Approximate controllability via adiabatic techniques for the three-inputs controlled Schrödinger equation

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APPROXIMATE CONTROLLABILITY VIA ADIABATIC TECHNIQUES FOR THE THREE-INPUTS CONTROLLED SCHRÖDINGER EQUATION*

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Abstract. We consider a system described by a controlled bilinear Schrödinger equation with three external inputs. We provide a constructive method to approximately steer the system from a given energy level to a superposition of energy levels corresponding to a given probability distribution. The method is based on adiabatic techniques and works if the spectrum of the Hamiltonian, as a function of the control parameters, admits conical intersections of eigenvalues. We provide sharp estimates of the relation between the error and the controllability time, and we show how to improve these estimates by selecting special control paths. As a byproduct of our results we show that conical intersections are stable with respect to general perturbations of the Hamiltonian and we also provide some results on the regularity of the eigenfamilies along paths locally around conical intersections.

Key words. Schrödinger equation, quantum control, controllability, adiabatic methods, conical intersections

AMS subject classifications. 93B05, 93C20, 81Q93

1. Introduction.

A typical issue in quantum control concerns the controllability of the bilinear Schrödinger equation

$$i\frac{d\psi}{dt} = \left(H_0 + \sum_{k=1}^{m} u_k(t)H_k\right)\psi(t), \tag{1}$$

where ψ belongs to the unit sphere of a (finite or infinite dimensional) complex separable Hilbert space $\mathcal{H}$ and $H_0, \ldots, H_m$ are self-adjoint operators on $\mathcal{H}$. Here $H_1, \ldots, H_m$ represent the action of external fields on the system, whose strength is given by the scalar-valued controls $u_1, \ldots, u_m$, while H_0 describes the uncontrolled dynamics of the system.

The controllability problem aims at establishing whether, for every pair of states ψ_0 and ψ_1 in the Hilbert sphere, there exist controls $u_k(\cdot)$ and a time T such that the solution of (1) with initial condition $\psi(0) = \psi_0$ satisfies $\psi(T) = \psi_1$.

While the case where $\mathcal{H}$ is a finite dimensional Hilbert space has been widely understood [3, 15], in the infinite dimensional case the answer is far from being given. In particular, negative results have been proved when $\mathcal{H}$ is infinite-dimensional (see [4, 30]). Hence one has to look for weaker controllability properties as, for instance, approximate controllability (see for instance [7, 9, 13, 23, 25]), or controllability between subfamilies of states (in particular the eigenstates of H_0, which are the most relevant physical states) or in suitably regular subspaces of the space of square-integrable functions (see [5, 6]).

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Unlike most of the known controllability results, mainly obtained by means of non-constructive arguments, the method proposed in this paper permits to explicitly select control inputs steering the system from the initial state to an arbitrarily small neighborhood of the given target state.

Adiabatic theory and conical intersections between eigenvalues constitute the main tools of the control strategy we propose in this paper.

Roughly speaking, the adiabatic theorem (see [8, 24, 28]) states that the occupation probabilities associated with the energy levels of a time-dependent Hamiltonian $H(\cdot)$ are approximately preserved along the evolution given by $i\dot{\psi}(t) = H(t)\psi(t)$, provided that $H(\cdot)$ varies slowly enough. This result works whenever the energy levels (i.e. the eigenvalues of $H(\cdot)$) are isolated for every t. On the other hand, if two eigenvalues intersect, and provided that $H(\cdot)$ is smooth enough, the passage through the intersections may determine (approximate) exchanges of the corresponding occupation probabilities (see [28, Corollary 2.5] and [17]). For these reasons, adiabatic methods are largely used in quantum control to induce population transfers (see for instance the techniques known as Stimulated Raman Adiabatic Passage (STIRAP), Stark-chirped rapid adiabatic passage (SCRAP)) and to prepare superposition states [20]. The applications of adiabatic methods in quantum control, as a tool for obtaining controllability results, have already been exploited in previous papers (see for instance [1, 10, 22, 33]). The general idea is to use slowly varying controls, taking advantage of the adiabatic theorem, and "climb" the energy levels through the conical intersections.

The method proposed in this paper is based on some ideas developed in [10] in the case $m = 2$ for self-adjoint Hamiltonians with real matrix elements. It exploits a generalization of [28, Corollary 2.5] stating that it is possible to arbitrarily recombine the probability weights associated with two subsequent energy levels by following (slowly) a suitable control path passing through a conical intersection between them. One of the main limits of the results of [10] consists in the fact that only Hamiltonians with real matrix elements (with respect to some suitable basis of the Hilbert space) are considered, and only bounded operators are admitted as control Hamiltonians. Many important classes of physical systems are thus excluded: for instance, spin systems in magnetic fields (described by Pauli matrices), and, in infinite dimension, Schrödinger Hamiltonians containing external fields coupled with the momentum. The purpose of this paper is to overcome this issue by adapting the control strategy introduced in [10] to the general case of self-adjoint Hamiltonians, assuming that three controlled Hamiltonians, relatively bounded with respect to the uncontrolled one, are employed. Preliminary results in this sense were discussed in [11].

The control strategy applies whenever a part of the spectrum of the Hamiltonian operator is uniformly separated from the rest of the spectrum (as a function of the control parameters), is discrete and, within it, each pair of subsequent eigenvalues intersect in a conical intersection. When there exists such a portion of the spectrum, called *separated discrete spectrum*, this control strategy permits to attain (approximately) a state having a prescribed distribution of probability (relative to the energy levels of the separated discrete spectrum) starting from an eigenstate. In particular this entails a controllability property, that we call *spread controllability*, which, although weaker than the usual approximate controllability property, is more practical. Indeed, the relative phases between pairs of components in the eigenbasis decomposition are essentially uncontrollable since they evolve according to the gaps between the corresponding energy levels. Furthermore, notice that this method allows us to control the population inside some portion of the discrete spectrum, if well separated from the rest, even in the presence of continuous spectrum, unlike many other classical methods.

Concerning the precision of the method, an application of the adiabatic theorem together with [28, Corollary 2.5] shows that the maximal error is of the order of the square root of the control speed. On the other hand the precision of the transfer may be remarkably improved if one follows some special paths in the space of controls; namely, such paths permit to attain a state with a prescribed probability distribution with an error of the order of the control speed. In practice, this means that in order to guarantee a given precision one may significantly reduce the duration of the process, whose extent constitutes one of the main disadvantages of the implementation of adiabatic techniques.

From a technical point of view, the choice of three instead of two controlled Hamiltonians leads to a different (and more involved) analysis of the properties of conical intersections and of the special paths introduced in the control algorithm. Also, many changes are due to the different regularity properties of the spectrum and of its related objects in the case of possibly unbounded controlled Hamiltonians. These properties are carefully investigated (see Appendix A) by using tools from perturbation theory. Notice that the choice of three controls is quite natural when looking for eigenvalues intersections, since it is well-known, for Hermitian matrices or within spaces of self-adjoint operators satisfying particular transversality conditions, that the set of operators admitting multiple eigenvalues is a submanifold of codimension three (see e.g. [2, 29, 31]). Moreover conical intersections do not constitute a pathological phenomenon since all eigenvalue intersections are generically conical in the finite dimensional case and in some physically relevant infinite dimensional models (for reasons of space, this result will be presented in a future work). Conical intersections are also structurally stable with respect to variations of the Hamiltonian operator, as shown in Theorem 23. Concerning the relation between conical intersections and controllability properties of the bilinear Schrödinger equation, let us finally mention [12].

The structure of the paper is the following. In Section 2 we introduce the notations used throughout the paper, the main assumptions and definitions, and we adapt the classical statement of the adiabatic theorem to our setting. In Section 3 we discuss some properties of conical intersections and related results that allow to propose the basic control strategy. In Section 4 we define special paths and, by means of a series of technical results, we show that they can be included in the control algorithm in order to improve its performance. As a byproduct, we get a structural stability result concerning conical intersections. Some numerical examples are provided in Section 5. In Section 6 we briefly mention some extensions of the control strategy and of the controllability results obtained earlier. Appendix A gathers the technical results concerning the regularity of the spectrum and of the spectral projections that are needed throughout the paper.

2. Notations and preliminary results.

We start this section by introducing the notations that will be used in the rest of the paper.

For a set $A \subset \mathbb{C}$ and $z \in \mathbb{C}$, we denote by $d(z, A) = \inf_{x \in A} |z - x|$ the distance between the point z and the set A.

For a function $f(\cdot)$ of a real parameter s, we use the following notation for its right and left limits at s_0:

$$f(s_0^{\pm}) = \lim_{s \to s_0^{\pm}} f(s).$$

Whenever $\gamma(s),\ s\in[s_1,s_2]$ is a curve on $\mathbb{R}^3$ and $Q(\cdot)$ is a function of $\mathbf{v}\in\mathbb{R}^3$ then, with abuse of notations, we denote by $\dot{Q}(\gamma(r))$ the derivative of the composition $Q(\gamma(\cdot))$ computed at r, that is $\dot{Q}(\gamma(r)) := \frac{d}{ds}Q(\gamma(s))|_{s=r} = \frac{dQ}{d\mathbf{v}}(\gamma(r))\frac{d\gamma}{ds}(r)$. Similarly, $Q^{(l)}(\gamma(r)) := \frac{d^l}{ds^l}Q(\gamma(s))|_{s=r}$.
The scalar product of two vectors $\mathbf{w}_1,\mathbf{w}_2$ in an euclidean space $\mathbb{R}^k$ is denoted by $\mathbf{w}_1\cdot\mathbf{w}_2$, while the norm of $\mathbf{w}\in\mathbb{R}^k$ is denoted by $|\mathbf{w}|$.
For a given vector $\mathbf{v}$ or matrix A the respective transpose is denoted by $\mathbf{v}^T$ and A^T.
The inverse of the transpose of an invertible square matrix A is denoted with A^{-T}.
Given a vector $\mathbf{v}=(v_1,v_2,v_3)\in\mathbb{C}^3$, we denote its complex conjugate (v_1^*,v_2^*,v_3^*) by $\mathbf{v}^*$ and its real and imaginary parts respectively by

$$\mathfrak{Re}(\mathbf{v}) = (\mathfrak{Re}(v_1),\mathfrak{Re}(v_2),\mathfrak{Re}(v_3)) \qquad \mathfrak{Im}(\mathbf{v}) = (\mathfrak{Im}(v_1),\mathfrak{Im}(v_2),\mathfrak{Im}(v_3)).$$

The symbol id is used to denote the identity operator on a vector space which is specified at each occurrence, whenever not clear from the context.
Given a linear operator A defined on a Hilbert space, its domain is denoted as $\mathcal{D}(A)$, the symbol $\sigma(A)$ denotes the spectrum of A, while the resolvent set $\rho(A)$ is the complement of $\sigma(A)$ in $\mathbb{C}$.

2.1. General setting. Let $\mathcal{H}$ be a separable complex Hilbert space with scalar product $\langle\cdot,\cdot\rangle$ and norm $\|\cdot\|$; let us introduce the following notion of relative boundedness between operators:

Definition 1 (A-smallness and A-boundedness). *Let A,B be two densely defined operators with domains $\mathcal{D}(A)\subset\mathcal{D}(B)$. We say that B is A-bounded if there exist $a,b>0$ such that $\|B\psi\|\le a\|A\psi\|+b\|\psi\|$ for every $\psi\in\mathcal{D}(A)$. B is said to be A-small if for every $\alpha>0$ there exists $\beta>0$ such that $\|B\psi\|\le\alpha\|A\psi\|+\beta\|\psi\|$ for every $\psi\in\mathcal{D}(A)$. (The latter notion is called* infinitesimal smallness with respect to *A in [26].)*

Given a self-adjoint operator A on $\mathcal{H}$, for every A-bounded operator B we define its norm with respect to A as

$$\|B\|_A = \sup_{\psi\in\mathcal{D}(A)} \frac{\|B\psi\|}{\|A\psi\|+\|\psi\|}. \tag{2}$$

This provides a norm in the space $\mathcal{L}(\mathcal{D}(A),\mathcal{H})$ of continuous linear operators from $\mathcal{D}(A)$ (endowed with the graph norm of A) to $\mathcal{H}$.

We consider the Hamiltonian

$$H(\mathbf{u}) = H_0 + u_1H_1 + u_2H_2 + u_3H_3,$$

with $\mathbf{u}=(u_1,u_2,u_3)\in\mathbb{R}^3$, and where $H_i,\ i=0,\dots,3$ satisfy the following assumption:

(H0) H_0 is a self-adjoint operator on a separable complex Hilbert space $\mathcal{H}$, and H_i are H_0-small self-adjoint operators on $\mathcal{H}$ for $i=1,2,3$. Moreover, H_0 is bounded from below, that is there exists a constant $C>0$ such that $\langle\psi,H_0\psi\rangle > -C\|\psi\|^2$ for every $\psi\in\mathcal{D}(H_0)$.

Under assumption **(H0)**, [26, Theorem X.12] guarantees that $H(\mathbf{u})$ is self-adjoint with domain $\mathcal{D}(H_0)$ and bounded from below (uniformly for $\mathbf{u}$ belonging to any compact subset of $\mathbb{R}^3$). Moreover, it is easy to see that for every $\mathbf{u}$, H_0 is $H(\mathbf{u})$-bounded, and therefore H_i is $H(\mathbf{u})$-small, for every $i=1,2,3$, with constants a,b (as in Definition 1) that depend continuously on $\mathbf{u}$.

Schrödinger Hamiltonians are typical Hamiltonian operators describing quantum phenomena and can be represented in the form $-\Delta + V$ on the Hilbert space $L^2(\Omega)$, where Ω is a domain of $\mathbb{R}^n$, Δ is the Laplacian on Ω (with Dirichlet or Neumann boundary conditions) and $V : \Omega \to \mathbb{R}$ has to be interpreted as a multiplicative operator on $L^2(\Omega)$. In particular such Hamiltonian operators are unbounded operators. In this context Hypothesis **(H0)** is thus intended to describe a Hamiltonian operator of the previous form that can be controlled by means of three external inputs so that $H_0 = -\Delta + V_0$ and $H_i = V_i$ for some multiplicative operators V_i, for $0 \leq i \leq 3$.

Finite dimensional representations of quantum systems are also common, for instance in the description of spin systems. In this case the Hamiltonian operator $H(\mathbf{u})$ is a Hermitian matrix. Consider for instance the case of a spin-1/2 particle immersed in a controlled magnetic field. In this case, H_i are the Pauli matrices, and the controls are the components of the magnetic field.

The dynamics of the quantum systems we consider are described by the time-dependent Schrödinger equation

$$i\frac{d\psi}{dt} = H(\mathbf{u}(t))\psi(t). \tag{3}$$

Such an equation has mild solutions under hypothesis **(H0)**, $\mathbf{u}(\cdot)$ piecewise $\mathcal{C}^1$ and with an initial condition in the domain of H_0 (see e.g. [26, Theorem X.70] and [4]).

We are interested in controlling (3) inside some portion of the discrete spectrum of $H(\mathbf{u})$. More precisely, we assume that (3) possesses a *separated discrete spectrum*, according to the following definition.

