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

4 FRANCESCA CARLOTTA CHITTARO [†] AND PAOLO MASON [‡]

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

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

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

17 **1. Introduction.** A typical issue in quantum control concerns the controllability
18 of the bilinear Schrödinger equation

19 (1)
$$i \frac{d\psi}{dt} = \left(H_0 + \sum_{k=1}^m u_k(t) H_k \right) \psi(t),$$

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

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

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

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

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

42 Roughly speaking, the adiabatic theorem (see [8, 24, 28]) states that the occupa-
 43 tion probabilities associated with the energy levels of a time-dependent Hamiltonian
 44 $H(\cdot)$ are approximately preserved along the evolution given by $i\dot{\psi}(t) = H(t)\psi(t)$, pro-
 45 vided that $H(\cdot)$ varies slowly enough. This result works whenever the energy levels
 46 (i.e. the eigenvalues of $H(\cdot)$) are isolated for every t . On the other hand, if two
 47 eigenvalues intersect, and provided that $H(\cdot)$ is smooth enough, the passage through
 48 the intersections may determine (approximate) exchanges of the corresponding occu-
 49 pation probabilities (see [28, Corollary 2.5] and [17]). For these reasons, adiabatic
 50 methods are largely used in quantum control to induce population transfers (see for
 51 instance the techniques known as Stimulated Raman Adiabatic Passage (STIRAP),
 52 Stark-chirped rapid adiabatic passage (SCRAP)) and to prepare superposition states
 53 [20]. The applications of adiabatic methods in quantum control, as a tool for ob-
 54 taining controllability results, have already been exploited in previous papers (see for
 55 instance [1, 10, 22, 33]). The general idea is to use slowly varying controls, taking
 56 advantage of the adiabatic theorem, and “climb” the energy levels through the conical
 57 intersections.

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

73 The control strategy applies whenever a part of the spectrum of the Hamiltonian
 74 operator is uniformly separated from the rest of the spectrum (as a function of the
 75 control parameters), is discrete and, within it, each pair of subsequent eigenvalues
 76 intersect in a conical intersection. When there exists such a portion of the spectrum,
 77 called *separated discrete spectrum*, this control strategy permits to attain (approx-
 78 imately) a state having a prescribed distribution of probability (relative to the energy
 79 levels of the separated discrete spectrum) starting from an eigenstate. In particular
 80 this entails a controllability property, that we call *spread controllability*, which, al-
 81 though weaker than the usual approximate controllability property, is more practical.
 82 Indeed, the relative phases between pairs of components in the eigenbasis decompo-
 83 sition are essentially uncontrollable since they evolve according to the gaps between
 84 the corresponding energy levels. Furthermore, notice that this method allows us to
 85 control the population inside some portion of the discrete spectrum, if well separated

86 from the rest, even in the presence of continuous spectrum, unlike many other classical
87 methods.

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

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

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

127 **2. Notations and preliminary results.** We start this section by introducing
128 the notations that will be used in the rest of the paper.

129 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
130 the point z and the set A .

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

$$133 \quad f(s_0^\pm) = \lim_{s \rightarrow s_0^\pm} f(s).$$

134 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,
 135 with abuse of notations, we denote by $\dot{Q}(\gamma(r))$ the derivative of the composition
 136 $Q(\gamma(\cdot))$ 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,
 137 $Q^{(l)}(\gamma(r)) := \frac{d^l}{ds^l}Q(\gamma(s))|_{s=r}$.

138 The scalar product of two vectors $\mathbf{w}_1, \mathbf{w}_2$ in an euclidean space \mathbb{R}^k is denoted by
 139 $\mathbf{w}_1 \cdot \mathbf{w}_2$, while the norm of $\mathbf{w} \in \mathbb{R}^k$ is denoted by $|\mathbf{w}|$.

140 For a given vector \mathbf{v} or matrix A the respective transpose is denoted by \mathbf{v}^T and A^T .

141 The inverse of the transpose of an invertible square matrix A is denoted with A^{-T} .

142 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
 143 \mathbf{v}^* and its real and imaginary parts respectively by

$$144 \quad \Re(\mathbf{v}) = (\Re(v_1), \Re(v_2), \Re(v_3)) \quad \Im(\mathbf{v}) = (\Im(v_1), \Im(v_2), \Im(v_3)).$$

145 The symbol id is used to denote the identity operator on a vector space which is
 146 specified at each occurrence, whenever not clear from the context.

147 Given a linear operator A defined on a Hilbert space, its domain is denoted as $\mathcal{D}(A)$,
 148 the symbol $\sigma(A)$ denotes the spectrum of A , while the resolvent set $\rho(A)$ is the
 149 complement of $\sigma(A)$ in \mathbb{C} .

150 **2.1. General setting.** Let \mathcal{H} be a separable complex Hilbert space with scalar
 151 product $\langle \cdot, \cdot \rangle$ and norm $\|\cdot\|$; let us introduce the following notion of relative bound-
 152 edness between operators:

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

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

$$161 \quad (2) \quad \|B\|_A = \sup_{\psi \in \mathcal{D}(A)} \frac{\|B\psi\|}{\|A\psi\| + \|\psi\|}.$$

162 This provides a norm in the space $\mathcal{L}(\mathcal{D}(A), \mathcal{H})$ of continuous linear operators from
 163 $\mathcal{D}(A)$ (endowed with the graph norm of A) to \mathcal{H} .

164 We consider the Hamiltonian

$$165 \quad H(\mathbf{u}) = H_0 + u_1 H_1 + u_2 H_2 + u_3 H_3,$$

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

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

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

177 Schrödinger Hamiltonians are typical Hamiltonian operators describing quantum
 178 phenomena and can be represented in the form $-\Delta + V$ on the Hilbert space $L^2(\Omega)$,
 179 where Ω is a domain of \mathbb{R}^n , Δ is the Laplacian on Ω (with Dirichlet or Neumann
 180 boundary conditions) and $V : \Omega \rightarrow \mathbb{R}$ has to be interpreted as a multiplicative operator
 181 on $L^2(\Omega)$. In particular such Hamiltonian operators are unbounded operators. In
 182 this context Hypothesis **(H0)** is thus intended to describe a Hamiltonian operator of
 183 the previous form that can be controlled by means of three external inputs so that
 184 $H_0 = -\Delta + V_0$ and $H_i = V_i$ for some multiplicative operators V_i , for $0 \leq i \leq 3$.

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

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

$$192 \quad (3) \quad i \frac{d\psi}{dt} = H(\mathbf{u}(t))\psi(t).$$

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

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

198 **DEFINITION 2.** *A separated discrete spectrum is a pair (ω, Σ) where ω is a do-
 199 main in \mathbb{R}^3 and Σ a map defined on ω that associates with each $\mathbf{u} \in \omega$ a subset
 200 $\Sigma(\mathbf{u})$ of the discrete spectrum of $H(\mathbf{u})$ such that there exist two continuous functions
 201 $f_1, f_2 : \omega \rightarrow \mathbb{R}$ satisfying*

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

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

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

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

220 **DEFINITION 4.** *Let $H(\cdot)$ satisfy hypothesis **(H0)**. We say that $\bar{\mathbf{u}} \in \mathbb{R}^3$ is a conical
 221 intersection between two subsequent eigenvalues λ_j and λ_{j+1} if $\lambda_j(\bar{\mathbf{u}}) = \lambda_{j+1}(\bar{\mathbf{u}})$ has*

222 *multiplicity two and there exists a constant $c > 0$ such that for any unit vector $\mathbf{v} \in \mathbb{R}^3$*
 223 *and $t > 0$ small enough we have that*

$$224 \quad \lambda_{j+1}(\bar{\mathbf{u}} + t\mathbf{v}) - \lambda_j(\bar{\mathbf{u}} + t\mathbf{v}) > ct.$$

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

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

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

$$236 \quad (4) \quad \dot{\lambda}_l(t) = \langle \phi_l(t), (\dot{u}_1(t)H_1 + \dot{u}_2(t)H_2 + \dot{u}_3(t)H_3)\phi_l(t) \rangle,$$

$$237 \quad (5) \quad (\lambda_m(t) - \lambda_l(t)) \langle \phi_l(t), \dot{\phi}_m(t) \rangle = \langle \phi_l(t), (\dot{u}_1(t)H_1 + \dot{u}_2(t)H_2 + \dot{u}_3(t)H_3)\phi_m(t) \rangle.$$

239 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 $\mathbf{v} =$
 240 (v_1, v_2, v_3) unit vector and $t \geq 0$. Then, thanks to (5) and since each H_i is H_0 -
 241 bounded, we have

$$242 \quad \lim_{t \rightarrow 0^+} \langle \phi_j(r_{\mathbf{v}}(t)), (v_1H_1 + v_2H_2 + v_3H_3)\phi_{j+1}(r_{\mathbf{v}}(t)) \rangle$$

$$243 \quad (6) \quad = \langle \phi_j^{\mathbf{v}}, (v_1H_1 + v_2H_2 + v_3H_3)\phi_{j+1}^{\mathbf{v}} \rangle = 0,$$

245 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.

246 **2.2. The adiabatic theorem.** In this section we recall a classical formulation
 247 of the time-adiabatic theorem ([8, 18, 24] adapted to our framework. For a general
 248 overview see the monograph [28]).

