-a\Im(\langle H_1\Psi|\Psi_{\mathrm{r}}\rangle),\\ \omega &= -b\Im(\langle\Psi|\Psi_{\mathrm{r}}\rangle). \end{cases}$$

Assume that there exists $\bar{s}\in]0,1[$ *such that the linearized system of* (1) *around the steady state* $\bar\Psi=\phi^{\bar u}$, $\bar u=f(\bar s)=u_{\mathrm{r}}(\bar sT)$ *and* $\bar\omega=-\lambda^{\bar u}$ *is controllable.*

Then for all $\eta>0$ *and* $\varepsilon>0$ *there exists* $\bar T>0$, *such that for all* $\Psi^0\in\mathbb{S}^{2n-1}$ *such that* $\|\Psi^0-\phi^0\|\leqslant 2-\eta$ *we have*

$$\forall T\geqslant\bar T,\qquad \min_{\alpha\in[0,2\pi]}\|\Psi(T)-\mathrm{e}^{\imath\alpha}\phi^0\|\leqslant\varepsilon.$$

The existence of the analytical map $u\mapsto(\phi^u,\lambda^u)$ comes from the following classical result of the perturbation theory for finite dimensional self-adjoint operators (Kato, 1966, p. 121):

Lemma 4. *Let us consider the* $n\times n$ *hermitian matrices* H_0 *and* H_1 *with entries in* $\mathbb{C}$ *and let us define*

$$H(u):=H_0+uH_1.$$

For each real $u\in\mathbb{R}$, *there exists an orthonormal basis* $(\phi^u_j)_{j\in\{1,\dots,n\}}$ *of* $\mathbb{C}^n$ *consisting of eigenvectors of* $H(u)$. *These orthonormal eigenvectors can be chosen as analytic functions of* $u\in\mathbb{R}$.

For the case of Fig. 3, it is then clear that the eigenvector $\phi^0=(1,0,0)$ of H_0 belongs to such an analytic branch. Moreover, simple numerical computations indicate that for $\bar u=0.1$, the linearized system around $\phi^{\bar u}$ is controllable. Moreover, since ϕ^0 is defined up a multiplication by $\mathrm{e}^{\imath\theta}$, $\theta\in[0,2\pi]$, one can always choose ϕ^0 such that $\|\Psi^0-\phi^0\|\leqslant 1$. Thus, all the conditions of Theorem 3 are fulfilled and we can adjust the final error by taking T large enough. One observes that, asymptotically when $\varepsilon>0$ tends to 0, the required time T to ensure a final error less than ε increases as $-k\log\varepsilon$ for some $k>0$. Such asymptotics for T can be interpreted as a kind of exponential convergence. Such exponential behaviors are often encountered (see, e.g., Martinez, 1994).

The proof of Theorem 3 relies on the following adiabatic theorem (see Elgart & Avron, 1999, for a tutorial presentation of different versions of adiabatic theorem).

Theorem 5. *Consider the solution* $[0,T]\ni t\mapsto\Psi_{\mathrm{r}}(t)$ *of* (Σ_{r}). *Then for all* $\varepsilon>0$, *there exists* $T_\varepsilon>0$ *such that for all* $T\geqslant T_\varepsilon$,

$$\forall t\in[0,T],\qquad \min_{\alpha\in[0,2\pi]}\|\Psi_{\mathrm{r}}(t)-\mathrm{e}^{\imath\alpha}\phi^{u_{\mathrm{r}}(t)}\|\leqslant\varepsilon.$$

The remaining part of this section is devoted to the proof of Theorem 3.