Definition 2. *A* separated discrete spectrum *is a pair (ω, Σ) where ω is a domain in $\mathbb{R}^3$ and Σ a map defined on ω that associates with each $\mathbf{u} \in \omega$ a subset $\Sigma(\mathbf{u})$ of the discrete spectrum of $H(\mathbf{u})$ such that there exist two continuous functions $f_1, f_2 : \omega \to \mathbb{R}$ satisfying*

- $f_1(\mathbf{u}) < f_2(\mathbf{u})$ *and* $\Sigma(\mathbf{u}) \subset [f_1(\mathbf{u}), f_2(\mathbf{u})] \qquad \forall \mathbf{u} \in \omega$.
- $\inf_{\mathbf{u}\in\omega} \inf_{\lambda\in\sigma(H(\mathbf{u}))\setminus\Sigma(\mathbf{u})} d(\lambda, [f_1(\mathbf{u}), f_2(\mathbf{u})])) > \Gamma$ *for some* $\Gamma > 0$.

Remark 3. *Thanks to Proposition 26 and Lemma 28, in order to guarantee the existence of a separated discrete spectrum for the Hamiltonian $H(\mathbf{u})$ satisfying* **(H0)**, *it is enough that there exist some open interval I and some point $\bar{\mathbf{u}}$ such that $\sigma(H(\bar{\mathbf{u}}))\cap I$ contains only a finite number of points. This in particular happens when $H(\bar{\mathbf{u}})$ has compact resolvent.*

Notation We label the eigenvalues belonging to a separated discrete spectrum $\Sigma(\mathbf{u})$ in such a way that $\Sigma(\mathbf{u}) = \{\lambda_{\hat{\jmath}}(\mathbf{u}), \ldots, \lambda_{\hat{\jmath}+k}(\mathbf{u})\}$ for some non-negative integers $\hat{\jmath}, k$, where $\lambda_{\hat{\jmath}}(\mathbf{u}) \leq \cdots \leq \lambda_{\hat{\jmath}+k}(\mathbf{u})$ are counted according to their multiplicity (note that the separation of Σ from the rest of the spectrum guarantees that k is constant). Moreover we denote by $\phi_{\hat{\jmath}}(\mathbf{u}), \ldots, \phi_{\hat{\jmath}+k}(\mathbf{u})$ an associated orthonormal family of eigenstates. Notice that in this notation $\lambda_{\hat{\jmath}}$ does not necessarily correspond to the $\hat{\jmath}$-th energy level of the system.

Our techniques rely on the existence of conical intersections between the eigenvalues, which constitute a well studied phenomenon in molecular physics (see for instance [8, 16, 17, 21, 32]). In this paper we will adopt the following definition, consistent with the one already given in [10] for the two-inputs case.

Definition 4. *Let $H(\cdot)$ satisfy hypothesis* **(H0)**. *We say that $\bar{\mathbf{u}} \in \mathbb{R}^3$ is a* conical intersection *between two subsequent eigenvalues λ_j and λ_{j+1} if $\lambda_j(\bar{\mathbf{u}}) = \lambda_{j+1}(\bar{\mathbf{u}})$ has* *multiplicity two and there exists a constant $c > 0$ such that for any unit vector $\mathbf{v} \in \mathbb{R}^3$ and $t > 0$ small enough we have that*

$$\lambda_{j+1}(\bar{\mathbf{u}} + t\mathbf{v}) - \lambda_j(\bar{\mathbf{u}} + t\mathbf{v}) > ct\,.$$

See Section 5 for some examples of conical intersections in both the finite and infinite-dimensional case.

To conclude this section, let us make some remarks on the regularity properties and the asymptotic behavior of the eigenfamilies of $H(\mathbf{u})$ in our setting. Notice that in general the regularity properties of the Hamiltonian induce similar regularity properties of the eigenfamilies (see e.g. Proposition 7 below). Moreover, it is well known that the eigenvectors can be chosen analytic along straight lines $\mathbf{u}(\cdot)$ possibly passing through eigenvalues intersections (see [19],[27, Theorem XII.13]).

Let I be an interval and consider a $\mathcal{C}^1$ curve $\mathbf{u} : I \to \mathbb{R}^3$. By direct computations we obtain that the following equations hold whenever $\lambda_l(t) \neq \lambda_m(t)$ are simple eigenvalues of $H(\mathbf{u}(t))$ with corresponding eigenstates $\phi_l(t), \phi_m(t)$:

$$\dot{\lambda}_l(t) = \langle \phi_l(t), \big(\dot{u}_1(t)H_1 + \dot{u}_2(t)H_2 + \dot{u}_3(t)H_3\big)\phi_l(t)\rangle, \tag{4}$$

$$(\lambda_m(t) - \lambda_l(t))\,\langle \phi_l(t), \dot{\phi}_m(t)\rangle = \langle \phi_l(t), \Big(\dot{u}_1(t)H_1 + \dot{u}_2(t)H_2 + \dot{u}_3(t)H_3\Big)\phi_m(t)\rangle. \tag{5}$$

Assume that $\lambda_j(\bar{\mathbf{u}}) = \lambda_{j+1}(\bar{\mathbf{u}})$ and consider the half-line $r_{\mathbf{v}}(t) = \bar{\mathbf{u}} + t\mathbf{v}$ with $\mathbf{v} = (v_1, v_2, v_3)$ unit vector and $t \geq 0$. Then, thanks to (5) and since each H_i is H_0-bounded, we have

$$\begin{aligned}\lim_{t\to 0^+} &\langle \phi_j(r_{\mathbf{v}}(t)), \big(v_1H_1 + v_2H_2 + v_3H_3\big)\phi_{j+1}(r_{\mathbf{v}}(t))\rangle \\ &= \langle \phi_j^{\mathbf{v}}, \big(v_1H_1 + v_2H_2 + v_3H_3\big)\phi_{j+1}^{\mathbf{v}}\rangle = 0,\end{aligned} \tag{6}$$

where $\phi_j^{\mathbf{v}}$ and $\phi_{j+1}^{\mathbf{v}}$ are the limits of $\phi_j(r_{\mathbf{v}}(t))$ and $\phi_{j+1}(r_{\mathbf{v}}(t))$ as t tends to zero.

2.2. The adiabatic theorem. In this section we recall a classical formulation of the time-adiabatic theorem ([8, 18, 24] adapted to our framework. For a general overview see the monograph [28].

Let $H(\mathbf{u}) = H_0 + \sum_{i=1}^3 u_iH_i$ satisfy **(H0)** and have a separated discrete spectrum (ω, Σ). Assume that the map $I = [\tau_0, \tau_f] \ni \tau \mapsto \mathbf{u}(\tau) = (u_1(\tau), u_2(\tau), u_3(\tau))$ belongs to $\mathcal{C}^2(I, \omega)$. We introduce a small parameter $\varepsilon > 0$ that controls the time scale, and the slow Hamiltonian $H(\mathbf{u}(\varepsilon t))$, $t \in [\tau_0/\varepsilon, \tau_f/\varepsilon]$. In these notations, τ is a geometric parameter used to describe the curve in the space of controls, while t is the actual time of the evolution along the control path.

We denote by $U^\varepsilon(t, t_0)$ the time evolution (from $t_0 = \tau_0/\varepsilon$ to $t = \tau/\varepsilon$) generated by $H(\mathbf{u}(\varepsilon t))$, and with $U_a^\varepsilon(t, t_0)$ the time evolution generated by the Hamiltonian $H_a(\varepsilon t)$, where $H_a(\tau) = H(\mathbf{u}(\tau)) - i\varepsilon P_*(\mathbf{u}(\tau))\dot{P}_*(\mathbf{u}(\tau)) - i\varepsilon P_*^\perp(\mathbf{u}(\tau))\dot{P}_*^\perp(\mathbf{u}(\tau))$ is the *adiabatic Hamiltonian*, $P_*(\mathbf{u})$ denotes the spectral projection of $H(\mathbf{u})$ on $\Sigma(\mathbf{u})$, and $P_*^\perp(\mathbf{u}) = \mathrm{id} - P_*(\mathbf{u})$. A crucial property of the adiabatic Hamiltonian is that the corresponding evolution decouples the dynamics relative to the subspace $P_*(\mathbf{u})\mathcal{H}$ from the remainder of the Hilbert space, in the sense that

$$P_*(\mathbf{u}(t))U_a^\varepsilon(t, t_0) = U_a^\varepsilon(t, t_0)P_*(\mathbf{u}(t_0)).$$

THEOREM 5 (Adiabatic Theorem). *Assume that $H(\mathbf{u}) = H_0 + \sum_{i=1}^3 u_iH_i$ satisfies* **(H0)** *and has a separated discrete spectrum (ω, Σ). Let $I \subset \mathbb{R}$ and $\mathbf{u} : I \to \omega$*

be a $\mathcal{C}^2$ curve. Then $P_* \in \mathcal{C}^2(I, \mathcal{L}(\mathcal{H}))$ and there exists a constant $C > 0$ such that for all $\tau_0, \tau \in I$, and setting $t_0 = \tau_0/\varepsilon, t = \tau/\varepsilon$, one has $\|U^\varepsilon(t,t_0) - U^\varepsilon_a(t,t_0)\| \leq C\varepsilon\left(1 + \varepsilon|t - t_0|\right)$. In particular

$$\|P_*(\mathbf{u}(t))U^\varepsilon(t,t_0) - U^\varepsilon(t,t_0)P_*(\mathbf{u}(t_0))\| \leq 2C\varepsilon\left(1 + \varepsilon|t - t_0|\right).$$

Let us now assume that $\Sigma = \{\lambda_j, \lambda_{j+1}\}$; we can take advantage of the adiabatic theorem to decouple the dynamics associated with the band Σ from those associated with the rest of the spectrum, in order to focus on the former.

Let $\mathcal{W}(\tau)$ denote the subspace spanned by the eigenstates associated with $\lambda_j(\mathbf{u}(\tau))$ and $\lambda_{j+1}(\mathbf{u}(\tau))$. Since $\mathcal{W}(\tau)$ is two-dimensional for any τ, it is possible to map it isomorphically on $\mathbb{C}^2$ and identify an effective Hamiltonian whose evolution is a representation of $U^\varepsilon_a(t,t_0)|_{\mathcal{W}(\varepsilon t_0)}$ on $\mathbb{C}^2$. In particular, if we can find a $\mathcal{C}^1$ eigenstate basis $\{\Phi_1(\mathbf{u}(\tau)), \Phi_2(\mathbf{u}(\tau))\}$ of $\mathcal{W}(\tau)$ (associated with a reordering $\{\Lambda_1(\mathbf{u}(\tau)), \Lambda_2(\mathbf{u}(\tau))\}$ of $\{\lambda_j(\mathbf{u}(\tau)), \lambda_{j+1}(\mathbf{u}(\tau))\}$), then the isomorphism $\mathcal{U}(\tau) : \mathcal{W}(\tau) \to \mathbb{C}^2$ is continuous. Represented in $\mathbb{C}^2$, the evolution $U^\varepsilon_a(\cdot, t_0)|_{\mathcal{W}(\varepsilon t_0)}$ is governed by the Hamiltonian $H^\varepsilon_{\text{eff}}(\varepsilon t)$, where $H^\varepsilon_{\text{eff}}(\cdot)$ is the *effective Hamiltonian*, whose form is

$$H^\varepsilon_{\text{eff}}(\tau) = \begin{pmatrix} \Lambda_1(\mathbf{u}(\tau)) & 0 \\ 0 & \Lambda_2(\mathbf{u}(\tau)) \end{pmatrix} - i\varepsilon \begin{pmatrix} \langle \Phi_1(\mathbf{u}(\tau)), \dot{\Phi}_1(\mathbf{u}(\tau))\rangle & \langle \Phi_2(\mathbf{u}(\tau)), \dot{\Phi}_1(\mathbf{u}(\tau))\rangle \\ \langle \Phi_1(\mathbf{u}(\tau)), \dot{\Phi}_2(\mathbf{u}(\tau))\rangle & \langle \Phi_2(\mathbf{u}(\tau)), \dot{\Phi}_2(\mathbf{u}(\tau))\rangle \end{pmatrix}, \tag{7}$$

with associated propagator $U^\varepsilon_{\text{eff}}(t,t_0) = \mathcal{U}(\varepsilon t)U^\varepsilon_a(t,t_0)\mathcal{U}^*(\varepsilon t_0)$.

Theorem 5 implies the following.

THEOREM 6. *Assume that $(\omega, \{\lambda_j, \lambda_{j+1}\})$ is a separated discrete spectrum and let $\mathbf{u} : I \to \omega$ be a $\mathcal{C}^2$ curve such that there exists a $\mathcal{C}^1$-varying basis of $\mathcal{W}(\cdot)$ made of eigenstates of $H(\mathbf{u}(\cdot))$. Then there exists a constant C such that for all $\tau_0, \tau \in I$, and setting $t_0 = \tau_0/\varepsilon, t = \tau/\varepsilon$,*

$$\|\left(U^\varepsilon(t,t_0) - \mathcal{U}^*(\varepsilon t)U^\varepsilon_{\text{eff}}(t,t_0)\mathcal{U}(\varepsilon t_0)\right)|_{\mathcal{W}(\varepsilon t_0)}\| \leq C\varepsilon(1 + \varepsilon|t - t_0|).$$

3. Conical Intersections and general control strategy.

3.1. Properties of conical intersections. Let $\lambda_j(\mathbf{u}), \lambda_{j+1}(\mathbf{u})$ denote two eigenvalues of $H(\mathbf{u})$, and assume that they are (locally) separated from the rest of the spectrum. It is well known that the projection $\boldsymbol{P}_{\mathbf{u}}$ associated with the sum of the corresponding eigenspaces is smooth with respect to $\mathbf{u}$. More in general, the result holds for any portion of the spectrum of $H(\mathbf{u})$, in presence of a gap (see e.g. [28]).

On the other hand, the projections P_j, P_{j+1}, associated respectively with λ_j and λ_{j+1}, are smooth with respect to $\mathbf{u}$ at any point such that $\lambda_j \neq \lambda_{j+1}$, but they are not necessarily continuous at the eigenvalues intersections. Nevertheless, along regular curves passing through a conical intersection, it is possible to extend these projections, obtaining operators whose regularity depends on the regularity of the curve, as stated in the following result, proved in Appendix A.

PROPOSITION 7. *Let $\gamma : I \to \mathbb{R}^3$, $I = [-R, 0]$, be a $\mathcal{C}^k(I)$ curve such that $\gamma(0) = \bar{\mathbf{u}}$ is a conical intersection between the eigenvalues λ_j and λ_{j+1} and $\dot{\gamma}(t) \neq 0$ for every $t \in I$, and consider its k-jet at the origin $\ell_k(t) = \gamma(0) + \sum_{j=1}^k \frac{1}{j!} t^j \frac{d^j}{dt^j}\gamma(t)|_{t=0}$. Then $P_j(\gamma(\cdot))$ is $\mathcal{C}^k$ on $[-R, 0)$, it is $\mathcal{C}^{k-1}$ at the singularity, and*

$$\lim_{t\to 0^-} \frac{d^l}{dt^l} P_j(\gamma(t)) = \lim_{t\to 0^-} \frac{d^l}{dt^l} P_j(\ell_k(t)), \qquad l = 0, \ldots, k-1,$$

where the limits above hold in the operator norm. The same result holds for $P_{j+1}(\gamma(\cdot))$.