249 Let $H(\mathbf{u}) = H_0 + \sum_{i=1}^3 u_i H_i$ satisfy **(H0)** and have a separated discrete spectrum
 250 (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
 251 to $\mathcal{C}^2(I, \omega)$. We introduce a small parameter $\varepsilon > 0$ that controls the time scale, and
 252 the slow Hamiltonian $H(\mathbf{u}(\varepsilon t))$, $t \in [\tau_0/\varepsilon, \tau_f/\varepsilon]$. In these notations, τ is a geometric
 253 parameter used to describe the curve in the space of controls, while t is the actual
 254 time of the evolution along the control path.

255 We denote by $U^\varepsilon(t, t_0)$ the time evolution (from $t_0 = \tau_0/\varepsilon$ to $t = \tau/\varepsilon$) generated
 256 by $H(\mathbf{u}(\varepsilon t))$, and with $U_a^\varepsilon(t, t_0)$ the time evolution generated by the Hamiltonian
 257 $H_a(\varepsilon t)$, 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
 258 *adiabatic Hamiltonian*, $P_*(\mathbf{u})$ denotes the spectral projection of $H(\mathbf{u})$ on $\Sigma(\mathbf{u})$, and
 259 $P_*^\perp(\mathbf{u}) = \text{id} - P_*(\mathbf{u})$. A crucial property of the adiabatic Hamiltonian is that the
 260 corresponding evolution decouples the dynamics relative to the subspace $P_*(\mathbf{u})\mathcal{H}$ from
 261 the remainder of the Hilbert space, in the sense that

$$262 \quad P_*(\mathbf{u}(t))U_a^\varepsilon(t, t_0) = U_a^\varepsilon(t, t_0)P_*(\mathbf{u}(t_0)).$$

263 **THEOREM 5 (Adiabatic Theorem).** *Assume that $H(\mathbf{u}) = H_0 + \sum_{i=1}^3 u_i H_i$ sat-*
 264 *isfies **(H0)** and has a separated discrete spectrum (ω, Σ) . Let $I \subset \mathbb{R}$ and $\mathbf{u} : I \rightarrow \omega$*

265 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
 266 for all $\tau_0, \tau \in I$, and setting $t_0 = \tau_0/\varepsilon, t = \tau/\varepsilon$, one has $\|U^\varepsilon(t, t_0) - U_a^\varepsilon(t, t_0)\| \leq$
 267 $C\varepsilon(1 + \varepsilon|t - t_0|)$. In particular

$$268 \quad \|P_*(\mathbf{u}(t))U^\varepsilon(t, t_0) - U^\varepsilon(t, t_0)P_*(\mathbf{u}(t_0))\| \leq 2C\varepsilon(1 + \varepsilon|t - t_0|).$$

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

272 Let $\mathcal{W}(\tau)$ denote the subspace spanned by the eigenstates associated with $\lambda_j(\mathbf{u}(\tau))$
 273 and $\lambda_{j+1}(\mathbf{u}(\tau))$. Since $\mathcal{W}(\tau)$ is two-dimensional for any τ , it is possible to map it
 274 isomorphically on \mathbb{C}^2 and identify an effective Hamiltonian whose evolution is a rep-
 275 resentation of $U_a^\varepsilon(t, t_0)|_{\mathcal{W}(\varepsilon t_0)}$ on \mathbb{C}^2 . In particular, if we can find a \mathcal{C}^1 eigenstate basis
 276 $\{\Phi_1(\mathbf{u}(\tau)), \Phi_2(\mathbf{u}(\tau))\}$ of $\mathcal{W}(\tau)$ (associated with a reordering $\{\Lambda_1(\mathbf{u}(\tau)), \Lambda_2(\mathbf{u}(\tau))\}$ of
 277 $\{\lambda_j(\mathbf{u}(\tau)), \lambda_{j+1}(\mathbf{u}(\tau))\}$), then the isomorphism $\mathcal{U}(\tau) : \mathcal{W}(\tau) \rightarrow \mathbb{C}^2$ is continuous. Rep-
 278 resented in \mathbb{C}^2 , the evolution $U_a^\varepsilon(\cdot, t_0)|_{\mathcal{W}(\varepsilon t_0)}$ is governed by the Hamiltonian $H_{\text{eff}}^\varepsilon(\varepsilon t)$,
 279 where $H_{\text{eff}}^\varepsilon(\cdot)$ is the *effective Hamiltonian*, whose form is

$$280 \quad (7) \quad H_{\text{eff}}^\varepsilon(\tau) = \begin{pmatrix} \Lambda_1(\mathbf{u}(\tau)) & 0 \\ 0 & \Lambda_2(\mathbf{u}(\tau)) \end{pmatrix} - i\varepsilon \begin{pmatrix} \langle \Phi_1(\mathbf{u}(\tau)), \dot{\Phi}_1(\mathbf{u}(\tau)) \rangle & \langle \Phi_2(\mathbf{u}(\tau)), \dot{\Phi}_1(\mathbf{u}(\tau)) \rangle \\ \langle \Phi_1(\mathbf{u}(\tau)), \dot{\Phi}_2(\mathbf{u}(\tau)) \rangle & \langle \Phi_2(\mathbf{u}(\tau)), \dot{\Phi}_2(\mathbf{u}(\tau)) \rangle \end{pmatrix},$$

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

282 Theorem 5 implies the following.

283 **THEOREM 6.** Assume that $(\omega, \{\lambda_j, \lambda_{j+1}\})$ is a separated discrete spectrum and let
 284 $\mathbf{u} : I \rightarrow \omega$ be a \mathcal{C}^2 curve such that there exists a \mathcal{C}^1 -varying basis of $\mathcal{W}(\cdot)$ made of
 285 eigenstates of $H(\mathbf{u}(\cdot))$. Then there exists a constant C such that for all $\tau_0, \tau \in I$, and
 286 setting $t_0 = \tau_0/\varepsilon, t = \tau/\varepsilon$,

$$287 \quad \|(U^\varepsilon(t, t_0) - \mathcal{U}^*(\varepsilon t)U_{\text{eff}}^\varepsilon(t, t_0)\mathcal{U}(\varepsilon t_0))|_{\mathcal{W}(\varepsilon t_0)}\| \leq C\varepsilon(1 + \varepsilon|t - t_0|).$$

288 3. Conical Intersections and general control strategy.

289 **3.1. Properties of conical intersections.** Let $\lambda_j(\mathbf{u}), \lambda_{j+1}(\mathbf{u})$ denote two eigen-
 290 values of $H(\mathbf{u})$, and assume that they are (locally) separated from the rest of the
 291 spectrum. It is well known that the projection $\mathbf{P}_{\mathbf{u}}$ associated with the sum of the
 292 corresponding eigenspaces is smooth with respect to \mathbf{u} . More in general, the result
 293 holds for any portion of the spectrum of $H(\mathbf{u})$, in presence of a gap (see e.g. [28]).

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

300 **PROPOSITION 7.** Let $\gamma : I \rightarrow \mathbb{R}^3, I = [-R, 0]$, be a $\mathcal{C}^k(I)$ curve such that $\gamma(0) = \bar{\mathbf{u}}$
 301 is a conical intersection between the eigenvalues λ_j and λ_{j+1} and $\dot{\gamma}(t) \neq 0$ for every
 302 $t \in I$, 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
 303 $P_j(\gamma(\cdot))$ is \mathcal{C}^k on $[-R, 0]$, it is \mathcal{C}^{k-1} at the singularity, and

$$304 \quad \lim_{t \rightarrow 0^-} \frac{d^l}{dt^l} P_j(\gamma(t)) = \lim_{t \rightarrow 0^-} \frac{d^l}{dt^l} P_j(\ell_k(t)), \quad l = 0, \dots, k-1,$$

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

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

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

$$311 \quad \mathcal{M}(\psi_1, \psi_2) = \begin{pmatrix} \langle \psi_1, H_1 \psi_2 \rangle & \langle \psi_1, H_1 \psi_2 \rangle^* & \langle \psi_2, H_1 \psi_2 \rangle - \langle \psi_1, H_1 \psi_1 \rangle \\ \langle \psi_1, H_2 \psi_2 \rangle & \langle \psi_1, H_2 \psi_2 \rangle^* & \langle \psi_2, H_2 \psi_2 \rangle - \langle \psi_1, H_2 \psi_1 \rangle \\ \langle \psi_1, H_3 \psi_2 \rangle & \langle \psi_1, H_3 \psi_2 \rangle^* & \langle \psi_2, H_3 \psi_2 \rangle - \langle \psi_1, H_3 \psi_1 \rangle \end{pmatrix}.$$

312 The following lemma can be proved by direct computation.

313 LEMMA 9. *The quantity $\det \mathcal{M}(\psi_1, \psi_2)$ is purely imaginary and the function $(\psi_1, \psi_2) \mapsto$ ■
 314 $\det \mathcal{M}(\psi_1, \psi_2)$ is invariant under unitary transformation of the argument, that is if
 315 $\begin{pmatrix} \widehat{\psi}_1 \\ \widehat{\psi}_2 \end{pmatrix} = \mathbb{U} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix}$ for a pair ψ_1, ψ_2 of orthonormal elements of $\mathcal{D}(H_0)$ and $\mathbb{U} \in U(2)$,
 316 then one has $\det \mathcal{M}(\widehat{\psi}_1, \widehat{\psi}_2) = \det \mathcal{M}(\psi_1, \psi_2)$.*