Proof. Take $\eta>0$, $\varepsilon>0$ and $T>0$. Denote by $\mathbb{R}\ni t\mapsto\tilde\Psi(t)$ the solution of the following closed-loop system

$$(\tilde\Sigma)\begin{cases} \imath(\mathrm{d}/\mathrm{d}t)\tilde\Psi &= (H_0+\tilde uH_1+\tilde\omega)\tilde\Psi,\\ \tilde\Psi(\bar sT) &= \Psi(\bar sT),\\ \tilde u &= \bar u-a\Im(\langle H_1\tilde\Psi|\mathrm{e}^{\imath(\bar\theta-(t-\bar sT)\lambda^{\bar u})}\phi^{\bar u}\rangle),\\ \tilde\omega &= -b\Im(\langle\tilde\Psi|\mathrm{e}^{\imath(\bar\theta-(t-\bar sT)\lambda^{\bar u})}\phi^{\bar u}\rangle), \end{cases}$$

where the angle $\bar\theta\in[0,2\pi]$ is such that

$$\|\Psi_{\mathrm{r}}(\bar sT)-\mathrm{e}^{\imath\bar\theta}\phi^{\bar u}\|=\min_{\alpha\in[0,2\pi]}\|\Psi_{\mathrm{r}}(\bar sT)-\mathrm{e}^{\imath\alpha}\phi^{\bar u}\|.$$

By the adiabatic Theorem 5 there exists $T_a>0$ such that for all $T\geqslant T_a$:

$$\forall t\in[0,T],\ \min_{\alpha\in[0,2\pi]}\|\Psi_{\mathrm{r}}(t)-\mathrm{e}^{\imath\alpha}\phi^{u_{\mathrm{r}}(t)}\|\leqslant\frac{\eta}{2}. \tag{12}$$

Since $\|\Psi-\Psi_{\mathrm{r}}\|$ is a time decreasing function we have

$$\|\Psi(\bar sT)-\Psi_{\mathrm{r}}(\bar sT)\|\leqslant\|\Psi(0)-\Psi_{\mathrm{r}}(0)\|\leqslant 2-\eta.$$

But for $T\geqslant T_a$, $\|\Psi_{\mathrm{r}}(\bar sT)-\mathrm{e}^{\imath\bar\theta}\phi^{\bar u}\|\leqslant\eta/2$. Thus, for $T\geqslant T_a$,

$$\|\Psi(\bar sT)-\mathrm{e}^{\imath\bar\theta}\phi^{\bar u}\|$$
$$\leqslant\|\Psi(\bar sT)-\Psi_{\mathrm{r}}(\bar sT)\|+\|\Psi_{\mathrm{r}}(\bar sT)-\mathrm{e}^{\imath\bar\theta}\phi^{\bar u}\|\leqslant 2-\eta/2.$$

Lemma 2 applied on $(\tilde\Sigma)$ provides a $T_b>0$ such that

$$\forall t\geqslant T_b,\quad \min_{\alpha\in[0,2\pi]}\|\tilde\Psi(\bar sT+t)-\mathrm{e}^{\imath\alpha}\phi^{\bar u}\|\leqslant\frac{\varepsilon}{3}. \tag{13}$$

One can always choose T_a large enough to ensure that for all $T\geqslant T_a$, $\bar sT+T_b\leqslant T$, $\bar s<1$ and T_b is independent of $T>T_a$. This last point will be crucial in the sequel: it results from the invariance with respect to time translation of Lemma 2 and from the independence of T_b versus $\bar\theta$ that depends a priori on T.

Let us compare now the solution of (Σ) and $(\tilde\Sigma)$ for $t\in[\bar sT,\bar sT+T_b]$. Both systems have for $t=\bar sT$ the same initial value. They are both closed-loop dynamics (dynamics (1) with the tracking feedback (3)). The only difference is the reference trajectory: $t\mapsto\Psi_{\mathrm{r}}(t)$ for (Σ) and $t\mapsto\mathrm{e}^{\imath(\bar\theta-(t-\bar sT)\lambda^{\bar u})}\phi^{\bar u}$ for $(\tilde\Sigma)$. Let us prove that

$$\lim_{T\to+\infty}\left(\sup_{t\in[\bar sT,\bar sT+T_b]}\|\Psi_{\mathrm{r}}(t)-\mathrm{e}^{\imath(\bar\theta-(t-\bar sT)\lambda^{\bar u})}\phi^{\bar u}\|\right)=0. \tag{14}$$