Conical intersections have a characterization in terms of the non-degeneracy of a particular matrix, which contains some geometric properties of the eigenspaces relative to the intersecting eigenvalues, as shown below.

Definition 8. *We define the* conicity matrix *associated with two orthonormal elements* $\psi_1, \psi_2 \in \mathcal{D}(H_0)$ *as*

$$\mathcal{M}(\psi_1,\psi_2) = \begin{pmatrix} \langle \psi_1, H_1\psi_2\rangle & \langle \psi_1, H_1\psi_2\rangle^* & \langle \psi_2, H_1\psi_2\rangle - \langle \psi_1, H_1\psi_1\rangle \\ \langle \psi_1, H_2\psi_2\rangle & \langle \psi_1, H_2\psi_2\rangle^* & \langle \psi_2, H_2\psi_2\rangle - \langle \psi_1, H_2\psi_1\rangle \\ \langle \psi_1, H_3\psi_2\rangle & \langle \psi_1, H_3\psi_2\rangle^* & \langle \psi_2, H_3\psi_2\rangle - \langle \psi_1, H_3\psi_1\rangle \end{pmatrix}.$$

The following lemma can be proved by direct computation.

Lemma 9. *The quantity* $\det \mathcal{M}(\psi_1,\psi_2)$ *is purely imaginary and the function* $(\psi_1,\psi_2) \mapsto \det \mathcal{M}(\psi_1,\psi_2)$ *is invariant under unitary transformation of the argument, that is if* $\begin{pmatrix} \widehat{\psi}_1 \\ \widehat{\psi}_2 \end{pmatrix} = \mathbb{U}\begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ *for a pair* ψ_1, ψ_2 *of orthonormal elements of* $\mathcal{D}(H_0)$ *and* $\mathbb{U} \in$ *U(2), then one has* $\det \mathcal{M}(\widehat{\psi}_1, \widehat{\psi}_2) = \det \mathcal{M}(\psi_1,\psi_2)$.

As a consequence of the result here above, the determinant of $\mathcal{M}(\psi_1,\psi_2)$ depends only on the complex space spanned by ψ_1 and ψ_2. Therefore, in a neighborhood of a conical intersection between the levels λ_j, λ_{j+1} we can define the following function:

$$F(\mathbf{u}) = \det \mathcal{M}(\psi_1,\psi_2) \tag{8}$$

where $\{\psi_1,\psi_2\}$ is an orthonormal basis for the sum of eigenspaces relative to λ_j, λ_{j+1}. In particular, outside the intersection we can take, for instance, $\psi_1 = \phi_j$ and $\psi_2 = \phi_{j+1}$. Thanks to the continuity of $\boldsymbol{P}_{\mathbf{u}}$, which follows from Proposition 26, we obtain that F is continuous (see [10]).

The following result characterizes conical intersections in terms of the conicity matrix.

Proposition 10. *Assume that* $(\omega, \{\lambda_j, \lambda_{j+1}\})$ *is a separated discrete spectrum with* $\lambda_j(\bar{\mathbf{u}}) = \lambda_{j+1}(\bar{\mathbf{u}})$*, for some* $\bar{\mathbf{u}} \in \omega$*. Let* $\{\psi_1,\psi_2\}$ *be an orthonormal basis of the eigenspace associated with the double eigenvalue. Then* $\bar{\mathbf{u}}$ *is a conical intersection if and only if* $\mathcal{M}(\psi_1,\psi_2)$ *is nonsingular.*

Proof. Define $r_{\mathbf{v}}(t) = \bar{\mathbf{u}} + t\mathbf{v}$, where $\mathbf{v}$ is a unit vector in $\mathbb{R}^3$, and let $\phi_j^{\mathbf{v}}, \phi_{j+1}^{\mathbf{v}}$ be the limits of $\phi_j(r_{\mathbf{v}}(t)), \phi_{j+1}(r_{\mathbf{v}}(t))$ as $t \to 0^+$ (recall that the eigenfunctions ϕ_j, ϕ_{j+1} can be chosen analytic along $r_{\mathbf{v}}$ for $t \geq 0$). Assume that the intersection is not conical. Then for every $\varepsilon > 0$ there is a unit vector $\mathbf{v}_\varepsilon = (v_1^\varepsilon, v_2^\varepsilon, v_3^\varepsilon)$ such that

$$\frac{d}{dt}\Big|_{t=0^+}\Big[\lambda_{j+1}(r_{\mathbf{v}_\varepsilon}(t)) - \lambda_j(r_{\mathbf{v}_\varepsilon}(t))\Big] \leq \varepsilon.$$

By (4) and (6) we deduce that, if $\mathbb{A}_\varepsilon$ is an orthogonal matrix having $\mathbf{v}_\varepsilon$ as first row, then the first row of the matrix $\mathbb{A}_\varepsilon \mathcal{M}(\phi_j^{\mathbf{v}_\varepsilon}, \phi_{j+1}^{\mathbf{v}_\varepsilon})$ is equal to $(0,0,a)$ for some a whose absolute value is smaller than ε. As a consequence

$$\left|\det \mathcal{M}(\phi_j^{\mathbf{v}_\varepsilon}, \phi_{j+1}^{\mathbf{v}_\varepsilon})\right| = \left|\det\left(\mathbb{A}_\varepsilon \mathcal{M}(\phi_j^{\mathbf{v}_\varepsilon}, \phi_{j+1}^{\mathbf{v}_\varepsilon})\right)\right| \leq C\varepsilon(\alpha|\lambda_j(\mathbf{u})| + \beta)^2,$$

with C, α and β suitable positive constants, where we have used the fact that H_i is $H(\mathbf{u})$-bounded for $i = 1,2,3$. By arbitrariness of ε, the conicity matrix is singular. Let us now prove the converse statement: assume that $\bar{\mathbf{u}}$ is a conical intersection and, by contradiction, that $\mathcal{M}(\psi_1,\psi_2)$ is singular for every orthonormal basis of the eigenspace associated with the double eigenvalue. We introduce the matrix

$$\widetilde{\mathcal{M}}(\psi_1,\psi_2)=\begin{pmatrix}\mathfrak{Re}\left(\langle\psi_1,H_1\psi_2\rangle\right) & \mathfrak{Im}\left(\langle\psi_1,H_1\psi_2\rangle\right) & \left(\langle\psi_2,H_1\psi_2\rangle-\langle\psi_1,H_1\psi_1\rangle\right)\\ \mathfrak{Re}\left(\langle\psi_1,H_2\psi_2\rangle\right) & \mathfrak{Im}\left(\langle\psi_1,H_2\psi_2\rangle\right) & \left(\langle\psi_2,H_2\psi_2\rangle-\langle\psi_1,H_2\psi_1\rangle\right)\\ \mathfrak{Re}\left(\langle\psi_1,H_3\psi_2\rangle\right) & \mathfrak{Im}\left(\langle\psi_1,H_3\psi_2\rangle\right) & \left(\langle\psi_2,H_3\psi_2\rangle-\langle\psi_1,H_3\psi_1\rangle\right)\end{pmatrix},$$

and we notice that $\det\mathcal{M}(\psi_1,\psi_2)=-2i\det\widetilde{\mathcal{M}}(\psi_1,\psi_2)$ so that $\mathcal{M}(\psi_1,\psi_2)$ is singular if and only if $\widetilde{\mathcal{M}}(\psi_1,\psi_2)$ is. The condition of conical intersection, together with (4) and (6), implies that $\mathbf{v}^T\widetilde{\mathcal{M}}(\phi_j^{\mathbf{v}},\phi_{j+1}^{\mathbf{v}})=(0,0,a)$ for some $a\neq 0$, so that the third column of the matrix $\widetilde{\mathcal{M}}(\phi_j^{\mathbf{v}},\phi_{j+1}^{\mathbf{v}})$ is never linearly dependent from the first two. In particular the matrix $\widetilde{\mathcal{M}}(\phi_j^{\mathbf{v}},\phi_{j+1}^{\mathbf{v}})$ is singular only if the first two columns of the matrix are linearly dependent. Thus, up to multiplying $\phi_j^{\mathbf{v}},\phi_{j+1}^{\mathbf{v}}$ by phase factors, we can always assume that $\langle\phi_j^{\mathbf{v}},H_i\phi_{j+1}^{\mathbf{v}}\rangle\in\mathbb{R},\ i=1,2,3.$

Let us now fix a unit vector $\mathbf{v}\in\mathbb{R}^3$ and let us call W the orthogonal complement in $\mathbb{R}^3$ of the vector $\left(\langle\phi_j^{\mathbf{v}},H_1\phi_{j+1}^{\mathbf{v}}\rangle,\langle\phi_j^{\mathbf{v}},H_2\phi_{j+1}^{\mathbf{v}}\rangle,\langle\phi_j^{\mathbf{v}},H_3\phi_{j+1}^{\mathbf{v}}\rangle\right)$. We have that $\mathbf{v}\in W$ and $\dim W\geq 2$. By direct computations it is easy to prove that, for every $\mathbf{w}\in W$, the limit basis $\{\phi_j^{\mathbf{w}},\phi_{j+1}^{\mathbf{w}}\}$ is equal to $\{\phi_j^{\mathbf{v}},\phi_{j+1}^{\mathbf{v}}\}$, up to exchanges between the two elements and up to phases.

For $\mathbf{w}\in W$ let us consider the vector

$$\Upsilon=\begin{pmatrix}\langle\phi_{j+1}^{\mathbf{w}},H_1\phi_{j+1}^{\mathbf{w}}\rangle-\langle\phi_j^{\mathbf{w}},H_1\phi_j^{\mathbf{w}}\rangle\\ \langle\phi_{j+1}^{\mathbf{w}},H_2\phi_{j+1}^{\mathbf{w}}\rangle-\langle\phi_j^{\mathbf{w}},H_2\phi_j^{\mathbf{w}}\rangle\\ \langle\phi_{j+1}^{\mathbf{w}},H_3\phi_{j+1}^{\mathbf{w}}\rangle-\langle\phi_j^{\mathbf{w}},H_3\phi_j^{\mathbf{w}}\rangle\end{pmatrix},$$

which corresponds to the third column of $\widetilde{\mathcal{M}}(\phi_j^{\mathbf{w}},\phi_{j+1}^{\mathbf{w}})$. Notice that the definition of Υ, up to a sign, does not depend on the choice of $\mathbf{w}\in W$, by previous remarks. Since $\Upsilon^\perp$, the orthogonal complement of Υ in $\mathbb{R}^3$, has dimension 2 there exists a non-zero $\widetilde{\mathbf{w}}\in W\cap\Upsilon^\perp$. By definition of $\widetilde{\mathbf{w}}$ we have that $\widetilde{\mathbf{w}}\cdot\Upsilon=0$.

We get a contradiction, thus the matrix $\widetilde{\mathcal{M}}(\phi_j^{\mathbf{v}},\phi_{j+1}^{\mathbf{v}})$ must be nonsingular, and therefore also $\mathcal{M}(\phi_j^{\mathbf{v}},\phi_{j+1}^{\mathbf{v}})$ has to. ∎

A peculiarity of conical intersections is that, when approaching the singularity from different directions, the eigenstates corresponding to the intersecting eigenvalues have different limits. The following proposition provides the relation between these limits.

Proposition 11. *Let $\bar{\mathbf{u}}$ be a conical intersection between λ_j and λ_{j+1}. Let $\mathbf{v}_0,\mathbf{v}\in\mathbb{R}^3$ be two unit vectors, and call ϕ_j^0,ϕ_{j+1}^0 the limits as $t\to 0^+$ of the eigenstates $\phi_j(r_0(t)),\phi_{j+1}(r_0(t))$ along a straight line $r_0(t)=\bar{\mathbf{u}}+t\mathbf{v}_0$, and $\phi_j^{\mathbf{v}},\phi_{j+1}^{\mathbf{v}}$ the limit basis along the straight line $r_{\mathbf{v}}(t)=\bar{\mathbf{u}}+t\mathbf{v}$. Then, up to phases, the following relation holds:*

$$\begin{pmatrix}\phi_j^{\mathbf{v}}\\ \phi_{j+1}^{\mathbf{v}}\end{pmatrix}=\begin{pmatrix}\cos\boldsymbol{\Xi} & e^{-i\beta}\sin\boldsymbol{\Xi}\\ -e^{i\beta}\sin\boldsymbol{\Xi} & \cos\boldsymbol{\Xi}\end{pmatrix}\begin{pmatrix}\phi_j^0\\ \phi_{j+1}^0\end{pmatrix}, \tag{9}$$

where the parameters $\boldsymbol{\Xi}=\boldsymbol{\Xi}(\mathbf{v})$ and $\beta=\beta(\mathbf{v})$ satisfy the following equations:

$$\tan 2\boldsymbol{\Xi}(\mathbf{v})=(-1)^\xi\frac{2|\langle\phi_j^0,H_{\mathbf{v}}\phi_{j+1}^0\rangle|}{\langle\phi_j^0,H_{\mathbf{v}}\phi_j^0\rangle-\langle\phi_{j+1}^0,H_{\mathbf{v}}\phi_{j+1}^0\rangle} \tag{10}$$

$$\beta(\mathbf{v})\overset{(\mathrm{mod}\,2\pi)}{=}\arg\langle\phi_j^0,H_{\mathbf{v}}\phi_{j+1}^0\rangle+\xi\pi, \tag{11}$$

where $H_{\mathbf{v}}=\sum_{i=1}^m H_i v_i$ and $\xi=0,1$.