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

$$320 \quad (8) \quad F(\mathbf{u}) = \det \mathcal{M}(\psi_1, \psi_2)$$

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

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

327 PROPOSITION 10. *Assume that $(\omega, \{\lambda_j, \lambda_{j+1}\})$ is a separated discrete spectrum
 328 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
 329 eigenspace associated with the double eigenvalue. Then $\bar{\mathbf{u}}$ is a conical intersection if
 330 and only if $\mathcal{M}(\psi_1, \psi_2)$ is nonsingular.*

331 *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
 332 the limits of $\phi_j(r_{\mathbf{v}}(t)), \phi_{j+1}(r_{\mathbf{v}}(t))$ as $t \rightarrow 0^+$ (recall that the eigenfunctions ϕ_j, ϕ_{j+1}
 333 can be chosen analytic along $r_{\mathbf{v}}$ for $t \geq 0$). Assume that the intersection is not conical.
 334 Then for every $\varepsilon > 0$ there is a unit vector $\mathbf{v}_{\varepsilon} = (v_1^{\varepsilon}, v_2^{\varepsilon}, v_3^{\varepsilon})$ such that

$$335 \quad \left. \frac{d}{dt} \right|_{t=0^+} \left[\lambda_{j+1}(r_{\mathbf{v}_{\varepsilon}}(t)) - \lambda_j(r_{\mathbf{v}_{\varepsilon}}(t)) \right] \leq \varepsilon.$$

336 By (4) and (6) we deduce that, if \mathbb{A}_{ε} is an orthogonal matrix having \mathbf{v}_{ε} as first row,
 337 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
 338 absolute value is smaller than ε . As a consequence

$$339 \quad |\det \mathcal{M}(\phi_j^{\mathbf{v}_{\varepsilon}}, \phi_{j+1}^{\mathbf{v}_{\varepsilon}})| = |\det (\mathbb{A}_{\varepsilon} \mathcal{M}(\phi_j^{\mathbf{v}_{\varepsilon}}, \phi_{j+1}^{\mathbf{v}_{\varepsilon}}))| \leq C\varepsilon(\alpha|\lambda_j(\mathbf{u})| + \beta)^2,$$

340 with C, α and β suitable positive constants, where we have used the fact that H_i is
 341 $H(\mathbf{u})$ -bounded for $i = 1, 2, 3$. By arbitrariness of ε , the conicity matrix is singular.
 342 Let us now prove the converse statement: assume that $\bar{\mathbf{u}}$ is a conical intersection

343 and, by contradiction, that $\mathcal{M}(\psi_1, \psi_2)$ is singular for every orthonormal basis of the
 344 eigenspace associated with the double eigenvalue. We introduce the matrix

$$345 \quad \widetilde{\mathcal{M}}(\psi_1, \psi_2) = \begin{pmatrix} \Re(\langle \psi_1, H_1 \psi_2 \rangle) & \Im(\langle \psi_1, H_1 \psi_2 \rangle) & (\langle \psi_2, H_1 \psi_2 \rangle - \langle \psi_1, H_1 \psi_1 \rangle) \\ \Re(\langle \psi_1, H_2 \psi_2 \rangle) & \Im(\langle \psi_1, H_2 \psi_2 \rangle) & (\langle \psi_2, H_2 \psi_2 \rangle - \langle \psi_1, H_2 \psi_1 \rangle) \\ \Re(\langle \psi_1, H_3 \psi_2 \rangle) & \Im(\langle \psi_1, H_3 \psi_2 \rangle) & (\langle \psi_2, H_3 \psi_2 \rangle - \langle \psi_1, H_3 \psi_1 \rangle) \end{pmatrix},$$

346 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
 347 if and only if $\widetilde{\mathcal{M}}(\psi_1, \psi_2)$ is. The condition of conical intersection, together with (4)
 348 and (6), implies that $\mathbf{v}^T \widetilde{\mathcal{M}}(\phi_j^{\mathbf{y}}, \phi_{j+1}^{\mathbf{y}}) = (0, 0, a)$ for some $a \neq 0$, so that the third
 349 column of the matrix $\widetilde{\mathcal{M}}(\phi_j^{\mathbf{y}}, \phi_{j+1}^{\mathbf{y}})$ is never linearly dependent from the first two. In
 350 particular the matrix $\widetilde{\mathcal{M}}(\phi_j^{\mathbf{y}}, \phi_{j+1}^{\mathbf{y}})$ is singular only if the first two columns of the
 351 matrix are linearly dependent. Thus, up to multiplying $\phi_j^{\mathbf{y}}, \phi_{j+1}^{\mathbf{y}}$ by phase factors, we
 352 can always assume that $\langle \phi_j^{\mathbf{y}}, H_i \phi_{j+1}^{\mathbf{y}} \rangle \in \mathbb{R}$, $i = 1, 2, 3$.

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

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

$$359 \quad \Upsilon = \begin{pmatrix} \langle \phi_{j+1}^{\mathbf{w}}, H_1 \phi_{j+1}^{\mathbf{w}} \rangle - \langle \phi_j^{\mathbf{w}}, H_1 \phi_j^{\mathbf{w}} \rangle \\ \langle \phi_{j+1}^{\mathbf{w}}, H_2 \phi_{j+1}^{\mathbf{w}} \rangle - \langle \phi_j^{\mathbf{w}}, H_2 \phi_j^{\mathbf{w}} \rangle \\ \langle \phi_{j+1}^{\mathbf{w}}, H_3 \phi_{j+1}^{\mathbf{w}} \rangle - \langle \phi_j^{\mathbf{w}}, H_3 \phi_j^{\mathbf{w}} \rangle \end{pmatrix},$$

360 which corresponds to the third column of $\widetilde{\mathcal{M}}(\phi_j^{\mathbf{w}}, \phi_{j+1}^{\mathbf{w}})$. Notice that the definition of
 361 Υ , up to a sign, does not depend on the choice of $\mathbf{w} \in W$, by previous remarks. Since
 362 Υ^\perp , the orthogonal complement of Υ in \mathbb{R}^3 , has dimension 2 there exists a non-zero
 363 $\widetilde{\mathbf{w}} \in W \cap \Upsilon^\perp$. By definition of $\widetilde{\mathbf{w}}$ we have that $\widetilde{\mathbf{w}} \cdot \Upsilon = 0$.

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

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

370 **PROPOSITION 11.** *Let $\bar{\mathbf{u}}$ be a conical intersection between λ_j and λ_{j+1} . Let $\mathbf{v}_0, \mathbf{v} \in$
 371 \mathbb{R}^3 be two unit vectors, and call ϕ_j^0, ϕ_{j+1}^0 the limits as $t \rightarrow 0^+$ of the eigenstates
 372 $\phi_j(r_0(t)), \phi_{j+1}(r_0(t))$ along a straight line $r_0(t) = \bar{\mathbf{u}} + t\mathbf{v}_0$, and $\phi_j^{\mathbf{y}}, \phi_{j+1}^{\mathbf{y}}$ the limit
 373 basis along the straight line $r_{\mathbf{v}}(t) = \bar{\mathbf{u}} + t\mathbf{v}$. Then, up to phases, the following relation
 374 holds:*

$$375 \quad (9) \quad \begin{pmatrix} \phi_j^{\mathbf{y}} \\ \phi_{j+1}^{\mathbf{y}} \end{pmatrix} = \begin{pmatrix} \cos \Xi & e^{-i\beta} \sin \Xi \\ -e^{i\beta} \sin \Xi & \cos \Xi \end{pmatrix} \begin{pmatrix} \phi_j^0 \\ \phi_{j+1}^0 \end{pmatrix},$$

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

$$377 \quad (10) \quad \tan 2\Xi(\mathbf{v}) = (-1)^\xi \frac{2|\langle \phi_j^0, H_{\mathbf{v}} \phi_{j+1}^0 \rangle|}{\langle \phi_j^0, H_{\mathbf{v}} \phi_j^0 \rangle - \langle \phi_{j+1}^0, H_{\mathbf{v}} \phi_{j+1}^0 \rangle}$$

$$378 \quad (11) \quad \beta(\mathbf{v}) \stackrel{(\text{mod } 2\pi)}{=} \arg \langle \phi_j^0, H_{\mathbf{v}} \phi_{j+1}^0 \rangle + \xi\pi,$$

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

381 *Proof.* First of all, we notice that all pairs of orthonormal eigenstates of $H(\bar{\mathbf{u}})$
 382 relative to the degenerate eigenvalue can be obtained through the action of the group
 383 $U(2)$ on the pair (ϕ_j^0, ϕ_{j+1}^0) . However, if one takes into account the equivalence relation
 384 $(e^{i\beta_1}\psi_1, e^{i\beta_2}\psi_2) \sim (\psi_1, \psi_2) \forall \beta_1, \beta_2 \in \mathbb{R}$, it is enough to consider the transformations
 385 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
 386 $\Xi(\mathbf{v}) = k\pi/2$ for some integer k , while $\beta(\mathbf{v})$ can be any real number. If \mathbf{v} is not
 387 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
 388 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)
 389 follow from $\langle \phi_j^y, H_{\mathbf{v}}\phi_{j+1}^y \rangle = 0$, once we replace ϕ_j^y, ϕ_{j+1}^y with the expression given
 390 in (9). \square