For T large, these two reference trajectories satisfy on $[\bar sT,\bar sT+T_b]$ almost the same differential equations (1) with almost the same initial conditions at $t=\bar sT$: $\max_{t\in[\bar sT,\bar sT+T_b]}|u_{\mathrm{r}}(t)-\bar u|$ and $|\Psi_{\mathrm{r}}(\bar sT)-\mathrm{e}^{\imath\bar\theta}\phi^{\bar u}|$ tend to 0 as T tends to $+\infty$. Since the interval length T_b does not depend on T, we have (14) by standard continuity arguments. For the same reasons, (14) implies for (Σ) and $(\tilde\Sigma)$:

$$\lim_{T\to+\infty}\left(\sup_{t\in[\bar sT,\bar sT+T_b]}\|\Psi(t)-\tilde\Psi(t)\|\right)=0. \tag{15}$$

Thus there exists $\bar{T} > T_a$ such that for all $T \geqslant \bar{T}$ we have via (14) and (15):

$$\|\Psi(\bar{s}T + T_b) - \tilde{\Psi}(\bar{s}T + T_b)\| \leqslant \frac{\varepsilon}{3},$$
$$\|\Psi_{\mathrm{r}}(\bar{s}T + T_b) - \mathrm{e}^{\imath(\bar{\theta} - T_b\lambda^{\bar{u}})}\phi^{\bar{u}}\| \leqslant \frac{\varepsilon}{3}.$$

Since

$$\begin{aligned}\|\Psi(\bar{s}T + T_b) - \Psi_{\mathrm{r}}(\bar{s}T + T_b)\| &\\ \leqslant \|\Psi(\bar{s}T + T_b) - \tilde{\Psi}(\bar{s}T + T_b)\| &\\ + \|\tilde{\Psi}(\bar{s}T + T_b) - \mathrm{e}^{\imath(\bar{\theta} - T_b\lambda^{\bar{u}})}\phi^{\bar{u}}\| &\\ + \|\mathrm{e}^{\imath(\bar{\theta} - T_b\lambda^{\bar{u}})}\phi^{\bar{u}} - \Psi_{\mathrm{r}}(\bar{s}T + T_b)\| &\end{aligned}$$

we have, for $T \geqslant \bar{T}$ $\|\Psi(\bar{s}T + T_b) - \Psi_{\mathrm{r}}(\bar{s}T + T_b)\| \leqslant \varepsilon$. Since $\|\Psi - \Psi_{\mathrm{r}}\|$ is a decreasing time function, we conclude that, for $T \geqslant \bar{T}$,

$$\|\Psi(T) - \Psi_{\mathrm{r}}(T)\| \leqslant \|\Psi(\bar{s}T + T_b) - \Psi_{\mathrm{r}}(\bar{s}T + T_b)\| \leqslant \varepsilon$$

since $\bar{s}T + T_b \leqslant T$.

5. Conclusion

In this paper, we propose and analyze via Theorems 1 and 3 a simple Lyapunov tracking feedback (3) for any finite dimension Schrödinger equation with a single physical control u. These theorems admit extensions to several controls and also to arbitrary analytic trajectories (Mirrahimi & Rouchon, 2004b). Such feedback design can be also applied to any infinite dimension system. However, extension of the previous convergence analysis is not immediate since it requires the pre-compactness of the closed-loop trajectories, a property that is difficult to prove in infinite dimension. Another natural question arises when we consider the key assumption required by Theorem 3. Assume that (1) is controllable. Does there always exist $\bar{u} \in \mathbb{R}$ such that around the eigenvector of $H_0 + \bar{u}H_1$, the linearized system is controllable. All the examples we tested validate this conjecture. Is it true for any controllable finite dimensional Schrödinger equation?

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