Proof. First of all, we notice that all pairs of orthonormal eigenstates of $H(\bar{\mathbf{u}})$ relative to the degenerate eigenvalue can be obtained through the action of the group $\mathsf{U}(2)$ on the pair (ϕ_j^0, ϕ_{j+1}^0). However, if one takes into account the equivalence relation $(e^{i\beta_1}\psi_1, e^{i\beta_2}\psi_2) \sim (\psi_1, \psi_2)\ \forall\ \beta_1, \beta_2 \in \mathbb{R}$, it is enough to consider the transformations of the form (9). If $\mathbf{v} = \pm\mathbf{v}_0$, then $\langle \phi_j^0, H_{\mathbf{v}}\phi_{j+1}^0\rangle = 0$ by (6), and we can assume $\boldsymbol{\Xi}(\mathbf{v}) = k\pi/2$ for some integer k, while $\beta(\mathbf{v})$ can be any real number. If $\mathbf{v}$ is not parallel to $\mathbf{v}_0$ then, as a consequence of Proposition 10, $\mathbf{v}^T\mathcal{M}(\phi_j^0, \phi_{j+1}^0)$ is not parallel to $\mathbf{v}_0^T\mathcal{M}(\phi_j^0, \phi_{j+1}^0)$, so that $\langle \phi_j^0, H_{\mathbf{v}}\phi_{j+1}^0\rangle \neq 0$. The two cases defined by (10)-(11) follow from $\langle \phi_j^{\mathbf{v}}, H_{\mathbf{v}}\phi_{j+1}^{\mathbf{v}}\rangle = 0$, once we replace $\phi_j^{\mathbf{v}}, \phi_{j+1}^{\mathbf{v}}$ with the expression given in (9). ∎

It can be seen that not all the solutions of (10)-(11) provide the correct transformation (9), which, nevertheless, is easy to detect. The good solutions of (10)-(11) constitute four branches which are continuous with respect to $\mathbf{v}$, and they can be constructed as follows. Let $\mathbf{w}(s)$, $s \in [0, \bar{s}]$, be a curve joining $\mathbf{v_0}$ to $\mathbf{v}$ such that $\mathbf{w}(s) \notin \{\mathbf{v}_0, -\mathbf{v}_0\}$ for every $s \in (0, \bar{s})$; for conical intersections, it is possible to associate with such a curve a continuous solution $(\boldsymbol{\Xi}(\mathbf{w}(s)), \beta(\mathbf{w}(s)))$ of (10)-(11) with $\boldsymbol{\Xi}(\mathbf{v}_0) = 0$ and compatible with (9). In particular, if we choose $\boldsymbol{\Xi}(\mathbf{v})$ satisfying (10) with $\xi = 0$, it is easy to see that $\boldsymbol{\Xi}(\mathbf{w}(s)) \in [-\pi/2, 0]$ for $s \in [0, \bar{s}]$, from which one deduces that the final value $\boldsymbol{\Xi}(\mathbf{v}) = \boldsymbol{\Xi}(\mathbf{w}(\bar{s}))$ is independent of the chosen path and continuously depends on $\mathbf{v}$. Moreover, it is easy to see that $\boldsymbol{\Xi}(-\mathbf{v}_0) = -\pi/2$. Similarly $\beta(\mathbf{v}) = \beta(\mathbf{w}(\bar{s}))$ is independent of the chosen path and continuous outside $\{\mathbf{v}_0, -\mathbf{v}_0\}$. Note that the fact that β is discontinuous at $-\mathbf{v}_0$ implies that the corresponding limit basis $(\phi_j^{\mathbf{v}}, \phi_{j+1}^{\mathbf{v}})$ has a discontinuity at $-\mathbf{v}_0$, that is, its limit depends on the path. We can repeat the same argument choosing $\boldsymbol{\Xi}(\mathbf{v})$ satisfying (10) with $\xi = 1$ and with initial condition $\boldsymbol{\Xi}(\mathbf{v}_0) = 0$. The other two continuous branches are obtained choosing the initial condition $\boldsymbol{\Xi}(\mathbf{v}_0) = \pi$.

3.2. The basic control algorithm. Let us consider the following controllability problem.

Let $H(\cdot)$ satisfy **(H0)** *and have a separated discrete spectrum (ω, Σ) with $\Sigma(\cdot) = \{\lambda_0(\cdot), \dots, \lambda_k(\cdot)\}$. Then, given $\eta > 0$, $\mathbf{u}^s, \mathbf{u}^f \in \omega$, $j \in \{0, \dots, k\}$ and $p \in [0,1]^{k+1}$ such that $\sum_{l=0}^k p_l^2 = 1$, find $T > 0$ and a path $\mathbf{u} : [0,T] \to \omega$ with $\mathbf{u}(0) = \mathbf{u}^s$ and $\mathbf{u}(T) = \mathbf{u}^f$ such that*

$$\|\psi(T) - \sum_{l=0}^{k} p_l e^{i\vartheta_l}\phi_l(\mathbf{u}^f)\| \leq \eta,$$

where $\psi(\cdot)$ is the solution of (3) with $\psi(0) = \phi_j(\mathbf{u}^s)$, and $\vartheta_0, \dots, \vartheta_k \in \mathbb{R}$ are some possibly unknown phases.

If all levels are connected by means of conical intersections occurring at different values of the control, the results obtained in the previous section provide the basic elements to construct a family of control paths solving the problem here above. This can be done by taking advantage of the following proposition, which describes the spreading of occupation probabilities induced when a path in the space of controls passes through a conical intersection.

PROPOSITION 12. *Let $\bar{\mathbf{u}}$ be a conical intersection between the eigenvalues λ_j, λ_{j+1}. Consider the curve $\gamma : [0,1] \to \omega$ defined by*

$$\gamma(t) = \begin{cases} \bar{\mathbf{u}} + (t - \bar{\tau})\mathbf{w}_0 & t \in [0, \bar{\tau}] \\ \bar{\mathbf{u}} + (t - \bar{\tau})\mathbf{v} & t \in [\bar{\tau}, 1] \end{cases},$$

for some $\bar\tau \in (0,1)$ and some unit vectors $\mathbf{w}_0, \mathbf{v}$. Then there exists $C > 0$ such that, for any $\varepsilon > 0$,

$$\|\psi(1/\varepsilon) - \pi_1 e^{i\vartheta_1}\phi_j(\gamma(1)) - \pi_2 e^{i\vartheta_2}\phi_{j+1}(\gamma(1))\| \leq C\sqrt{\varepsilon}$$

where $\vartheta_1,\ \vartheta_2 \in \mathbb{R}$, $\psi(\cdot)$ is the solution of equation (3) with $\psi(0) = \phi_j(\gamma(0))$ corresponding to the control $\mathbf{u} : [0, 1/\varepsilon] \to \omega$ defined by $\mathbf{u}(t) = \gamma(\varepsilon t)$,

$$\pi_1 = |\cos(\mathbf{\Xi}(\mathbf{v}))|,\ \ \pi_2 = |\sin(\mathbf{\Xi}(\mathbf{v}))|,$$

and $\mathbf{\Xi}(\cdot)$ is the only solution of equation (10) with $\xi = 0$ such that $\mathbf{\Xi}(\mathbf{v}) \in (-\pi/2, 0]$ for $\mathbf{v} \neq -\mathbf{w}_0$, and $\mathbf{\Xi}(-\mathbf{w}_0) = -\pi/2$, where the limit basis in (10) is given by the limits $\phi_j(\gamma(\bar\tau^-)), \phi_{j+1}(\gamma(\bar\tau^-))$, respectively.

Proof. We consider the Hamiltonian $H(\mathbf{u}(t))$, $t \in [0, 1/\varepsilon]$. Since the control function $\mathbf{u}(\cdot)$ is not $\mathcal{C}^2$ at the singularity, we cannot directly apply the adiabatic theorem. Instead, we consider separately the evolution on the two subintervals (in time t) $[0, \bar\tau/\varepsilon]$ and $[\bar\tau/\varepsilon, 1/\varepsilon]$. Since the eigenstates $\phi_j(\mathbf{u}(t)), \phi_{j+1}(\mathbf{u}(t))$ are piecewise $\mathcal{C}^1$, we can apply [28, Corollary 2.5] and obtain that there exists a phase θ_1 (depending on ε) such that

$$\|\psi(\bar\tau/\varepsilon) - e^{i\theta_1}\phi_j(\gamma(\bar\tau^-))\| \leq C'\sqrt{\varepsilon},$$

for some constant $C' > 0$. By Proposition 11, this implies that

$$\|\psi(\bar\tau/\varepsilon) - e^{i\theta_1}\Big(\cos\mathbf{\Xi}(\mathbf{v})\ \phi_j(\gamma(\bar\tau^+)) - e^{-i\beta(\mathbf{v})}\sin\mathbf{\Xi}(\mathbf{v})\ \phi_{j+1}(\gamma(\bar\tau^+))\Big)\| \leq C'\sqrt{\varepsilon},$$

with $\mathbf{\Xi}(\mathbf{v})$ as in the statement of the proposition and $\beta(\mathbf{v}) = \arg\langle\phi_j^0, H_{\mathbf{v}}\phi_{j+1}^0\rangle$. By applying [28, Corollary 2.5] also in the time interval $(\bar\tau/\varepsilon, 1/\varepsilon)$ we get the thesis. ☐

For control purposes, it is interesting to consider the problem of determining a path that induces the desired transition in the case in which the initial probability is concentrated in the first level and the final occupation probabilities π_1^2 and π_2^2 are prescribed. For a given line reaching the conical intersection, the outward directions that provide the required spreading of probability are given in the following proposition. The proof easily follows from Proposition 11.

PROPOSITION 13. *Let $\bar{\mathbf{u}}$ be a conical intersection between the eigenvalues λ_j, λ_{j+1}, and let π_1, π_2 be positive constants such that $\pi_1^2 + \pi_2^2 = 1$. Consider the line $r(t) = \bar{\mathbf{u}} + (t - \bar\tau)\mathbf{w}_0$, $t \in [0, \bar\tau]$, for a unit vector $\mathbf{w}_0 \in \mathbb{R}^3$ and some $\bar\tau \in (0,1)$, and set $\phi_j^0 = \phi_j(r(\bar\tau^-))$ and $\phi_{j+1}^0 = \phi_{j+1}(r(\bar\tau^-))$.*

Then the locus formed by the directions $\mathbf{v} \in \mathbb{R}^3$ that give rise to transformation (9) with $\pi_1 = |\cos\Xi(\mathbf{v})|$ and $\pi_2 = |\sin\Xi(\mathbf{v})|$ is given by the following expression whenever $\pi_1 \notin \{0, 1\}$

$$\widetilde{\mathcal{M}}(\phi_j^0, \phi_{j+1}^0)^{-T}(\mathcal{K}),$$

where $\mathcal{K} = \left\{(x,y,z) \in \mathbb{R}^3 : \sqrt{x^2+y^2} = \frac{\pi_1\pi_2}{\pi_1^2-\pi_2^2}z\right\}$. Otherwise, if $\pi_1 = 0$ then $\mathbf{v} = \mathbf{w}_0$ and if $\pi_1 = 1$ then $\mathbf{v} = -\mathbf{w}_0$.

The controllability problem presented at the beginning of this section can be solved taking advantage of the results shown above. The strategy consists in constructing a piecewise $\mathcal{C}^2$ path joining $\mathbf{u}^s$ with $\mathbf{u}^f$ that passes through the conical intersections $\bar{\mathbf{u}}_j$ between the j-th and the $(j+1)$-th levels, $j = 0, \ldots, k-1$, and avoids any other degeneracy point. The tangent directions at the conical intersection are chosen according to the probability weights p_j^2, as explained in Proposition 13.

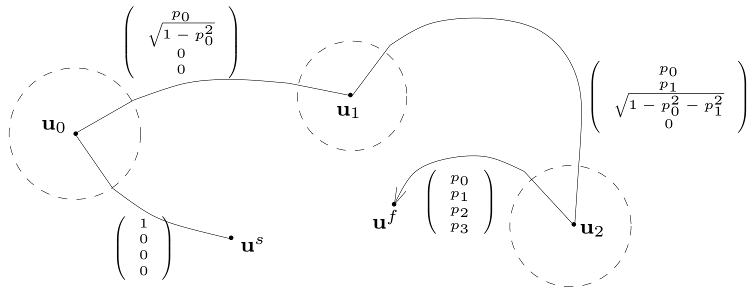

FIG. 1. *Construction of the path $\gamma(\cdot)$. The corners at the points $\mathbf{u}_i$, corresponding to conical intersections, are chosen in such a way that they induce the desired spreading.*

For simplicity we assume that $\psi(0) = \phi_0(\mathbf{u}^s)$; in the other cases a path can be obtained similarly. We set $\gamma(0) = \mathbf{u}^s$ and, for some $0 < \tau_0 < 1$ we choose $\gamma|_{[0,\tau_0]}$ in such a way that $\gamma(\tau_0) = \bar{\mathbf{u}}_0$ and all the eigenvalues $\lambda_l(\gamma(\tau))$ are simple for every $l = 0,\dots,k$ and $\tau \in [0,\tau_0)$. Moreover, $\gamma(\cdot)$ is chosen tangent to a segment in a neighborhood of $\bar{\mathbf{u}}_0$. The rest of the path is then constructed recursively as follows. Assume that the path has been defined up to time τ_j, for some $j = 0,\dots,k-2$, with $\gamma(\tau_j) = \bar{\mathbf{u}}_j$, and that it is tangent to a segment of direction $\mathbf{v}_j^-$ in a neighborhood of $\bar{\mathbf{u}}_j$. Then $\gamma|_{[\tau_j,\tau_{j+1}]}$, where $\tau_{j+1} \in (\tau_j, 1)$, is chosen to be tangent, in a neighborhood of $\bar{\mathbf{u}}_j$, to a segment directed as $\mathbf{v}_j^+$, where $\mathbf{v}_j^+$ is obtained applying Proposition 13 with $\mathbf{w}_0 = \mathbf{v}_j^-$, $\pi_1 = p_j/\sqrt{\sum_{l=j}^k p_l^2}$ and $\pi_2 = \sqrt{1-\pi_1^2}$. Moreover $\gamma|_{[\tau_j,\tau_{j+1}]}$ is such that $\gamma(\tau_{j+1}) = \bar{\mathbf{u}}_{j+1}$ and is tangent to a straight line on a neighborhood of $\bar{\mathbf{u}}_{j+1}$. The last arc defined on $(\tau_{k-1}, 1]$ is simply constructed by joining $\bar{\mathbf{u}}_{k-1}$ with $\mathbf{u}^f$, taking care of choosing $\gamma(\cdot)$ tangent to the outward direction obtained through Proposition 13, in a neighborhood of $\bar{\mathbf{u}}_{k-1}$. To avoid highly non-homogeneous parameterizations, the path $\gamma(\cdot)$ can be reparameterized by arc-length. The geometric construction of the path is represented in Figure 1.

Let us now reparameterize the time by setting $t = \tau/\varepsilon$, for some small positive ε. When we are far from all the conical intersections it follows from Theorem 5 that the evolution of $H(\gamma(\varepsilon t))$ conserves the occupation probabilities relative to each energy level λ_l, $l = 0,\dots,k$, with an approximation of order ε. Similarly, in a neighborhood of the conical intersection between λ_j and λ_{j+1}, $j = 0,\dots,k-1$, the evolution of $H(\gamma(\varepsilon t))$ conserves the occupation probabilities relative to each non-intersecting energy level with an approximation of order ε. The occupation probabilities relative to the j−th and $(j+1)$−th levels are instead estimated by combining Theorem 5 with the estimate provided by Proposition 12.

Summing up, we obtain the estimate

$$\|\psi(1/\varepsilon) - \sum_{l=0}^{k} p_l e^{i\vartheta_l}\phi_l(\mathbf{u}^f)\| \le C\sqrt{\varepsilon},$$

for some $\vartheta_0,\dots,\vartheta_k \in \mathbb{R}$ and some $C > 0$ depending on the path $\gamma(\cdot)$ and on the gaps in the spectrum.

4. An improvement of the efficiency of the algorithm: the non-mixing field. The problem of reducing transition times is quite important in quantum control, in particular for the need of preventing decoherence. In this section we show how to construct special paths in the space of controls that permit to speed up the process:

indeed, the error accumulated when following these paths is inversely proportional to the total time of the transition, while the basic strategy described in Proposition 12 guarantees an error scaling with the inverse of the square root of the total time, so that shorter times are sufficient to guarantee a prescribed accuracy.

Let us consider a pair $\{\lambda_j, \lambda_{j+1}\}$ of eigenvalues separated from the rest of the spectrum in a certain open set $\omega \subset \mathbb{R}^3$, according to Definition 2, and intersecting only at $\bar{\mathbf{u}} \in \omega$ where they form a conical intersection. We are interested in the dynamics inside the subspace $\boldsymbol{P}_{\mathbf{u}}\mathcal{H}$, where $\boldsymbol{P}_{\mathbf{u}}$ denotes the projection associated with the two levels $\{\lambda_j(\mathbf{u}), \lambda_{j+1}(\mathbf{u})\}$ for $\mathbf{u} \in \omega$. To improve the algorithm described in the previous section, the idea is to cancel the off-diagonal terms in the effective Hamiltonian (7), which are responsible of the error of order $\sqrt{\varepsilon}$ in the estimates given in [28, Corollary 2.5] and in Proposition 12. In order to do that, we choose some special trajectories in ω along which the term $\langle \phi_j, \dot{\phi}_{j+1}\rangle$ is null.