391 It can be seen that not all the solutions of (10)-(11) provide the correct trans-
 392 formation (9), which, nevertheless, is easy to detect. The good solutions of (10)-(11)
 393 constitute four branches which are continuous with respect to \mathbf{v} , and they can be
 394 constructed as follows. Let $\mathbf{w}(s)$, $s \in [0, \bar{s}]$, be a curve joining \mathbf{v}_0 to \mathbf{v} such that
 395 $\mathbf{w}(s) \notin \{\mathbf{v}_0, -\mathbf{v}_0\}$ for every $s \in (0, \bar{s})$; for conical intersections, it is possible to as-
 396 sociate with such a curve a continuous solution $(\Xi(\mathbf{w}(s)), \beta(\mathbf{w}(s)))$ of (10)-(11) with
 397 $\Xi(\mathbf{v}_0) = 0$ and compatible with (9). In particular, if we choose $\Xi(\mathbf{v})$ satisfying (10)
 398 with $\xi = 0$, it is easy to see that $\Xi(\mathbf{w}(s)) \in [-\pi/2, 0]$ for $s \in [0, \bar{s}]$, from which
 399 one deduces that the final value $\Xi(\mathbf{v}) = \Xi(\mathbf{w}(\bar{s}))$ is independent of the chosen path
 400 and continuously depends on \mathbf{v} . Moreover, it is easy to see that $\Xi(-\mathbf{v}_0) = -\pi/2$.
 401 Similarly $\beta(\mathbf{v}) = \beta(\mathbf{w}(\bar{s}))$ is independent of the chosen path and continuous outside
 402 $\{\mathbf{v}_0, -\mathbf{v}_0\}$. Note that the fact that β is discontinuous at $-\mathbf{v}_0$ implies that the corre-
 403 sponding limit basis (ϕ_j^y, ϕ_{j+1}^y) has a discontinuity at $-\mathbf{v}_0$, that is, its limit depends
 404 on the path. We can repeat the same argument choosing $\Xi(\mathbf{v})$ satisfying (10) with
 405 $\xi = 1$ and with initial condition $\Xi(\mathbf{v}_0) = 0$. The other two continuous branches are
 406 obtained choosing the initial condition $\Xi(\mathbf{v}_0) = \pi$.

407 **3.2. The basic control algorithm.** Let us consider the following controllability
 408 problem.

409 *Let $H(\cdot)$ satisfy (H0) and have a separated discrete spectrum (ω, Σ) with $\Sigma(\cdot) =$
 410 $\{\lambda_0(\cdot), \dots, \lambda_k(\cdot)\}$. Then, given $\eta > 0$, $\mathbf{u}^s, \mathbf{u}^f \in \omega$, $j \in \{0, \dots, k\}$ and $p \in [0, 1]^{k+1}$
 411 such that $\sum_{l=0}^k p_l^2 = 1$, find $T > 0$ and a path $\mathbf{u} : [0, T] \rightarrow \omega$ with $\mathbf{u}(0) = \mathbf{u}^s$ and
 412 $\mathbf{u}(T) = \mathbf{u}^f$ such that*

$$413 \quad \|\psi(T) - \sum_{l=0}^k p_l e^{i\vartheta_l} \phi_l(\mathbf{u}^f)\| \leq \eta,$$

414 *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
 415 possibly unknown phases.*

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

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

$$424 \quad \gamma(t) = \begin{cases} \bar{\mathbf{u}} + (t - \bar{\tau})\mathbf{w}_0 & t \in [0, \bar{\tau}] \\ \bar{\mathbf{u}} + (t - \bar{\tau})\mathbf{v} & t \in [\bar{\tau}, 1] \end{cases},$$

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

$$427 \quad \|\psi(1/\varepsilon) - \pi_1 e^{i\vartheta_1} \phi_j(\gamma(1)) - \pi_2 e^{i\vartheta_2} \phi_{j+1}(\gamma(1))\| \leq C\sqrt{\varepsilon}$$

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

$$430 \quad \pi_1 = |\cos(\Xi(\mathbf{v}))|, \quad \pi_2 = |\sin(\Xi(\mathbf{v}))|,$$

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

434 *Proof.* We consider the Hamiltonian $H(\mathbf{u}(t))$, $t \in [0, 1/\varepsilon]$. Since the control
 435 function $\mathbf{u}(\cdot)$ is not \mathcal{C}^2 at the singularity, we cannot directly apply the adiabatic
 436 theorem. Instead, we consider separately the evolution on the two subintervals (in
 437 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
 438 \mathcal{C}^1 , we can apply [28, Corollary 2.5] and obtain that there exists a phase θ_1 (depending
 439 on ε) such that

$$440 \quad \|\psi(\bar{\tau}/\varepsilon) - e^{i\theta_1} \phi_j(\gamma(\bar{\tau}^-))\| \leq C'\sqrt{\varepsilon},$$

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

$$442 \quad \|\psi(\bar{\tau}/\varepsilon) - e^{i\theta_1} \left(\cos \Xi(\mathbf{v}) \phi_j(\gamma(\bar{\tau}^+)) - e^{-i\beta(\mathbf{v})} \sin \Xi(\mathbf{v}) \phi_{j+1}(\gamma(\bar{\tau}^+)) \right)\| \leq C'\sqrt{\varepsilon},$$

443 with $\Xi(\mathbf{v})$ 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
 444 applying [28, Corollary 2.5] also in the time interval $(\bar{\tau}/\varepsilon, 1/\varepsilon]$ we get the thesis. \square

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

451 **PROPOSITION 13.** *Let $\bar{\mathbf{u}}$ be a conical intersection between the eigenvalues λ_j, λ_{j+1} ,
 452 and let π_1, π_2 be positive constants such that $\pi_1^2 + \pi_2^2 = 1$. Consider the line $r(t) =$
 453 $\bar{\mathbf{u}} + (t - \bar{\tau})\mathbf{w}_0$, $t \in [0, \bar{\tau}]$, for a unit vector $\mathbf{w}_0 \in \mathbb{R}^3$ and some $\bar{\tau} \in (0, 1)$, and set
 454 $\phi_j^0 = \phi_j(r(\bar{\tau}^-))$ and $\phi_{j+1}^0 = \phi_{j+1}(r(\bar{\tau}^-))$.*

455 *Then the locus formed by the directions $\mathbf{v} \in \mathbb{R}^3$ that give rise to transformation (9)
 456 with $\pi_1 = |\cos \Xi(\mathbf{v})|$ and $\pi_2 = |\sin \Xi(\mathbf{v})|$ is given by the following expression whenever
 457 $\pi_1 \notin \{0, 1\}$*

$$458 \quad \widetilde{\mathcal{M}}(\phi_j^0, \phi_{j+1}^0)^{-T}(\mathcal{K}),$$

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

461 The controllability problem presented at the beginning of this section can be solved
 462 taking advantage of the results shown above. The strategy consists in constructing
 463 a piecewise \mathcal{C}^2 path joining \mathbf{u}^s with \mathbf{u}^f that passes through the conical intersections
 464 $\bar{\mathbf{u}}_j$ between the j -th and the $(j + 1)$ -th levels, $j = 0, \dots, k - 1$, and avoids any
 465 other degeneracy point. The tangent directions at the conical intersection are chosen
 466 according to the probability weights p_j^2 , as explained in Proposition 13.

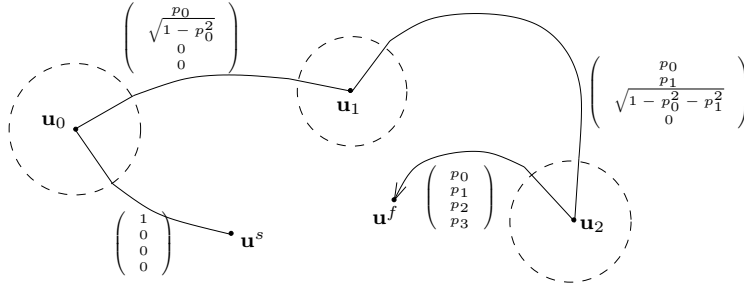


FIG. 1. Construction of the path $\gamma(\cdot)$. The corners at the points \mathbf{u}_i , corresponding to conical intersections, are chosen in such a way that they induce the desired spreading.

467 For simplicity we assume that $\psi(0) = \phi_0(\mathbf{u}^s)$; in the other cases a path can be
 468 obtained similarly. We set $\gamma(0) = \mathbf{u}^s$ and, for some $0 < \tau_0 < 1$ we choose $\gamma|_{[0, \tau_0]}$
 469 in such a way that $\gamma(\tau_0) = \bar{\mathbf{u}}_0$ and all the eigenvalues $\lambda_l(\gamma(\tau))$ are simple for every
 470 $l = 0, \dots, k$ and $\tau \in [0, \tau_0)$. Moreover, $\gamma(\cdot)$ is chosen tangent to a segment in a
 471 neighborhood of $\bar{\mathbf{u}}_0$. The rest of the path is then constructed recursively as follows.
 472 Assume that the path has been defined up to time τ_j , for some $j = 0, \dots, k-2$, with
 473 $\gamma(\tau_j) = \bar{\mathbf{u}}_j$, and that it is tangent to a segment of direction \mathbf{v}_j^- in a neighborhood of
 474 $\bar{\mathbf{u}}_j$. Then $\gamma|_{[\tau_j, \tau_{j+1}]}$, where $\tau_{j+1} \in (\tau_j, 1)$, is chosen to be tangent, in a neighborhood
 475 of $\bar{\mathbf{u}}_j$, to a segment directed as \mathbf{v}_j^+ , where \mathbf{v}_j^+ is obtained applying Proposition 13 with
 476 $\mathbf{w}_0 = \mathbf{v}_j^-$, $\pi_1 = p_j / \sqrt{\sum_{l=j}^k p_l^2}$ and $\pi_2 = \sqrt{1 - \pi_1^2}$. Moreover $\gamma|_{[\tau_j, \tau_{j+1}]}$ is such that
 477 $\gamma(\tau_{j+1}) = \bar{\mathbf{u}}_{j+1}$ and is tangent to a straight line on a neighborhood of $\bar{\mathbf{u}}_{j+1}$. The last
 478 arc defined on $(\tau_{k-1}, 1]$ is simply constructed by joining $\bar{\mathbf{u}}_{k-1}$ with \mathbf{u}^f , taking care
 479 of choosing $\gamma(\cdot)$ tangent to the outward direction obtained through Proposition 13,
 480 in a neighborhood of $\bar{\mathbf{u}}_{k-1}$. To avoid highly non-homogeneous parameterizations, the
 481 path $\gamma(\cdot)$ can be reparameterized by arc-length. The geometric construction of the
 482 path is represented in Figure 1.

483 Let us now reparameterize the time by setting $t = \tau/\varepsilon$, for some small positive ε .
 484 When we are far from all the conical intersections it follows from Theorem 5 that the
 485 evolution of $H(\gamma(\varepsilon t))$ conserves the occupation probabilities relative to each energy
 486 level λ_l , $l = 0, \dots, k$, with an approximation of order ε . Similarly, in a neighborhood
 487 of the conical intersection between λ_j and λ_{j+1} , $j = 0, \dots, k-1$, the evolution of
 488 $H(\gamma(\varepsilon t))$ conserves the occupation probabilities relative to each non-intersecting en-
 489 ergy level with an approximation of order ε . The occupation probabilities relative to
 490 the j -th and $(j+1)$ -th levels are instead estimated by combining Theorem 5 with
 491 the estimate provided by Proposition 12.

492 Summing up, we obtain the estimate

$$493 \quad \|\psi(1/\varepsilon) - \sum_{l=0}^k p_l e^{i\vartheta_l} \phi_l(\mathbf{u}^f)\| \leq C\sqrt{\varepsilon},$$

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

496 **4. An improvement of the efficiency of the algorithm: the non-mixing**
 497 **field.** The problem of reducing transition times is quite important in quantum con-
 498 trol, in particular for the need of preventing decoherence. In this section we show how
 499 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 $\mathbf{P}_{\mathbf{u}}\mathcal{H}$, where $\mathbf{P}_{\mathbf{u}}$ 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 $\mathbf{m}(\psi_1, \psi_2)$ and its components $\langle \psi_1, H_i \psi_2 \rangle$ as m_i , and we define the vector

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

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

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

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*

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

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 $\mu(\rho, \mathbf{v}) = \mathbf{m}(\phi_j(\rho, \mathbf{v}), \phi_{j+1}(\rho, \mathbf{v}))$, 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.

542 LEMMA 17. Assume that $\bar{\mathbf{u}} = 0$ is a conical intersection. Then the inequality
 543 $|\mu(\rho, \mathbf{v}) \cdot \mathbf{v}| \leq C\rho$ holds in a neighborhood of 0 for some constant $C > 0$ uniform with
 544 respect to \mathbf{v} .

545 *Proof.* Up to shifting H_0 by a multiple of the identity we may assume $\lambda_j(0) =$
 546 $\lambda_{j+1}(0) = 0$. Then

$$547 \quad \rho\mu(\rho, \mathbf{v}) \cdot \mathbf{v} = \rho \langle \phi_j(\rho, \mathbf{v}), (v_1 H_1 + v_2 H_2 + v_3 H_3) \phi_{j+1}(\rho, \mathbf{v}) \rangle$$

$$548 \quad = -\langle \phi_j(\rho, \mathbf{v}), H_0 \phi_{j+1}(\rho, \mathbf{v}) \rangle = -\langle \phi_j(\rho, \mathbf{v}) - \mathbf{P}_0 \phi_j(\rho, \mathbf{v}), H_0 \phi_{j+1}(\rho, \mathbf{v}) \rangle.$$

550 Assumption **(H0)** implies that

$$551 \quad \|H_0 \phi_{j+1}(\rho, \mathbf{v})\| \leq |\lambda_{j+1}(\rho \mathbf{v})| + \rho \sum_{i=1}^3 \|H_i \phi_{j+1}(\rho, \mathbf{v})\| \leq c\rho,$$

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

$$554 \quad |\langle \phi_j(\rho, \mathbf{v}) - \mathbf{P}_0 \phi_j(\rho, \mathbf{v}), H_0 \phi_{j+1}(\rho, \mathbf{v}) \rangle| \leq C\rho^2,$$

555 for a suitable $C > 0$, hence we get the thesis. \square

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

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

561 *Proof.* Direct computations lead to the equations

$$562 \quad \dot{\rho} = \mathcal{X}_\mu \cdot \mathbf{v}, \quad \dot{\mathbf{v}} = \frac{1}{\rho} (\mathcal{X}_\mu - (\mathcal{X}_\mu \cdot \mathbf{v}) \mathbf{v}).$$

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

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

$$570 \quad |\mathcal{X}_\mu \cdot \mathbf{v}| = |\mathcal{X}_\mu \cdot (\mathbf{v} - (\mathbf{v} \cdot \hat{\mathbf{v}})\hat{\mathbf{v}})| = \sqrt{1 - (\mathbf{v} \cdot \hat{\mathbf{v}})^2} |\mathcal{X}_\mu| \geq (1 - \hat{c}^2 \rho^2) |\mathcal{X}_\mu|$$

571 and

$$572 \quad |\mathcal{X}_\mu - (\mathcal{X}_\mu \cdot \mathbf{v}) \mathbf{v}|^2 = |\mathcal{X}_\mu|^2 - (\mathcal{X}_\mu \cdot \mathbf{v})^2 \leq 2\hat{c}^2 \rho^2 |\mathcal{X}_\mu|^2.$$

573 The thesis follows. \square

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

577 PROPOSITION 19. For every unit vector \mathbf{v} in \mathbb{R}^3 there exists an integral curve
 578 $\gamma : [-\eta, 0] \rightarrow \omega$ of \mathcal{X}_P with $\gamma(0) = 0$, $\eta > 0$, such that $\lim_{t \rightarrow 0^-} \frac{\dot{\gamma}(t)}{\|\dot{\gamma}(t)\|} = \mathbf{v}$.

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

585 We remark moreover that, if $\gamma : [t_0, t_1] \rightarrow \mathbb{R}^3$ is an integral curve of the non-mixing
 586 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
 587 field, it holds

$$588 \quad (14) \quad P_j(\gamma(t))\dot{P}_{j+1}(\gamma(t)) = 0 \quad P_{j+1}(\gamma(t))\dot{P}_j(\gamma(t)) = 0 \quad \forall t \in [t_0, t_1].$$

589 We have the following.

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

593 *Proof.* Let $\gamma : [-T, 0] \rightarrow \mathbb{R}^3$ be an integral curve of $\mathcal{X}_{\mathcal{P}}$ such that $\gamma(0) = \bar{\mathbf{u}}$ is
 594 a conical intersection between λ_j and λ_{j+1} . Outside the singularity, the eigenstates
 595 are well defined, up to a phase. To fix the phase, we set $\psi_j(t) = \frac{P_j(\gamma(t))\hat{\psi}}{\|P_j(\gamma(t))\hat{\psi}\|}$, for
 596 some $\hat{\psi} \in \mathcal{H}$ satisfying $P_j(\gamma(t))\hat{\psi} \neq 0$ on $[0, T]$ (up to reducing T). Thus $\psi_j(t)$ is a
 597 normalized eigenstate of $H(\gamma(t))$ relative to $\lambda_j(\gamma(t))$. In order to prove that $\psi_j(t)$ is
 598 \mathcal{C}^1 it is enough to prove that $P_j(\gamma(t))$ is. Since $P_j(\gamma(t)) + P_{j+1}(\gamma(t)) = \mathbf{P}_{\gamma(t)}$ for $t \in$
 599 $[-T, 0)$, and by (14), we get that $\mathbf{P}_{\gamma(t)}\dot{P}_j(\gamma(t)) = P_j(\gamma(t))\dot{P}_j(\gamma(t)) = P_j(\gamma(t))\dot{\mathbf{P}}_{\gamma(t)}$.
 600 Therefore

$$601 \quad \dot{P}_j(\gamma(t)) = \dot{\mathbf{P}}_{\gamma(t)}P_j(\gamma(t)) + \mathbf{P}_{\gamma(t)}\dot{P}_j(\gamma(t)) = \dot{\mathbf{P}}_{\gamma(t)}P_j(\gamma(t)) + P_j(\gamma(t))\dot{\mathbf{P}}_{\gamma(t)},$$

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

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

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

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

611 *Proof.* Let $\gamma : [-T, 0] \rightarrow \mathbb{R}^3$ be an integral curve of $\mathcal{X}_{\mathcal{P}}$ such that $\gamma(0) = \bar{\mathbf{u}}$ and
 612 $|\dot{\gamma}(t)| > 0$ for every $t \in [-T, 0]$ (this is true up to choosing T sufficiently small), and
 613 define the eigenstates $\psi_j(\cdot), \psi_{j+1}(\cdot)$ as in Proposition 20.