We denote the first column of the conicity matrix $\mathcal{M}(\psi_1, \psi_2)$ by $\boldsymbol{m}(\psi_1, \psi_2)$ and its components $\langle \psi_1, H_i \psi_2\rangle$ as m_i, and we define the vector

$$X(\psi_1, \psi_2) = \mathfrak{Im}(\boldsymbol{m}(\psi_1, \psi_2)) \times \mathfrak{Re}(\boldsymbol{m}(\psi_1, \psi_2)) = \mathfrak{Im}\,(m_2 m_3^*, m_3 m_1^*, m_1 m_2^*)^T \tag{12}$$

where $\times$ denotes the cross product.

REMARK 14. *Let us remark that the vector $X(\psi_1, \psi_2)$ is invariant under phase changes in the argument, that is $X(\psi_1, \psi_2) = X(e^{i\beta_1}\psi_1, e^{i\beta_2}\psi_2)$. Notice however that $X(\psi_1, \psi_2) = -X(\psi_2, \psi_1)$.*

DEFINITION 15. *Given a conical intersection $\bar{\mathbf{u}}$, the vector field*

$$\mathcal{X}_P(\mathbf{u}) = X(\phi_j(\mathbf{u}), \phi_{j+1}(\mathbf{u})),$$

defined in $\omega \setminus \{\bar{\mathbf{u}}\}$, is called the non-mixing field associated with $\bar{\mathbf{u}}$.

The non-mixing field is smooth in its domain of definition. From (5) and (12), we have $\langle \phi_j, \dot{\phi}_{j+1}\rangle = 0$ along its integral curves. Moreover, a simple computation leads to

$$X(\psi_1, \psi_2) \cdot \begin{pmatrix} \langle \psi_2, H_1\psi_2\rangle - \langle \psi_1, H_1\psi_1\rangle \\ \langle \psi_2, H_2\psi_2\rangle - \langle \psi_1, H_2\psi_1\rangle \\ \langle \psi_2, H_3\psi_2\rangle - \langle \psi_1, H_3\psi_1\rangle \end{pmatrix} = \frac{1}{2i}\det \mathcal{M}(\psi_1, \psi_2), \tag{13}$$

which implies the following result.

PROPOSITION 16. *Let $\bar{\mathbf{u}}$ be a conical intersection and $\gamma(\cdot) \subset \omega\setminus\{\bar{\mathbf{u}}\}$ be an integral curve of the non-mixing field. Then*

$$\frac{d}{dt}\big[\lambda_{j+1}(\gamma(t)) - \lambda_j(\gamma(t))\big] = \frac{1}{2i}F(\gamma(t)),$$

where $F(\cdot)$ is defined in (8). In particular, all the integral curves of the non-mixing field starting from a punctured neighborhood of the conical intersection reach it in finite time (up to a time reversal).

Without loss of generality, we can assume that $\bar{\mathbf{u}} = 0$. Denote every $\mathbf{u} \in \mathbb{R}^3$ by $\mathbf{u} = \rho\mathbf{v}$, where ρ is its module and $\mathbf{v}$ the versor. Let us call $\mu(\rho, \mathbf{v}) = \boldsymbol{m}(\phi_j(\rho, \mathbf{v}), \phi_{j+1}(\rho, \mathbf{v}))$, where $\phi_j(\rho, \mathbf{v}), \phi_{j+1}(\rho, \mathbf{v})$ denotes a choice of the eigenstates relative respectively to $\lambda_j(\rho\mathbf{v})$ and $\lambda_{j+1}(\rho\mathbf{v})$ (extended by continuity for $\rho = 0$). We remark that $\mu(\rho, \mathbf{v})$ is defined up to a phase. Finally, set $\mathcal{X}_\mu(\rho, \mathbf{v}) = \mathcal{X}_P(\rho\mathbf{v})$. Notice that, for different values of $\mathbf{v}$, $\mathcal{X}_\mu(\rho, \mathbf{v})$ has a priori different limits as ρ tends to 0.

The following estimates hold.

LEMMA 17. *Assume that $\bar{\mathbf{u}} = 0$ is a conical intersection. Then the inequality $|\mu(\rho, \mathbf{v}) \cdot \mathbf{v}| \le C\rho$ holds in a neighborhood of 0 for some constant $C > 0$ uniform with respect to $\mathbf{v}$.*

Proof. Up to shifting H_0 by a multiple of the identity we may assume $\lambda_j(0) = \lambda_{j+1}(0) = 0$. Then

$$\begin{aligned}\rho\mu(\rho, \mathbf{v}) \cdot \mathbf{v} &= \rho \langle \phi_j(\rho, \mathbf{v}), (v_1 H_1 + v_2 H_2 + v_3 H_3)\phi_{j+1}(\rho, \mathbf{v})\rangle \\ &= -\langle \phi_j(\rho, \mathbf{v}), H_0 \phi_{j+1}(\rho, \mathbf{v})\rangle = -\langle \phi_j(\rho, \mathbf{v}) - \boldsymbol{P}_0 \phi_j(\rho, \mathbf{v}), H_0 \phi_{j+1}(\rho, \mathbf{v})\rangle.\end{aligned}$$

Assumption **(H0)** implies that

$$\|H_0 \phi_{j+1}(\rho, \mathbf{v})\| \le |\lambda_{j+1}(\rho \mathbf{v})| + \rho \sum_{i=1}^{3} \|H_i \phi_{j+1}(\rho, \mathbf{v})\| \le c\rho,$$

for some $c > 0$, locally around the intersection. By smoothness of the projection, we get that

$$\left|\langle \phi_j(\rho, \mathbf{v}) - \boldsymbol{P}_0 \phi_j(\rho, \mathbf{v}), H_0 \phi_{j+1}(\rho, \mathbf{v})\rangle\right| \le C\rho^2,$$

for a suitable $C > 0$, hence we get the thesis. ∎

We are now ready to prove the following result, which provides some information on the behavior of the trajectories of the non-mixing field.

PROPOSITION 18. *With the notations introduced above and for ρ small enough, there exist three constants $c_1, c_2, c_3 > 0$ such that $c_1 \le |\dot{\rho}| \le c_2$ and $|\dot{\mathbf{v}}| \le c_3$ along the trajectories of the non-mixing field.*

Proof. Direct computations lead to the equations

$$\dot{\rho} = \mathcal{X}_\mu \cdot \mathbf{v}, \quad \dot{\mathbf{v}} = \frac{1}{\rho}\left(\mathcal{X}_\mu - (\mathcal{X}_\mu \cdot \mathbf{v})\,\mathbf{v}\right).$$

The upper bound for $|\dot{\rho}|$ comes easily from the $H(\mathbf{u})$-boundedness of H_i for every i.

From (13) we get that $|\mathcal{X}_\mu| \ge c$ for some $c > 0$ in a neighborhood of the singularity, which implies that the sinus of the angle between $\mathfrak{Im}(\mu(\rho, \mathbf{v}))$ and $\mathfrak{Re}(\mu(\rho, \mathbf{v}))$ is uniformly far from zero. As a consequence of this fact and of Lemma 17, for any unit vector $\mathbf{z}$ in the plane spanned by $\mathfrak{Im}(\mu(\rho, \mathbf{v}))$ and $\mathfrak{Re}(\mu(\rho, \mathbf{v}))$ one has $|\mathbf{z} \cdot \mathbf{v}| \le \hat{c}\rho$ for some $\hat{c} > 0$ and ρ small enough. The orthogonal projection of $\mathbf{v}$ on that plane may be written as $(\mathbf{v} \cdot \hat{\mathbf{v}})\hat{\mathbf{v}}$, where $\hat{\mathbf{v}}$ is a unit vector. Then

$$|\mathcal{X}_\mu \cdot \mathbf{v}| = |\mathcal{X}_\mu \cdot (\mathbf{v} - (\mathbf{v} \cdot \hat{\mathbf{v}})\hat{\mathbf{v}})| = \sqrt{1 - (\mathbf{v} \cdot \hat{\mathbf{v}})^2}\,|\mathcal{X}_\mu| \ge (1 - \hat{c}^2\rho^2)|\mathcal{X}_\mu|$$

and

$$|\mathcal{X}_\mu - (\mathcal{X}_\mu \cdot \mathbf{v})\,\mathbf{v}|^2 = |\mathcal{X}_\mu|^2 - (\mathcal{X}_\mu \cdot \mathbf{v})^2 \le 2\hat{c}^2\rho^2|\mathcal{X}_\mu|^2.$$

The thesis follows. ∎

The following proposition is a generalization of [10, Proposition 5.9] in the three dimensional case. The proof follows the same lines, thanks to Proposition 18, and is thus omitted.

PROPOSITION 19. *For every unit vector $\mathbf{v}$ in $\mathbb{R}^3$ there exists an integral curve $\gamma : [-\eta, 0] \to \omega$ of $\mathcal{X}_P$ with $\gamma(0) = 0$, $\eta > 0$, such that $\lim_{t \to 0^-} \frac{\dot{\gamma}(t)}{\|\dot{\gamma}(t)\|} = \mathbf{v}$.*

Thanks to Proposition 18, the integral curves of the non-mixing field are $\mathcal{C}^1$ up to the singularity included. In particular, they satisfy the hypotheses of Proposition 7 with $k=1$, so that the projections $P_j(\mathbf{u})$ and $P_{j+1}(\mathbf{u})$ on the eigenspaces relative to the intersecting eigenvalues are $\mathcal{C}^1$ along the integral curves of the non-mixing field outside the singularity, and can be continuously extended at the singularity. On the other hand, $\boldsymbol{P}_{\mathbf{u}}$ is C^1 along such curves, singularity included.

We remark moreover that, if $\gamma:[t_0,t_1]\to\mathbb{R}^3$ is an integral curve of the non-mixing field such that $\lambda_j(\gamma(t))\neq\lambda_{j+1}(\gamma(t))$ for $t\in[t_0,t_1)$, by definition of the non-mixing field, it holds

$$P_j(\gamma(t))\dot{P}_{j+1}(\gamma(t))=0 \qquad P_{j+1}(\gamma(t))\dot{P}_j(\gamma(t))=0 \qquad \forall\, t\in[t_0,t_1). \tag{14}$$

We have the following.

Proposition 20. *Along every integral curve of the non-mixing field, there is a choice of the eigenstates relative to the intersecting eigenvalues which is $\mathcal{C}^1$ up to the singularity included.*

Proof. Let $\gamma:[-T,0]\to\mathbb{R}^3$ be an integral curve of $\mathcal{X}_P$ such that $\gamma(0)=\bar{\mathbf{u}}$ is a conical intersection between λ_j and λ_{j+1}. Outside the singularity, the eigenstates are well defined, up to a phase. To fix the phase, we set $\psi_j(t)=\frac{P_j(\gamma(t))\widehat{\psi}}{\|P_j(\gamma(t))\widehat{\psi}\|}$, for some $\widehat{\psi}\in\mathcal{H}$ satisfying $P_j(\gamma(t))\widehat{\psi}\neq 0$ on $[0,T]$ (up to reducing T). Thus $\psi_j(t)$ is a normalized eigenstate of $H(\gamma(t))$ relative to $\lambda_j(\gamma(t))$. In order to prove that $\psi_j(t)$ is $\mathcal{C}^1$ it is enough to prove that $P_j(\gamma(t))$ is. Since $P_j(\gamma(t))+P_{j+1}(\gamma(t))=\boldsymbol{P}_{\gamma(t)}$ for $t\in[-T,0)$, and by (14), we get that $\boldsymbol{P}_{\gamma(t)}\dot{P}_j(\gamma(t))=P_j(\gamma(t))\dot{P}_j(\gamma(t))=P_j(\gamma(t))\dot{\boldsymbol{P}}_{\gamma(t)}$. Therefore

$$\dot{P}_j(\gamma(t))=\dot{\boldsymbol{P}}_{\gamma(t)}P_j(\gamma(t))+\boldsymbol{P}_{\gamma(t)}\dot{P}_j(\gamma(t))=\dot{\boldsymbol{P}}_{\gamma(t)}P_j(\gamma(t))+P_j(\gamma(t))\dot{\boldsymbol{P}}_{\gamma(t)},$$

where the right hand side has limit for $t\to 0^-$.

We can repeat the same procedure to show that there is a choice for $\psi_{j+1}(t)$ such that $\dot{\psi}_{j+1}(t)$ has limit for $t\to 0^-$. ∎

A suitable improvement of the regularity properties provided by Proposition 20 is actually needed in order to apply Theorem 6 along the integral curves of the non-mixing field, around conical intersections. This is achieved by the next result.

Proposition 21. *In a neighborhood of a conical intersection, the integral curves of its associated non-mixing field are $\mathcal{C}^\infty$ up to the singularity included. Moreover, we can choose $\mathcal{C}^\infty$ eigenstates ψ_j,ψ_{j+1} along such a curve, up to the singularity included.*

Proof. Let $\gamma:[-T,0]\to\mathbb{R}^3$ be an integral curve of $\mathcal{X}_P$ such that $\gamma(0)=\bar{\mathbf{u}}$ and $|\dot{\gamma}(t)|>0$ for every $t\in[-T,0]$ (this is true up to choosing T sufficiently small), and define the eigenstates $\psi_j(\cdot),\psi_{j+1}(\cdot)$ as in Proposition 20.

For simplicity, we denote by $\lambda_j(t),\lambda_{j+1}(t)$ and $P_j(t),P_{j+1}(t)$ the j-th and $(j+1)$-th eigenvalues and the corresponding spectral projections at $\gamma(t)$. We prove by induction that, for every positive integer h, $\gamma(\cdot),\lambda_l(\cdot),P_l(\cdot)$ and $H_iP_l(\cdot)$ are $\mathcal{C}^h$ on $[-T,0]$, where $l=j,j+1$ and $i=1,2,3$. The proposition then follows immediately.

For every non-negative integer h, whenever the h-th order derivatives of $P_l(\cdot)$ and $H_iP_l(\cdot)$ are well defined, the following inequality holds

$$\begin{aligned}\|H_i(P_l^{(h)}(s)-P_l^{(h)}(t))\| \leq &\|H_i\|_{H(\gamma(t))}\big(\|H(\gamma(s))P_l^{(h)}(s)-H(\gamma(t))P_l^{(h)}(t)\| \\ &+\sum_i|\gamma_i(s)-\gamma_i(t)|\|H_iP_l^{(h)}(s)\|+\|P_l^{(h)}(s)-P_l^{(h)}(t)\|\big).\end{aligned}$$

In particular, thanks to Proposition 20 and since H_i is $H(\gamma(s))$-bounded (uniformly with respect to s), this yields the continuity of $H_iP_l(\cdot)$ on $[-T,0]$ and the initialization step of the induction. Let us now take $h>0$; we prove that, if $\lambda_l(\cdot),P_l(\cdot)$ are $\mathcal{C}^h$ and $H_iP_l(\cdot)$ is $\mathcal{C}^{h-1}$, then $H_iP_l^{(h)}(\cdot)$ is continuous. Indeed, by differentiating h times the equality $H(\gamma(\cdot))P_l(\cdot)=\lambda_l(\cdot)P_l(\cdot)$ and exploiting the regularity assumptions on $\lambda_l(\cdot)$, $P_l(\cdot)$ and $H_iP_l(\cdot)$ we get that $H(\gamma(\cdot))P_l^{(h)}(\cdot)$ is continuous in $[-T,0]$. Since H_i is $H(\gamma(s))$-bounded we deduce that $\|H_iP_l^{(h)}(s)\|$ is uniformly bounded on $[-T,0]$. Then, the continuity of $H_iP_l^{(h)}(\cdot)$ follows from the above inequality.