614 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
 615 eigenvalues and the corresponding spectral projections at $\gamma(t)$. We prove by induction
 616 that, for every positive integer h , $\gamma(\cdot), \lambda_l(\cdot), P_l(\cdot)$ and $H_i P_l(\cdot)$ are \mathcal{C}^h on $[-T, 0]$, where
 617 $l = j, j+1$ and $i = 1, 2, 3$. The proposition then follows immediately.

618 For every non-negative integer h , whenever the h -th order derivatives of $P_l(\cdot)$ and
 619 $H_i P_l(\cdot)$ are well defined, the following inequality holds

$$620 \quad \|H_i(P_l^{(h)}(s) - P_l^{(h)}(t))\| \leq \|H_i\|_{H(\gamma(t))} (\|H(\gamma(s))P_l^{(h)}(s) - H(\gamma(t))P_l^{(h)}(t)\|$$

$$621 \quad + \sum_i |\gamma_i(s) - \gamma_i(t)| \|H_i P_l^{(h)}(s)\| + \|P_l^{(h)}(s) - P_l^{(h)}(t)\|).$$

622

623 In particular, thanks to Proposition 20 and since H_i is $H(\gamma(s))$ -bounded (uniformly
 624 with respect to s), this yields the continuity of $H_i P_l(\cdot)$ on $[-T, 0]$ and the initialization
 625 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
 626 $H_i P_l(\cdot)$ is \mathcal{C}^{h-1} , then $H_i P_l^{(h)}(\cdot)$ is continuous. Indeed, by differentiating h times
 627 the equality $H(\gamma(\cdot))P_l(\cdot) = \lambda_l(\cdot)P_l(\cdot)$ and exploiting the regularity assumptions on
 628 $\lambda_l(\cdot), P_l(\cdot)$ and $H_i P_l(\cdot)$ we get that $H(\gamma(\cdot))P_l^{(h)}(\cdot)$ is continuous in $[-T, 0]$. Since
 629 H_i is $H(\gamma(s))$ -bounded we deduce that $\|H_i P_l^{(h)}(s)\|$ is uniformly bounded on $[-T, 0]$.
 630 Then, the continuity of $H_i P_l^{(h)}(\cdot)$ follows from the above inequality.

631 Assume now that $\gamma(\cdot), \lambda_l(\cdot), P_l(\cdot)$ and $H_i P_l(\cdot)$ have been proved to be \mathcal{C}^h , for
 632 $h \leq k - 1$. Then, by definition of $\mathcal{X}_{\mathcal{P}}$ it turns out that $\gamma(\cdot)$ is \mathcal{C}^k in $[-T, 0]$ and,
 633 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 .
 634 Note that $P_l(\cdot) = \mathbf{P}_{\gamma(\cdot)} P_l(\cdot)$, where $\mathbf{P}_{\gamma(\cdot)}$ is \mathcal{C}^k in $[-T, 0]$, because of the regularity of
 635 $\gamma(\cdot)$. Then, by inductive hypothesis, $P_l(\cdot)$ is \mathcal{C}^k if and only if $\mathbf{P}_{\gamma(\cdot)} P_l^{(k)}(\cdot)$ is continuous
 636 in $[-T, 0]$. We can develop $\mathbf{P}_{\gamma(t)} P_j^{(k)}(\gamma(t))$ as

$$637 \quad \mathbf{P}_{\gamma(t)} P_j^{(k)}(\gamma(t)) = P_j(t) \mathbf{P}_{\gamma(t)}^{(k)} - P_j(t) P_{j+1}^{(k)}(t) + P_{j+1}(t) P_j^{(k)}(t).$$

638 The first term in the right-hand side is continuous in $[-T, 0]$. By (14), it follows that
 639 $\frac{d^{k-1}}{dt^{k-1}} \left(P_j(t) \dot{P}_{j+1}(t) \right) \equiv 0$. Then, by inductive hypothesis, we get that $P_j(t) P_{j+1}^{(k)}(t)$
 640 is continuous in $[-T, 0]$. By a symmetric argument, $P_{j+1}(t) \dot{P}_j^{(k)}(t)$ is continuous
 641 in $[-T, 0]$. We deduce that $\mathbf{P}_{\gamma(t)} P_j^{(k)}(\gamma(t))$ is continuous in $[-T, 0]$, and so is $P_j^{(k)}(\cdot)$
 642 (and, by symmetry, $P_{j+1}^{(k)}(\cdot)$). Since, as shown above, $H_i P_l^{(k)}(\cdot)$ is continuous in $[-T, 0]$
 643 for $l = j, j + 1$ and $i = 1, 2, 3$, the proof of the proposition is concluded. \square

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

647 **THEOREM 22.** *Let $H(\mathbf{u}) = H_0 + u_1 H_1 + u_2 H_2 + u_3 H_3$ satisfy hypotheses (H0).
 648 Assume that $(\omega, \{\lambda_0, \dots, \lambda_k\})$ is a separated discrete spectrum for $H(\mathbf{u})$ and that there
 649 exist conical intersections $\bar{\mathbf{u}}_j \in \omega$, $j = 0, \dots, k - 1$, between the eigenvalues λ_j, λ_{j+1} ,
 650 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
 651 λ_l , $l = 0, \dots, k$ are non degenerate at \mathbf{u}^s and \mathbf{u}^f , for every $\bar{\phi} \in \{\phi_0(\mathbf{u}^s), \dots, \phi_k(\mathbf{u}^s)\}$,
 652 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
 653 $\gamma(\cdot) : [0, 1] \rightarrow \mathbb{R}^m$ with $\gamma(0) = \mathbf{u}^s$ and $\gamma(1) = \mathbf{u}^f$, such that for every $\varepsilon > 0$*

$$654 \quad (15) \quad \|\psi(1/\varepsilon) - \sum_{j=0}^k p_j e^{i\vartheta_j} \phi_j(\mathbf{u}^f)\| \leq C\varepsilon,$$

655 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
 656 some phases depending on ε and γ .

657 *Proof.* The strategy is analogous to the one presented in Section 3.2 and is based
 658 on the construction of a suitable piecewise smooth path joining \mathbf{u}^s with \mathbf{u}^f that
 659 passes through all the conical intersection; in particular, we assume that the path
 660 $\gamma : [0, 1] \rightarrow \omega$ 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
 661 some $0 < \tau_0 < \dots < \tau_{k-1} < 1$. The only difference concerns the construction of
 662 the path in the neighborhoods of the conical intersections: indeed, in these regions
 663 the path is chosen to be tangent to the non-mixing field. At the intersection, the

664 inner and outer directions are selected according to Proposition 13, as explained
 665 in Section 3.2, and the existence of corresponding trajectories tangent to the non-
 666 mixing field is guaranteed by Proposition 19. Far from all the conical intersections the
 667 evolution of $H(\gamma(\varepsilon t))$ conserves the occupation probabilities relative to each energy
 668 level λ_l , $l = 0, \dots, k$, with an approximation of order ε . Let us now estimate the
 669 probability distribution obtained after the passage through the conical intersection
 670 $\bar{\mathbf{u}}_0$. Since the path is tangent to the non-mixing field, we can apply Theorem 6 in order
 671 to study the evolution inside the space $\mathbf{P}_{\mathbf{u}(t)}\mathcal{H}$, where $\mathbf{P}_{\mathbf{u}(t)}$ is the spectral projection
 672 associated with the two levels $\{\lambda_0(\mathbf{u}), \lambda_1(\mathbf{u})\}$. For τ in a left neighborhood of τ_0 , the
 673 effective Hamiltonian and its associated evolution operator $U_{\text{eff}}^\varepsilon$ are diagonal, and this
 674 implies the existence of a phase θ_0 (depending on ε) and of a positive constant C_0
 675 such that $\|\psi(\tau_0/\varepsilon) - e^{i\theta_0}\phi_0(\gamma(\tau_0^-))\| \leq C_0\varepsilon$, where $\psi(\cdot)$ is the solution of equation (3)
 676 with $\psi(0) = \phi_0(\gamma(0))$ corresponding to the control $\mathbf{u}(t) = \gamma(\varepsilon t)$, defined on $[0, 1/\varepsilon]$.
 677 By Proposition 11, this implies that

$$678 \quad \|\psi(\tau_0/\varepsilon) - e^{i\theta_0} \left(\cos \Xi(\mathbf{v}) \phi_0(\gamma(\tau_0^+)) - e^{-i\beta(\mathbf{v})} \sin \Xi(\mathbf{v}) \phi_1(\gamma(\tau_0^+)) \right)\| \leq C_0\varepsilon,$$

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

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

$$683 \quad \|\psi(\tau/\varepsilon) - e^{i\alpha_0} p_0 \phi_0(\gamma(\tau)) - e^{i\alpha_1} \sqrt{1 - p_0^2} \phi_1(\gamma(\tau))\| \leq \hat{C}_0\varepsilon.$$