Assume now that $\gamma(\cdot),\lambda_l(\cdot),P_l(\cdot)$ and $H_iP_l(\cdot)$ have been proved to be $\mathcal{C}^h$, for $h\leq k-1$. Then, by definition of $\mathcal{X}_P$ it turns out that $\gamma(\cdot)$ is $\mathcal{C}^k$ in $[-T,0]$ and, applying (4), we obtain that $\lambda_l(\cdot)$ is $\mathcal{C}^k$ in $[-T,0]$ too. Let us show that $P_l(\cdot)$ is $\mathcal{C}^k$. Note that $P_l(\cdot)=\boldsymbol{P}_{\gamma(\cdot)}P_l(\cdot)$, where $\boldsymbol{P}_{\gamma(\cdot)}$ is $\mathcal{C}^k$ in $[-T,0]$, because of the regularity of $\gamma(\cdot)$. Then, by inductive hypothesis, $P_l(\cdot)$ is $\mathcal{C}^k$ if and only if $\boldsymbol{P}_{\gamma(\cdot)}P_l^{(k)}(\cdot)$ is continuous in $[-T,0]$. We can develop $\boldsymbol{P}_{\gamma(t)}P_j^{(k)}(\gamma(t))$ as

$$\boldsymbol{P}_{\gamma(t)}P_j^{(k)}(t)=P_j(t)\boldsymbol{P}_{\gamma(t)}^{(k)}-P_j(t)P_{j+1}^{(k)}(t)+P_{j+1}(t)P_j^{(k)}(t).$$

The first term in the right-hand side is continuous in $[-T,0]$. By (14), it follows that $\frac{d^{k-1}}{dt^{k-1}}\left(P_j(t)\dot P_{j+1}(t)\right)\equiv 0$. Then, by inductive hypothesis, we get that $P_j(t)P_{j+1}^{(k)}(t)$ is continuous in $[-T,0]$. By a symmetric argument, $P_{j+1}(t)\dot P_j^{(k)}(t)$ is continuous in $[-T,0]$. We deduce that $\boldsymbol{P}_{\gamma(t)}P_j^{(k)}(\gamma(t))$ is continuous in $[-T,0]$, and so is $P_j^{(k)}(\cdot)$ (and, by symmetry, $P_{j+1}^{(k)}(\cdot)$). Since, as shown above, $H_iP_l^{(k)}(\cdot)$ is continuous in $[-T,0]$ for $l=j,j+1$ and $i=1,2,3$, the proof of the proposition is concluded. ∎

We are now ready to state the main result of this section, namely we show how the curves tangent to the non-mixing field allow to improve the performances of the control algorithm presented in Section 3.2.

THEOREM 22. *Let $H(\mathbf{u})=H_0+u_1H_1+u_2H_2+u_3H_3$ satisfy hypotheses* **(H0)**. *Assume that $(\omega,\{\lambda_0,\dots,\lambda_k\})$ is a separated discrete spectrum for $H(\mathbf{u})$ and that there exist conical intersections $\bar{\mathbf{u}}_j\in\omega$, $j=0,\dots,k-1$, between the eigenvalues λ_j,λ_{j+1}, with $\lambda_l(\bar{\mathbf{u}}_j)$ simple if $l\neq j,j+1$. Then, for every $\mathbf{u}^s$ and $\mathbf{u}^f$ such that the eigenvalues λ_l, $l=0,\dots,k$ are non degenerate at $\mathbf{u}^s$ and $\mathbf{u}^f$, for every $\bar\phi\in\{\phi_0(\mathbf{u}^s),\dots,\phi_k(\mathbf{u}^s)\}$, and $p\in[0,1]^{k+1}$ such that $\sum_{j=0}^k p_j^2=1$, there exist $C>0$ and a continuous control $\gamma(\cdot):[0,1]\to\mathbb{R}^m$ with $\gamma(0)=\mathbf{u}^s$ and $\gamma(1)=\mathbf{u}^f$, such that for every $\varepsilon>0$*

$$\|\psi(1/\varepsilon)-\sum_{j=0}^{k}p_je^{i\vartheta_j}\phi_j(\mathbf{u}^f)\|\leq C\varepsilon, \tag{15}$$

where $\psi(\cdot)$ is the solution of (3) with $\psi(0)=\bar\phi$, $\mathbf{u}(t)=\gamma(\varepsilon t)$, and $\vartheta_0,\dots,\vartheta_k\in\mathbb{R}$ are some phases depending on ε and γ.

Proof. The strategy is analogous to the one presented in Section 3.2 and is based on the construction of a suitable piecewise smooth path joining $\mathbf{u}^s$ with $\mathbf{u}^f$ that passes through all the conical intersection; in particular, we assume that the path $\gamma:[0,1]\to\omega$ satisfies $\gamma(0)=\mathbf{u}^s$, $\gamma(1)=\mathbf{u}^f$ and $\gamma(\tau_j)=\bar{\mathbf{u}}_j$, $j=0,\dots,k-1$, for some $0<\tau_0<\dots<\tau_{k-1}<1$. The only difference concerns the construction of the path in the neighborhoods of the conical intersections: indeed, in these regions the path is chosen to be tangent to the non-mixing field. At the intersection, the inner and outer directions are selected according to Proposition 13, as explained in Section 3.2, and the existence of corresponding trajectories tangent to the non-mixing field is guaranteed by Proposition 19. Far from all the conical intersections the evolution of $H(\gamma(\varepsilon t))$ conserves the occupation probabilities relative to each energy level λ_l, $l = 0, \dots, k$, with an approximation of order ε. Let us now estimate the probability distribution obtained after the passage through the conical intersection $\bar{\mathbf{u}}_0$. Since the path is tangent to the non-mixing field, we can apply Theorem 6 in order to study the evolution inside the space $\boldsymbol{P}_{\mathbf{u}(t)}\mathcal{H}$, where $\boldsymbol{P}_{\mathbf{u}(t)}$ is the spectral projection associated with the two levels $\{\lambda_0(\mathbf{u}), \lambda_1(\mathbf{u})\}$. For τ in a left neighborhood of τ_0, the effective Hamiltonian and its associated evolution operator $U^{\varepsilon}_{\text{eff}}$ are diagonal, and this implies the existence of a phase θ_0 (depending on ε) and of a positive constant C_0 such that $\|\psi(\tau_0/\varepsilon) - e^{i\theta_0}\phi_0(\gamma(\tau_0^-))\| \le C_0\varepsilon$, where $\psi(\cdot)$ is the solution of equation (3) with $\psi(0) = \phi_0(\gamma(0))$ corresponding to the control $\mathbf{u}(t) = \gamma(\varepsilon t)$, defined on $[0, 1/\varepsilon]$. By Proposition 11, this implies that

$$\|\psi(\tau_0/\varepsilon) - e^{i\theta_0}\left(\cos\boldsymbol{\Xi}(\mathbf{v})\ \phi_0(\gamma(\tau_0^+)) - e^{-i\beta(\mathbf{v})}\sin\boldsymbol{\Xi}(\mathbf{v})\ \phi_1(\gamma(\tau_0^+))\right)\| \le C_0\varepsilon,$$

with $\boldsymbol{\Xi}(\mathbf{v})$ and $\beta(\mathbf{v})$ satisfying equations (10)-(11), and $\mathbf{v}$ is the outer direction.

Since the effective Hamiltonian is diagonal also for τ belonging to a right neighborhood of τ_0, we conclude that there exist two phases α_0 and α_1 (depending on τ and ε) and a positive constant $\hat{C}_0$ such that

$$\|\psi(\tau/\varepsilon) - e^{i\alpha_0}p_0\ \phi_0(\gamma(\tau)) - e^{i\alpha_1}\sqrt{1-p_0^2}\ \phi_1(\gamma(\tau))\| \le \hat{C}_0\varepsilon.$$

Since analogous estimates hold for the passages through any other conical intersection and outside the corresponding neighborhoods the theorem is proved. ∎

To conclude this section, we present below a result providing some information on the structural stability of conical intersections based on the properties of the non-mixing fields.

THEOREM 23. *Assume that $H(\mathbf{u}) = H_0 + u_1H_1 + u_2H_2 + u_3H_3$ satisfies* **(H0)** *and admits a separated discrete spectrum $(\omega, \{\lambda_j, \lambda_{j+1}\})$. Let $\bar{\mathbf{u}} \in \omega$ be a conical intersection for $H(\mathbf{u})$ between the eigenvalues λ_j and λ_{j+1}. Then for every $\varepsilon > 0$ there exists $\delta > 0$ such that, if $\hat{H}(\mathbf{u}) = \hat{H}_0 + u_1\hat{H}_1 + u_2\hat{H}_2 + u_3\hat{H}_3$ satisfies* **(H0)** *and*

$$\sum_{i=0}^{3}\|\hat{H}_i - H_i\|_{H_0} \le \delta,$$

then the operator $\hat{H}(\mathbf{u})$ has a separated discrete spectrum $(\omega, \{\hat{\lambda}_j, \hat{\lambda}_{j+1}\})$ and it possesses a conical intersection of eigenvalues at $\hat{\mathbf{u}}$, with $|\bar{\mathbf{u}} - \hat{\mathbf{u}}| \le \varepsilon$.

Proof. First of all, by equivalence of all norms $\|\cdot\|_{H(\mathbf{u})}$, without loss of generality we can assume that $\bar{\mathbf{u}} = 0$. We notice that our assumptions guarantee that in a neighborhood of the conical intersection the eigenvalues λ_j and λ_{j+1} are well separated from the rest of the spectrum. Continuous dependence of the eigenvalues with respect to perturbations of the Hamiltonian (see Lemma 28) ensures that, if δ is small, then $\hat{H}(\cdot)$ admits two eigenvalues $\hat{\lambda}_j, \hat{\lambda}_{j+1}$ close to λ_j, λ_{j+1}. Moreover $\{\hat{\lambda}_j, \hat{\lambda}_{j+1}\}$ is separated from the rest of the spectrum, locally around $\bar{\mathbf{u}}$. From the conicity of the intersection between λ_j and λ_{j+1}, there exists $\varepsilon > 0$ small enough such that $|F(\mathbf{u})| \ge c$ for some $c > 0$ on $B(\bar{\mathbf{u}}, \varepsilon)$ and, moreover, by Proposition 18 the vector field $\mathcal{X}_P$ (up to the sign) points inside the ball $B(\bar{\mathbf{u}}, \varepsilon)$ at every point of its boundary. If δ is small enough then $\hat\lambda_j \neq \hat\lambda_{j+1}$ on $\partial B(\bar{\mathbf{u}}, \varepsilon)$ and the gap between the two eigenvalues can be assumed to be of order ε. Therefore we can define the conicity matrix $\hat{\mathcal{M}}$ associated with $\hat H(\cdot)$ and the function $\hat F(\mathbf{u}) = \det \hat{\mathcal{M}}(\psi_j(\mathbf{u}), \psi_{j+1}(\mathbf{u}))$, where $\{\psi_j(\mathbf{u}), \psi_{j+1}(\mathbf{u})\}$ is an orthonormal basis for the sum of eigenspaces relative to $\{\hat\lambda_j(\mathbf{u}), \hat\lambda_{j+1}(\mathbf{u})\}$. Since the conicity matrix depends continuously on the control operators, with respect to the norm $\|\cdot\|_{H_0}$, and as a consequence of Lemma 9 and Proposition 26, we can take δ small enough such that $|\hat F(\mathbf{u})| \geq c/2$ on $B(\bar{\mathbf{u}}, \varepsilon)$. This allows us to define, whenever $\hat\lambda_j \neq \hat\lambda_{j+1}$, the non-mixing field $\hat{\mathcal{X}}_P$ associated with $\hat H(\cdot)$ and corresponding to the band $\{\hat\lambda_j, \hat\lambda_{j+1}\}$; thanks to Proposition 16, up to a time reversal the time derivative of $\hat\lambda_{j+1} - \hat\lambda_j$ along the integral curves of $\hat{\mathcal{X}}_P$ is smaller than $-c/4$. By Corollary 27 if δ is small enough, then $\hat{\mathcal{X}}_P$ points inside $B(\bar{\mathbf{u}}, \varepsilon)$ at every point of $\partial B(\bar{\mathbf{u}}, \varepsilon)$. Any trajectory $\hat\gamma(\cdot)$ of $\hat{\mathcal{X}}_P$ starting from $B(\bar{\mathbf{u}}, \varepsilon)$ remains inside $B(\bar{\mathbf{u}}, \varepsilon)$ in its interval of definition and reaches in finite time a point $\hat{\mathbf{u}}$ corresponding to a double eigenvalue $\hat\lambda_j(\hat{\mathbf{u}}) = \hat\lambda_{j+1}(\hat{\mathbf{u}})$. The conclusion follows from Proposition 10. ∎

5. Examples. Let us first consider a finite dimensional example; let $H(\mathbf{u})$ be the Hamiltonian in $i\mathfrak{u}(3)$ defined by

$$(16) \qquad H_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad H_1 = \begin{pmatrix} 1 & i & 0 \\ -i & 0 & 1 \\ 0 & 1 & -1 \end{pmatrix}, \quad H_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad H_3 = \begin{pmatrix} -1 & 1 & -1 \\ 1 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}.$$

The Hamiltonian $H(\cdot)$ admits a double eigenvalue at $\mathbf{u} = 0$ corresponding to the two lowest levels. A simple computation leads to $\det \mathcal{M}(e_1, e_2) = -2i$ where $e_1 = (1,0,0)^T, e_2 = (0,1,0)^T$ form a basis of the double eigenspace at 0. Thus the eigenvalue intersection is conical. Moreover, at the point $\mathbf{u} = (1/2, -1/4, 0)$, the second and third eigenvalues degenerate, and the intersection is conical: indeed, the determinant of the conicity matrix corresponding to these two levels is equal to $4i/3$.

Figure 2 describes the behavior of the trajectories of the non-mixing field relative to the first two eigenvalues of $H(\cdot)$. Consistently with the results shown above, the flow corresponding to the non-mixing vector field allows to identify two conical intersections, one of them being the origin, among the first two levels. In particular, the trajectories converge or diverge from them, locally.

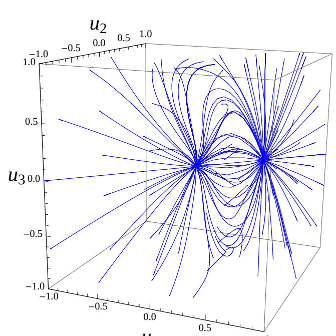

FIG. 2. *Trajectories of the non-mixing field relative to the two lowest eigenvalues for the Hamiltonian corresponding to* (16)

Let us consider the case in which the initial value of the control is $\mathbf{u}_0 = (-1, 0, 0)$. We want to approximately send an initial state ψ concentrated in the lowest energy level into a state whose probability distribution with respect to the three states is

$(1/3, 1/6, 1/2)$. To do that, we first pass through the conical intersection between the two lowest levels, leaving a probability of $1/3$ on the lowest one and sending $2/3$ of probability to the other; afterwards, we pass through the conical intersection between the two highest levels in order to send $1/2$ of the total probability to the third level; finally, we come back to the initial point.

Figure 3, on the left, shows the chosen path, which follows the non-mixing field in a neighborhood of the conical intersection. On the right the distribution of probability is depicted. The simulations were run on arc-length parametrized curves, with a parameter $\varepsilon = 0.001$.

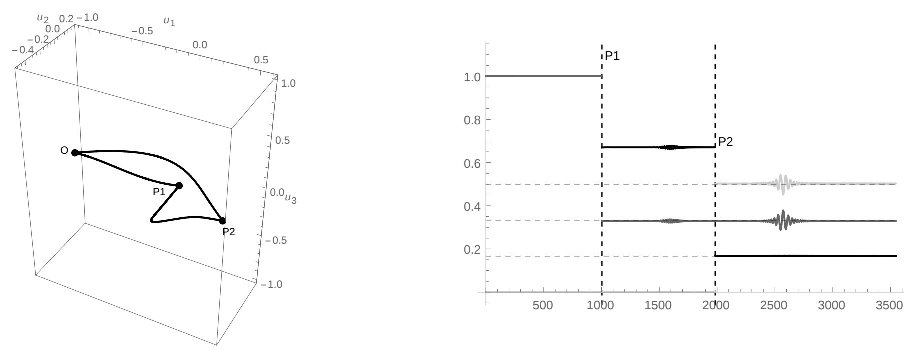

FIG. 3. *Control path and probability distributions for the Hamiltonian corresponding to* (16). *We use black for the probability of being in the second energy state, and the lighter shade of gray for the probability of being in the highest one. The starting point is labeled as O and the conical intersections* $(0,0,0)$ *and* $(1/2, -1/4, 0)$ *respectively as* $P1, P2$.

Consider now the Hamiltonian $H(\mathbf{u}) = -\Delta + u_1 V_1 + u_2 V_2 - i u_3 (\nabla \mathbf{A} + \mathbf{A}\nabla)$, where

$$V_1(x) = x_2^2 + x_3^2,\ V_2(x) = x_2 x_3,\ A = (0, -x_3/2, x_2/2)^T,$$
$$x = (x_1, x_2, x_3) \in \Omega = (0,1) \times (0, \sqrt{3}) \times (0, \sqrt{5})$$

with zero Dirichlet boundary conditions. We recall that the third controlled operator acts on the elements of its domain as follows $-i(\nabla \mathbf{A} + \mathbf{A}\nabla)\psi = -i\,\mathbf{A}\cdot\nabla\psi - i\,\mathrm{div}(\mathbf{A}\psi)$. This operator has the form of a vector potential coupled with the momentum. By classical results (see [26, 27]), it is easy to check that $H(\mathbf{u})$ satisfies hypothesis **(H0)** and has a purely discrete spectrum with a finite number of eigenvalues in each compact subset of $\mathbb{R}$ (this, together with Lemma 28, guarantees that $H(\mathbf{u})$ possesses a separated discrete spectrum).

We claim that $H(0)$ (representing the potential well in Ω) admits conical intersections of eigenvalues. The eigenvalues and the eigenfunctions of $H(0)$ take the form

$$\lambda_{j_1,j_2,j_3} = \pi^2\Big(j_1^2 + \frac{j_2^2}{3} + \frac{j_3^2}{5}\Big), \quad \psi_{j_1,j_2,j_3}(x) = \frac{2\sqrt{2}}{\sqrt[4]{15}} \sin(j_1 \pi x_1) \sin\Big(\frac{j_2 \pi x_2}{\sqrt{3}}\Big) \sin\Big(\frac{j_3 \pi x_3}{\sqrt{5}}\Big)$$

where j_1, j_2, j_3 are strictly positive integers. In particular it is easy to check that the fourth and the fifth lowest eigenvalues take the same value $\lambda_{1,1,3} = \lambda_{1,2,2}$ at the origin, and, since the determinant of the conicity matrix is approximately $0.029i$, we deduce that the intersection is conical.

Let us consider an initial control $\mathbf{u}_0 = (1, 0, 0)$ and an initial state concentrated on the fourth energy level of $H(\mathbf{u}_0)$. Our aim is to induce an approximate transition to a state distributed between the fourth and fifth level of $H(\mathbf{u}_0)$ with probability 2/3 and 1/3, respectively. We follow arc-length parametrized curves with a parameter $\varepsilon = 0.003$, and we compare the transition obtained following control paths with a different behavior around the singularity. Namely, we consider a path which is locally an integral curve of the non-mixing field (top-left in Figure 4) and one which is piecewise affine in the sense of Proposition 11 (bottom-left in Figure 4). The corresponding probability distributions as functions of the time are shown in Figure 4, on the right side. Both paths induce quite precisely the desired transition, although for long times the accuracy degrades. We remark that the most significant difference between the two strategies is given by the fact that the second one induces a less accurate spread of probability at the passage through the conical intersection, as expected.

Note that, to compute the evolution of the controlled system, we truncated the infinite dimensional system to the lowest 20 and to the lowest 30 energy levels. These two choices did not exhibit significant differences: this suggests that the truncation up to the first 20 energy levels well describes the behavior of the infinite dimensional system. Figure 4 is obtained choosing this truncation.

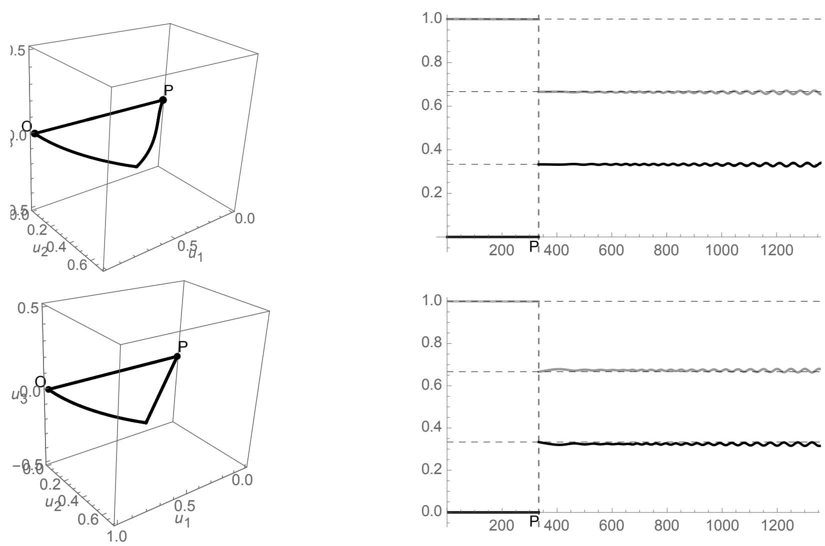

FIG. 4. *Control paths and probability distributions for $H(\mathbf{u}) = -\Delta + u_1V_1 + u_2V_2 - iu_3(\nabla\mathbf{A} + \mathbf{A}\nabla)$. We reproduce in gray the probability of being in the fourth energy level and in black the probability of being in the fifth one. The starting point is labeled as O and the conical intersection as P.*

6. Final remarks. The integral curves of the non-mixing field are not the only paths guaranteeing the estimate (15): suitable approximations (in the sense precised just below) of these curves also ensure an adiabatic approximation of order ε. Indeed, let us consider an arc-length parametrized curve $\gamma^P(\tau)$, tangent to the non-mixing field, that reaches a conical intersection between λ_j and λ_{j+1} at time $\tau = 0$, and let γ be a $\mathcal{C}^3$ curve such that $|\gamma(\tau) - \gamma^P(\tau)| \leq C\tau^3$, for τ small enough and some positive constant C. Let $t = \tau/\varepsilon$ and consider the effective Hamiltonians evaluated along the two curves. It is then easy to see, by simple computations and because of Proposition 7, that the difference between the two effective Hamiltonians is less or equal than $C'\varepsilon^2 t$ for some $C' > 0$. This term, integrated over a time interval of order

$1/\varepsilon$, gives a difference of order ε.

An interesting controllability problem alternative to the one introduced in Section 3.2 aims at sending (approximately) an initial state $\psi^s = \sum_{j=0}^{k} c_j \phi_j(\mathbf{u}^s)$ to a final state concentrated in a single energy level. This problem may appear completely equivalent to the previous one, but is actually more delicate. Indeed, a natural way to induce the desired transition would be to run backward in time a path constructed as in Section 3.2. However, a simple computation shows that, at each passage through a conical intersection, the components corresponding to the intersecting eigenvalues recombine in a concentrated state only if their relative phase coincides with the one induced by the unitary transformation of the limit basis (that is, the phase $\beta(\mathbf{v})$ of Proposition 11). On the other hand, the computation of dynamical phases, coming from the integration of the energy on intervals whose length is of order $1/\varepsilon$, is very sensitive to changes in the speed ε. This is in principle possible, but it compromises the constructiveness of the algorithm.

Similarly, by means of non-constructive arguments (for instance, by exploiting the rational independence of the gaps between the eigenvalues underlined in [12, Lemma 14]) one can obtain the following controllability property, stronger than the one considered in Section 3.2.

Under assumption **(H0)**, *assuming that the Hamiltonian possesses a separated discrete spectrum in which all energy levels are connected through conical intersections, and for any given initial and target states ψ^s, ψ^f distributed in Σ and $\eta > 0$, there exists a control input steering the system from ψ^s to a final state whose distance from ψ^f is less than η.*

It is opinion of the authors that all the results here above still hold in a non-linear sufficiently smooth setting, that is for Hamiltonians of the form $H(\mathbf{u})$ whose derivatives with respect to the parameter $\mathbf{u}$ are $H(0)$-small up to a suitable order and under hypothesis **(H1)**. This case is interesting, since it covers relevant physical models, such as those described by Hamiltonians with controlled electromagnetic potentials. Preliminary results in this sense have been obtained in [14].

Appendix A. Regularity properties and proof of Proposition 7.

Let $\mathcal{H}$ be a complex separable Hilbert space; all operators in the following are assumed to be operators on $\mathcal{H}$. In this section we derive some regularity results on the eigenvalues and the eigenstates of self-adjoint operators with respect to the norm defined in (2) (see e.g. [19] for similar regularity properties). Such results will be used in particular to prove Proposition 7.

The resolvent of A in $\zeta \in \rho(A)$ is denoted by $R(A,\zeta) = (A - \zeta \mathrm{id})^{-1}$; we recall that it is a bounded linear operator that maps $\mathcal{H}$ into $\mathcal{D}(A)$, and that, given two self-adjoint operators A_1, A_2 with the same domain, their resolvents satisfy the Second Resolvent Identity

$$R(A_2,\zeta) - R(A_1,\zeta) = R(A_1,\zeta)(A_1 - A_2)R(A_2,\zeta). \tag{17}$$

The identity

$$\|(X - \zeta \mathrm{id})^{-1}\| = d(\zeta, \sigma(X))^{-1} \tag{18}$$

holds for self-adjoint operators (see e.g. [19]).

Let us state the following technical lemma, which will be largely used in the following. Its proof easily comes from the definition of $\|\cdot\|_A$ and is thus omitted.

LEMMA 24. *Let A, B be self-adjoint operators with B A-bounded and $\zeta \in \rho(A)$. Then the following inequality holds:*

$$\|BR(A,\zeta)\| \leq \Big(1 + (|\zeta| + 1)\,\|R(A,\zeta)\|\Big)\|B\|_A. \tag{19}$$

The following result shows that the resolvent set for a self-adjoint operator A possesses some continuity properties with respect to small perturbation in the space $\mathcal{L}(\mathcal{D}(A), \mathcal{H})$.

LEMMA 25. *Let A_1 be a self-adjoint operator. Let $\mathcal{Z} \subset \rho(A_1)$ be a compact set. There exists a $\delta > 0$ such that, if a self-adjoint operator A_2 satisfies $\|A_1 - A_2\|_{A_1} \leq \delta$, then A_1 and A_2 have the same domain, $\mathcal{Z} \subset \rho(A_2)$ and the inequality*

$$\|R(A_2,\zeta) - R(A_1,\zeta)\| \leq C\|A_1 - A_2\|_{A_1} \tag{20}$$

holds true on $\mathcal{Z}$ for some constant C depending on $\mathcal{Z}$ and A_1.

Proof. To ensure that $\mathcal{D}(A_1) = \mathcal{D}(A_2)$ it is clearly enough to assume $\delta < 1$. To conclude the proof we proceed as follows. As a consequence of (18), $\|R(A_1,\zeta)\|$ is uniformly bounded on $\mathcal{Z}$. This, together with (19), implies that $\|(A_2 - A_1)R(A_1,\zeta)\| < C'\|A_1 - A_2\|_{A_1}$ for some $C' > 0$. Since

$$R(A_2,\zeta) = R(A_1,\zeta)\left(\mathrm{id} + (A_2 - A_1)R(A_1,\zeta)\right)^{-1}$$

whenever the right-hand side is well defined, we deduce that $\mathcal{Z} \subset \rho(A_2)$ and that $\|R(A_2,\zeta)\| \leq 2\|R(A_1,\zeta)\|$ on $\mathcal{Z}$, provided that δ is small enough. Finally, by applying (17), we get (20). ∎

Let $\Sigma \subset \sigma(A)$ be constituted by a finite number of eigenvalues of the self-adjoint operator A. For every positively-oriented closed path $\Gamma \subset \mathbb{C}$ encircling Σ, and not encircling any other element in $\sigma(A)$, the projection P onto the sum of the eigenspaces relative to Σ is given by

$$P = -(2\pi i)^{-1} \oint_\Gamma R(A,\zeta)\, d\zeta. \tag{21}$$

PROPOSITION 26. *Let A_1 be a self-adjoint operator. Assume that $\Sigma_1 = \sigma(A_1) \cap (\zeta_1, \zeta_2)$ is constituted by k eigenvalues, counted with multiplicity, and that $\zeta_1, \zeta_2 \notin \sigma(A_1)$. Then for every $\epsilon > 0$ there exists a $\delta > 0$, depending on ζ_1, ζ_2 and A_1, such that if A_2 is self-adjoint and $\|A_1 - A_2\|_{A_1} \leq \delta$, then*

i) $\Sigma_2 = \sigma(A_2) \cap (\zeta_1, \zeta_2)$ is constituted by k eigenvalues, counted with multiplicity;

ii) Calling $P^{A_1}_{\Sigma_1}$ the spectral projection onto the sum of eigenspaces of A_1 relative to Σ_1 and $P^{A_2}_{\Sigma_2}$ the spectral projection onto the sum of eigenspaces of A_2 relative to Σ_2, it holds $\|P^{A_1}_{\Sigma_1} - P^{A_2}_{\Sigma_2}\| \leq \epsilon$.