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

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

689 **THEOREM 23.** *Assume that $H(\mathbf{u}) = H_0 + u_1H_1 + u_2H_2 + u_3H_3$ satisfies **(H0)**
 690 and admits a separated discrete spectrum $(\omega, \{\lambda_j, \lambda_{j+1}\})$. Let $\bar{\mathbf{u}} \in \omega$ be a conical
 691 intersection for $H(\mathbf{u})$ between the eigenvalues λ_j and λ_{j+1} . Then for every $\varepsilon > 0$
 692 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*

$$693 \quad \sum_{i=0}^3 \|\hat{H}_i - H_i\|_{H_0} \leq \delta,$$

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

696 *Proof.* First of all, by equivalence of all norms $\|\cdot\|_{H(\mathbf{u})}$, without loss of generality
 697 we can assume that $\bar{\mathbf{u}} = 0$. We notice that our assumptions guarantee that in a
 698 neighborhood of the conical intersection the eigenvalues λ_j and λ_{j+1} are well sepa-
 699 rated from the rest of the spectrum. Continuous dependence of the eigenvalues with
 700 respect to perturbations of the Hamiltonian (see Lemma 28) ensures that, if δ is small,
 701 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
 702 separated from the rest of the spectrum, locally around $\bar{\mathbf{u}}$. From the conicity of the
 703 intersection between λ_j and λ_{j+1} , there exists $\varepsilon > 0$ small enough such that $|F(\mathbf{u})| \geq c$
 704 for some $c > 0$ on $B(\bar{\mathbf{u}}, \varepsilon)$ and, moreover, by Proposition 18 the vector field \mathcal{X}_P (up

705 to the sign) points inside the ball $B(\bar{\mathbf{u}}, \varepsilon)$ at every point of its boundary. If δ is small
 706 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
 707 assumed to be of order ε . Therefore we can define the conicity matrix $\hat{\mathcal{M}}$ associated
 708 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 $\{\psi_j(\mathbf{u}), \psi_{j+1}(\mathbf{u})\}$
 709 is an orthonormal basis for the sum of eigenspaces relative to $\{\hat{\lambda}_j(\mathbf{u}), \hat{\lambda}_{j+1}(\mathbf{u})\}$. Since
 710 the conicity matrix depends continuously on the control operators, with respect to
 711 the norm $\|\cdot\|_{H_0}$, and as a consequence of Lemma 9 and Proposition 26, we can take
 712 δ small enough such that $|\hat{F}(\mathbf{u})| \geq c/2$ on $B(\bar{\mathbf{u}}, \varepsilon)$. This allows us to define, whenever
 713 $\hat{\lambda}_j \neq \hat{\lambda}_{j+1}$, the non-mixing field $\hat{\mathcal{X}}_{\mathcal{P}}$ associated with $\hat{H}(\cdot)$ and corresponding to the
 714 band $\{\hat{\lambda}_j, \hat{\lambda}_{j+1}\}$; thanks to Proposition 16, up to a time reversal the time derivative
 715 of $\hat{\lambda}_{j+1} - \hat{\lambda}_j$ along the integral curves of $\hat{\mathcal{X}}_{\mathcal{P}}$ is smaller than $-c/4$. By Corollary 27
 716 if δ is small enough, then $\hat{\mathcal{X}}_{\mathcal{P}}$ points inside $B(\bar{\mathbf{u}}, \varepsilon)$ at every point of $\partial B(\bar{\mathbf{u}}, \varepsilon)$. Any
 717 trajectory $\hat{\gamma}(\cdot)$ of $\hat{\mathcal{X}}_{\mathcal{P}}$ starting from $B(\bar{\mathbf{u}}, \varepsilon)$ remains inside $B(\bar{\mathbf{u}}, \varepsilon)$ in its interval of
 718 definition and reaches in finite time a point $\hat{\mathbf{u}}$ corresponding to a double eigenvalue
 719 $\hat{\lambda}_j(\hat{\mathbf{u}}) = \hat{\lambda}_{j+1}(\hat{\mathbf{u}})$. The conclusion follows from Proposition 10. \square

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

$$722 \quad (16) \quad H_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad H_1 = \begin{pmatrix} 1 & i & 0 \\ -i & 0 & 1 \\ 0 & 1 & -1 \end{pmatrix}, \quad H_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 1 & 0 \\ -i & 0 & 0 \end{pmatrix}, \quad H_3 = \begin{pmatrix} -1 & 1 & -1 \\ 1 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}.$$

723 The Hamiltonian $H(\cdot)$ admits a double eigenvalue at $\mathbf{u} = 0$ corresponding to the
 724 two lowest levels. A simple computation leads to $\det \mathcal{M}(e_1, e_2) = -2i$ where $e_1 =$
 725 $(1, 0, 0)^T, e_2 = (0, 1, 0)^T$ form a basis of the double eigenspace at 0. Thus the eigen-
 726 value intersection is conical. Moreover, at the point $\mathbf{u} = (1/2, -1/4, 0)$, the second and
 727 third eigenvalues degenerate, and the intersection is conical: indeed, the determinant
 728 of the conicity matrix corresponding to these two levels is equal to $4i/3$.

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

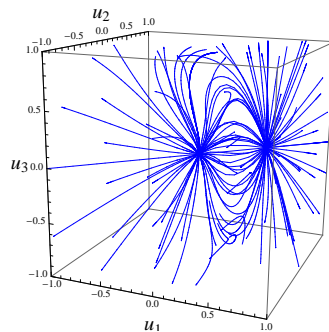


FIG. 2. Trajectories of the non-mixing field relative to the two lowest eigenvalues for the Hamiltonian corresponding to (16)

733

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

737 (1/3, 1/6, 1/2). To do that, we first pass through the conical intersection between the
 738 two lowest levels, leaving a probability of 1/3 on the lowest one and sending 2/3 of
 739 probability to the other; afterwards, we pass through the conical intersection between
 740 the two highest levels in order to send 1/2 of the total probability to the third level;
 741 finally, we come back to the initial point.

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

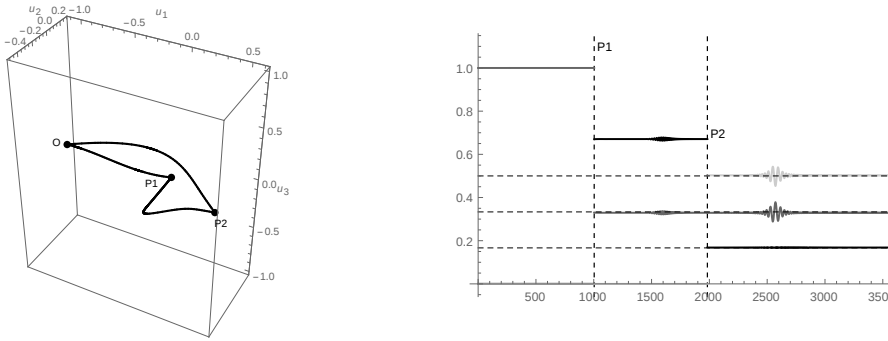


FIG. 3. Control path and probability distributions for the Hamiltonian corresponding to (16). We use black for the probability of being in the second energy state, and the lighter shade of gray for the probability of being in the highest one. The starting point is labeled as O and the conical intersections $(0, 0, 0)$ and $(1/2, -1/4, 0)$ respectively as P_1, P_2 .

746 Consider now the Hamiltonian $H(\mathbf{u}) = -\Delta + u_1V_1 + u_2V_2 - iu_3(\nabla\mathbf{A} + \mathbf{A}\nabla)$,
 747 where

$$748 \quad V_1(x) = x_2^2 + x_3^2, \quad V_2(x) = x_2x_3, \quad A = (0, -x_3/2, x_2/2)^T,$$

$$749 \quad x = (x_1, x_2, x_3) \in \Omega = (0, 1) \times (0, \sqrt{3}) \times (0, \sqrt{5})$$

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

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

$$760 \quad \lambda_{j_1, j_2, j_3} = \pi^2 \left(j_1^2 + \frac{j_2^2}{3} + \frac{j_3^2}{5} \right), \quad \psi_{j_1, j_2, j_3}(x) = \frac{2\sqrt{2}}{\sqrt[4]{15}} \sin(j_1\pi x_1) \sin\left(\frac{j_2\pi x_2}{\sqrt{3}}\right) \sin\left(\frac{j_3\pi x_3}{\sqrt{5}}\right)$$

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

765 Let us consider an initial control $\mathbf{u}_0 = (1, 0, 0)$ and an initial state concentrated
 766 on the fourth energy level of $H(\mathbf{u}_0)$. Our aim is to induce an approximate transition

767 to a state distributed between the fourth and fifth level of $H(\mathbf{u}_0)$ with probability $2/3$
 768 and $1/3$, respectively. We follow arc-length parametrized curves with a parameter $\varepsilon =$
 769 0.003 , and we compare the transition obtained following control paths with a different
 770 behavior around the singularity. Namely, we consider a path which is locally an
 771 integral curve of the non-mixing field (top-left in Figure 4) and one which is piecewise
 772 affine in the sense of Proposition 11 (bottom-left in Figure 4). The corresponding
 773 probability distributions as functions of the time are shown in Figure 4, on the right
 774 side. Both paths induce quite precisely the desired transition, although for long times
 775 the accuracy degrades. We remark that the most significant difference between the
 776 two strategies is given by the fact that the second one induces a less accurate spread
 777 of probability at the passage through the conical intersection, as expected.