Proof. Let Γ be the circle in the complex plane centered on the real axis and passing through ζ_1 and ζ_2, and consider the projection $P^{A_2}_{\Sigma_2} = -(2\pi i)^{-1} \oint_\Gamma R(A_2,\zeta)\, d\zeta$. From (20) we obtain that

$$\left\|P^{A_1}_{\Sigma_1} - P^{A_2}_{\Sigma_2}\right\| \leq (2\pi)^{-1} \oint_\Gamma \|R(A_1,\zeta) - R(A_2,\zeta)\|\; d\zeta \leq \hat{C}\delta$$

for some $\hat{C} > 0$ (depending on Γ and A_1). In particular, $\|P^{A_1}_{\Sigma_1} - P^{A_2}_{\Sigma_2}\| < 1$ for δ small enough, which easily implies that $\dim \mathrm{Range}(P^{A_2}_{\Sigma_2}) = \dim \mathrm{Range}(P^{A_1}_{\Sigma_1}) = k$ (see [27, page 14]), therefore Σ_2 contains exactly k eigenvalues, counted with multiplicity, i.e. *i)* holds true. By possibly choosing a smaller δ, *ii)* also holds true. ∎

The following result immediately follows from Proposition 26.

COROLLARY 27. *Let λ be a simple eigenvalue of a self-adjoint operator A_1. Then for every $\epsilon > 0$ there exists $\delta > 0$ such that any self-adjoint operator A_2 satisfying $\|A_1 - A_2\|_{A_1} \leq \delta$ admits a unique eigenvalue μ with $|\lambda - \mu| < \epsilon$. Moreover, there exists a choice $\phi_\lambda^{A_1}, \phi_\mu^{A_2}$ for the corresponding eigenstates such that $\|\phi_\lambda^{A_1} - \phi_\mu^{A_2}\| \leq \epsilon$.*

The next result provides an estimate concerning regularity properties of the eigenvalues.

LEMMA 28. *Let A_1 be a self-adjoint operator such that $\sigma(A_1) \cap I$ is discrete and without finite accumulation points for some open, possibly unbounded, interval I. If $\delta > 0$ is small enough and A_2 is a self-adjoint operator satisfying $\|A_2 - A_1\|_{A_1} \leq \delta$, then the eigenvalues of A_2 contained in I are close to those of A_1, in the following sense. Up to appropriately indexing on a subset of $\mathbb{Z}$ the eigenvalues (counted with multiplicity) in $\sigma(A_j) \cap I$, for $j = 1, 2$, and denoting them with $\mu_i(A_j)$ we have $|\mu_i(A_1) - \mu_i(A_2)| \leq \epsilon(1 + |\mu_i(A_1)|)$, where $\epsilon = e^{\frac{\delta}{1-\delta}} - 1$.*

Proof. Let A_1 satisfy the hypotheses of the lemma, and let A_2 be a self-adjoint operator with $\|A_1 - A_2\|_{A_1} \leq \delta$, where without loss of generality we assume that $\delta < 1$; define $A(t) = A_1 + t(A_2 - A_1)$, for $t \in [0, 1]$. Let $\lambda_i(t)$ be the analytic branch of the eigenvalues of $A(t)$ emanating from $\lambda_i(0) = \mu_i(A_1)$, and denote by $\phi_i(t)$ a corresponding analytic eigenstate. By hypothesis

$$\|(A_2 - A_1)\phi_i(t)\| \leq \delta\|A_1\phi_i(t)\| + \delta \leq \delta|\lambda_i(t)| + \delta t\|(A_2 - A_1))\phi_i(t)\| + \delta,$$

which implies that $\|(A_2 - A_1)\phi_i(t)\| \leq \frac{\delta}{1-\delta}(|\lambda_i(t)| + 1)$. From

$$|\dot\lambda_i(t)| = |\langle\phi_i(t), (A_2 - A_1)\phi_i(t)\rangle| \leq \|(A_2 - A_1)\phi_i(t)\|$$

we easily get the thesis. ∎

Consider a control-dependent Hamiltonian $H(\mathbf{u})$ satisfying assumption **(H0)**. It is easy to see that for any $\mathbf{u}_1, \mathbf{u}_2$ the norms $\|\cdot\|_{H(\mathbf{u}_1)}, \|\cdot\|_{H(\mathbf{u}_2)}$ are equivalent, thanks to the H_0-smallness of the control Hamiltonians. From Lemma 28, and the equivalence of the norms $\|\cdot\|_{H(\mathbf{u})}$, the eigenvalues $\lambda_i(\cdot)$ of $H(\cdot)$ are locally Lipschitz, and the corresponding Lipschitz constants locally depend on the magnitude of $\lambda_i(\cdot)$. Moreover, we remark the following fact: let $\bar{\mathbf{u}}$ be a conical intersection between the eigenvalues λ_j and λ_{j+1}, that satisfy a gap condition, according to Definition 2. By the definition of conical intersection and the Lipschitz continuity of the eigenvalues we can conclude that there exist a suitably small neighborhood U of $\bar{\mathbf{u}}$ and two constants $C_1 > 0$ and $C_2 > 0$ such that

$$\lambda_{j+1}(\mathbf{u}) - \lambda_j(\mathbf{u}) \geq C_1|\mathbf{u} - \bar{\mathbf{u}}| \quad \forall\, \mathbf{u} \in U \tag{22}$$

and

$$|\lambda_i(\mathbf{u}) - \lambda_i(\mathbf{u}')| \leq C_2|\mathbf{u} - \mathbf{u}'| \quad \forall\, \mathbf{u}, \mathbf{u}' \in U,\ i = j, j+1. \tag{23}$$

We are now ready to prove Proposition 7.

Proof of Proposition 7. For simplicity, throughout this proof we will write $R(\mathbf{u}, \xi)$ to denote the resolvent $R(H(\mathbf{u}), \xi)$. The property that the projections $P_J(\gamma(t))$, $J = j, j+1$, are $\mathcal{C}^k$ at any $t \in [-R, 0)$ whenever $\gamma(\cdot)$ is $\mathcal{C}^k$ has been shown e.g. in [28]. It comes from (21) and a recursive application of the identity

$$\frac{d}{dt}R(f(t), \xi) = R(f(t), \xi)\Big(\frac{d}{dt}H(f(t))\Big)R(f(t), \xi), \tag{24}$$

valid for any differentiable path f taking values in $\mathbb{R}^3$, together with (19).

It remains to study the regularity of the projections at the singularity. We first consider the case $k=1$. Without loss of generality we assume $|\dot\gamma(0)|=1$. Let $\rho = C_1/4$, where C_1 is as in (22), and for every $t\in[-R,0)$ consider the circle $\Gamma_t\subset\mathbb{C}$ of radius ρt centered at $\lambda_j(\gamma(t))$. There exists $0<T\le R$ such that for every $t\in[-T,0)$

$$|\lambda_{j+1}(\gamma(t))-\lambda_j(\gamma(t))|\ge \frac{3}{4}C_1 t = 3\rho t$$

so that $|\lambda_{j+1}(\gamma(t))-\zeta|\ge 2\rho t$ for every $\zeta\in\Gamma_t$. Thus $d(\zeta,\sigma(H(\gamma(t))))=\rho t$ and, by (23) and the definition of $\ell_1(\cdot)$, $d(\zeta,\sigma(H(\ell_1(t))))\ge \rho t/2$, up to reducing T. Therefore, from (18), for $\zeta\in\Gamma_t$ it holds

$$\|R(\gamma(t),\zeta)\| = \frac{1}{\rho t}, \qquad \|R(\ell_1(t),\zeta)\|\le \frac{2}{\rho t}. \tag{25}$$

It is left to prove that $\oint_{\Gamma_t}(R(\gamma(t),\zeta)-R(\ell_1(t),\zeta))\,d\zeta$ tends to 0. Estimate (19) gives

$$\|(H(\ell_1(t))-H(\gamma(t)))R(\gamma(t),\zeta)\|\le C\left|\frac{\ell_1(t)-\gamma(t)}{t}\right|$$

for some $C>0$, which, together with (17) and (25) yields the thesis.

Let us now tackle the general case; the proof follows similar arguments. We define the circuit Γ_τ as above, and we notice that for every fixed $\tau\in(-T,0)$ there is a neighborhood I_τ of τ such that (25) can be replaced by the similar estimate

$$\|R(\gamma(t),\zeta)\|\le \frac{2}{\rho t}, \qquad \|R(\ell_k(t),\zeta)\|\le \frac{2}{\rho t}, \tag{26}$$

holding for every $\zeta\in\Gamma_\tau$ and $t\in I_\tau$. By applying (17) we get, for every $t\in I_\tau$ and $l\le k-1$,

$$\frac{d^l}{dt^l}P_j(\gamma(t))-\frac{d^l}{dt^l}P_j(\ell(t)) = -(2\pi i)^{-1}\oint_{\Gamma_\tau}\frac{d^l}{dt^l}\Big[R(\ell_k(t),\zeta)(H(\ell_k(t))-H(\gamma(t)))R(\gamma(t),\zeta)\Big]\,d\zeta.$$

The proof can then be easily completed by applying recursively the identity (24) together with the estimates (26) and (19), and by exploiting the regularity of $\gamma(\cdot)$ and the definition of $\ell_k(\cdot)$. ◻

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REFERENCES

[1] R. Adami and U. Boscain. Controllability of the Schrödinger equation via intersection of eigenvalues. In *Proceedings of the 44th IEEE Conference on Decision and Control, December 12-15*, pages 1080–1085, 2005.
[2] A. A. Agrachev. Spaces of symmetric operators with multiple ground states. *Funct. Anal. Appl.*, 45(4):241–251, 2011.
[3] F. Albertini and D. D'Alessandro. Notions of controllability for bilinear multilevel quantum systems. *IEEE Trans. Automat. Control*, 48(8):1399–1403, 2003.
[4] J. M. Ball, J. E. Marsden, and M. Slemrod. Controllability for distributed bilinear systems. *SIAM J. Control Optim.*, 20(4):575–597, 1982.
[5] K. Beauchard and J.-M. Coron. Controllability of a quantum particle in a moving potential well. *J. Funct. Anal.*, 232(2):328–389, 2006.

[6] K. Beauchard and C. Laurent. Local controllability of 1D linear and nonlinear Schrödinger equations with bilinear control. *J. Math. Pures Appl. (9)*, 94(5):520–554, 2010.
[7] A. M. Bloch, R. W. Brockett, and C. Rangan. Finite controllability of infinite-dimensional quantum systems. *IEEE Trans. Automat. Control*, 55(8):1797–1805, 2010.
[8] M. Born and V. Fock. Beweis des adiabatensatzes. *Zeitschrift für Physik A Hadrons and Nuclei*, 51(3–4):165–180, 1928.
[9] U. Boscain, M. Caponigro, T. Chambrion, and M. Sigalotti. A weak spectral condition for the controllability of the bilinear Schrödinger equation with application to the control of a rotating planar molecule. *Communications in Mathematical Physics*, 2(311):423–455, 2012.
[10] U. Boscain, F. Chittaro, P. Mason, and M. Sigalotti. Adiabatic control of the Schrödinger equation via conical intersections of the eigenvalues. *IEEE Trans. Automat. Control*, 57(8):1970–1983, 2012.
[11] U. Boscain, F. Chittaro, P. Mason, and M. Sigalotti. Controllability of the Schrödinger equation via adiabatic methods and conical intersections of the eigenvalues. In *Proceedings of the 51st IEEE Conference on Decision and Control, December 10-13*, pages 3044–3049, 2012.
[12] U. Boscain, J.-P. Gauthier, F. Rossi, and M. Sigalotti. Approximate controllability, exact controllability, and conical eigenvalue intersections for quantum mechanical systems. *Communications in Mathematical Physics*, 333(3):1225–1239, 2015.
[13] T. Chambrion, P. Mason, M. Sigalotti, and U. Boscain. Controllability of the discrete-spectrum Schrödinger equation driven by an external field. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 26(1):329–349, 2009.
[14] F. Chittaro and P. Mason. Approximate controllability by adiabatic methods of the Schrödinger equation with nonlinear hamiltonian. In *Proceedings of the 54th IEEE Conference on Decision and Control, December 15-18*, pages 7771–7776, 2015.
[15] D. D'Alessandro. *Introduction to quantum control and dynamics.* Applied Mathematics and Nonlinear Science Series. Boca Raton, FL: Chapman, Hall/CRC., 2008.
[16] C. Fermanian Kammerer and C. Lasser. Propagation through generic level crossings : a surface hopping semigroup. *SIAM J. of Math. Anal.*, 140(1):103–133, 2008.
[17] G. A. Hagedorn. Molecular propagation through electron energy level crossings. *Mem. Amer. Math. Soc.*, 111(536):vi+130, 1994.
[18] T. Kato. On the adiabatic theorems of quantum mechanics. *Phys. Soc. Japan*, 5:435–439, 1950.
[19] T. Kato. *Perturbation theory for linear operators.* Die Grundlehren der mathematischen Wissenschaften, Band 132. Springer-Verlag New York, Inc., New York, 1966.
[20] M. Lapert, S. Guérin, and D. Sugny. Field-free quantum cogwheel by shaping of rotational wave packets. *Phys. Rev. A*, 83:013403 (5 pages), 2011.
[21] C. Lasser and S. Teufel. Propagation through conical crossings: an asymptotic semigroup. *Comm. Pure Appl. Math.*, 58(9):1188–1230, 2005.
[22] Z. Leghtas, A. Sarlette, and P. Rouchon. Adiabatic passage and ensemble control of quantum systems. *Journal of Physics B*, 44(15), 2011.
[23] M. Mirrahimi. Lyapunov control of a quantum particle in a decaying potential. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 26(5):1743–1765, 2009.
[24] G. Nenciu. On the adiabatic theorem of quantum mechanics. *J. Phys A*, 13:15–18, 1980.
[25] V. Nersesyan. Global approximate controllability for Schrödinger equation in higher Sobolev norms and applications. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 27(3):901–915, 2010.
[26] M. Reed and B. Simon. *Methods of modern mathematical physics. II. Fourier analysis, self-adjointness.* Academic Press [Harcourt Brace Jovanovich Publishers], New York, 1975.
[27] M. Reed and B. Simon. *Methods of modern mathematical physics. IV. Analysis of operators.* Academic Press [Harcourt Brace Jovanovich Publishers], New York, 1978.
[28] S. Teufel. *Adiabatic perturbation theory in quantum dynamics*, volume 1821 of *Lecture Notes in Mathematics.* Springer-Verlag, Berlin, 2003.
[29] M. Teytel. How rare are multiple eigenvalues? *Comm. Pure Appl. Math.*, 52(8):917–934, 1999.
[30] G. Turinici. On the controllability of bilinear quantum systems. In M. Defranceschi and C. Le Bris, editors, *Mathematical models and methods for ab initio Quantum Chemistry*, volume 74 of *Lecture Notes in Chemistry.* Springer, 2000.
[31] J. Von Neumann and E. Wigner. Über das Verhalten von Eigenwerten bei adiabatischen Prozessen. *Physikalische Zeitschrift*, 30:467–470, 1929.
[32] D. R. Yarkony. Diabolical conical intersections. *Reviews of Modern Physics*, 68:985–1013, 1996.
[33] L. Yatsenko, S. Guérin, and H. Jauslin. Topology of adiabatic passage. *Phys. Rev. A*, 65:043407 (7 pages), 2002.