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

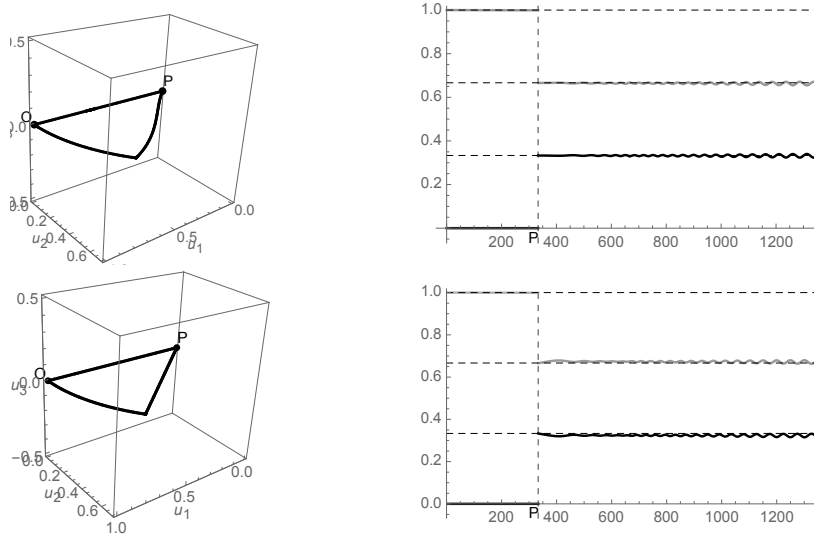


FIG. 4. Control paths and probability distributions for $H(\mathbf{u}) = -\Delta + u_1V_1 + u_2V_2 - iu_3(\nabla\mathbf{A} + \mathbf{A}\nabla)$. We reproduce in gray the probability of being in the fourth energy level and in black the probability of being in the fifth one. The starting point is labeled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

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

793 $1/\varepsilon$, gives a difference of order ε .

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

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

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

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

822 Appendix A. Regularity properties and proof of Proposition 7.

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

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

$$832 \quad (17) \quad R(A_2, \zeta) - R(A_1, \zeta) = R(A_1, \zeta)(A_1 - A_2)R(A_2, \zeta).$$

833 The identity

$$834 \quad (18) \quad \|(X - \zeta \text{id})^{-1}\| = d(\zeta, \sigma(X))^{-1}$$

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

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

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

$$840 \quad (19) \quad \|BR(A, \zeta)\| \leq \left(1 + (|\zeta| + 1) \|R(A, \zeta)\|\right) \|B\|_A.$$

841 The following result shows that the resolvent set for a self-adjoint operator A
 842 possesses some continuity properties with respect to small perturbation in the space
 843 $\mathcal{L}(\mathcal{D}(A), \mathcal{H})$.

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

$$847 \quad (20) \quad \|R(A_2, \zeta) - R(A_1, \zeta)\| \leq C \|A_1 - A_2\|_{A_1}$$

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

849 *Proof.* To ensure that $\mathcal{D}(A_1) = \mathcal{D}(A_2)$ it is clearly enough to assume $\delta < 1$. To
 850 conclude the proof we proceed as follows. As a consequence of (18), $\|R(A_1, \zeta)\|$ is
 851 uniformly bounded on \mathcal{Z} . This, together with (19), implies that $\|(A_2 - A_1)R(A_1, \zeta)\| <$
 852 $C' \|A_1 - A_2\|_{A_1}$ for some $C' > 0$. Since

$$853 \quad R(A_2, \zeta) = R(A_1, \zeta) (\text{id} + (A_2 - A_1)R(A_1, \zeta))^{-1}$$

854 whenever the right-hand side is well defined, we deduce that $\mathcal{Z} \subset \rho(A_2)$ and that
 855 $\|R(A_2, \zeta)\| \leq 2\|R(A_1, \zeta)\|$ on \mathcal{Z} , provided that δ is small enough. Finally, by apply-
 856 ing (17), we get (20). \square

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

$$861 \quad (21) \quad P = -(2\pi i)^{-1} \oint_{\Gamma} R(A, \zeta) d\zeta.$$

862 PROPOSITION 26. Let A_1 be a self-adjoint operator. Assume that $\Sigma_1 = \sigma(A_1) \cap$
 863 (ζ_1, ζ_2) is constituted by k eigenvalues, counted with multiplicity, and that $\zeta_1, \zeta_2 \notin$
 864 $\sigma(A_1)$. Then for every $\epsilon > 0$ there exists a $\delta > 0$, depending on ζ_1, ζ_2 and A_1 , such
 865 that if A_2 is self-adjoint and $\|A_1 - A_2\|_{A_1} \leq \delta$, then

- 866 *i)* $\Sigma_2 = \sigma(A_2) \cap (\zeta_1, \zeta_2)$ is constituted by k eigenvalues, counted with multiplicity;
 867 *ii)* Calling $P_{\Sigma_1}^{A_1}$ the spectral projection onto the sum of eigenspaces of A_1 relative
 868 to Σ_1 and $P_{\Sigma_2}^{A_2}$ the spectral projection onto the sum of eigenspaces of A_2
 869 relative to Σ_2 , it holds $\|P_{\Sigma_1}^{A_1} - P_{\Sigma_2}^{A_2}\| \leq \epsilon$.

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

$$873 \quad \left\|P_{\Sigma_1}^{A_1} - P_{\Sigma_2}^{A_2}\right\| \leq (2\pi)^{-1} \oint_{\Gamma} \|R(A_1, \zeta) - R(A_2, \zeta)\| d\zeta \leq \hat{C}\delta$$

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

878 The following result immediately follows from Proposition 26.

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

883 The next result provides an estimate concerning regularity properties of the eigen-
 884 values.

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

892 *Proof.* Let A_1 satisfy the hypotheses of the lemma, and let A_2 be a self-adjoint
 893 operator with $\|A_1 - A_2\|_{A_1} \leq \delta$, where without loss of generality we assume that
 894 $\delta < 1$; define $A(t) = A_1 + t(A_2 - A_1)$, for $t \in [0, 1]$. Let $\lambda_i(t)$ be the analytic branch
 895 of the eigenvalues of $A(t)$ emanating from $\lambda_i(0) = \mu_i(A_1)$, and denote by $\phi_i(t)$ a
 896 corresponding analytic eigenstate. By hypothesis

$$897 \quad \|(A_2 - A_1)\phi_i(t)\| \leq \delta\|A_1\phi_i(t)\| + \delta \leq \delta|\lambda_i(t)| + \delta t\|(A_2 - A_1)\phi_i(t)\| + \delta,$$

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

$$899 \quad |\dot{\lambda}_i(t)| = |\langle \phi_i(t), (A_2 - A_1)\phi_i(t) \rangle| \leq \|(A_2 - A_1)\phi_i(t)\|$$

900 we easily get the thesis. \square

901 Consider a control-dependent Hamiltonian $H(\mathbf{u})$ satisfying assumption **(H0)**. It
 902 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
 903 the H_0 -smallness of the control Hamiltonians. From Lemma 28, and the equivalence
 904 of the norms $\|\cdot\|_{H(\mathbf{u})}$, the eigenvalues $\lambda_i(\cdot)$ of $H(\cdot)$ are locally Lipschitz, and the
 905 corresponding Lipschitz constants locally depend on the magnitude of $\lambda_i(\cdot)$. Moreover,
 906 we remark the following fact: let $\bar{\mathbf{u}}$ be a conical intersection between the eigenvalues
 907 λ_j and λ_{j+1} , that satisfy a gap condition, according to Definition 2. By the definition
 908 of conical intersection and the Lipschitz continuity of the eigenvalues we can conclude
 909 that there exist a suitably small neighborhood U of $\bar{\mathbf{u}}$ and two constants $C_1 > 0$ and
 910 $C_2 > 0$ such that

$$911 \quad (22) \quad \lambda_{j+1}(\mathbf{u}) - \lambda_j(\mathbf{u}) \geq C_1|\mathbf{u} - \bar{\mathbf{u}}| \quad \forall \mathbf{u} \in U$$

912 and

$$913 \quad (23) \quad |\lambda_i(\mathbf{u}) - \lambda_i(\mathbf{u}')| \leq C_2|\mathbf{u} - \mathbf{u}'| \quad \forall \mathbf{u}, \mathbf{u}' \in U, \quad i = j, j + 1.$$

914 We are now ready to prove Proposition 7.

915 *Proof of Proposition 7.* For simplicity, throughout this proof we will write $R(\mathbf{u}, \xi)$
 916 to denote the resolvent $R(H(\mathbf{u}), \xi)$. The property that the projections $P_j(\gamma(t))$, $J =$
 917 $j, j + 1$, 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
 918 comes from (21) and a recursive application of the identity

$$919 \quad (24) \quad \frac{d}{dt}R(f(t), \xi) = R(f(t), \xi) \left(\frac{d}{dt}H(f(t)) \right) R(f(t), \xi),$$

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

921 It remains to study the regularity of the projections at the singularity. We first
 922 consider the case $k = 1$. Without loss of generality we assume $|\dot{\gamma}(0)| = 1$. Let
 923 $\rho = C_1/4$, where C_1 is as in (22), and for every $t \in [-R, 0)$ consider the circle
 924 $\Gamma_t \subset \mathbb{C}$ of radius ρt centered at $\lambda_j(\gamma(t))$. There exists $0 < T \leq R$ such that for every
 925 $t \in [-T, 0)$

$$926 \quad |\lambda_{j+1}(\gamma(t)) - \lambda_j(\gamma(t))| \geq \frac{3}{4}C_1 t = 3\rho t$$

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

$$930 \quad (25) \quad \|R(\gamma(t), \zeta)\| = \frac{1}{\rho t}, \quad \|R(\ell_1(t), \zeta)\| \leq \frac{2}{\rho t}.$$

931 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

$$932 \quad \|(H(\ell_1(t)) - H(\gamma(t)))R(\gamma(t), \zeta)\| \leq C \left| \frac{\ell_1(t) - \gamma(t)}{t} \right|$$

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

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

$$937 \quad (26) \quad \|R(\gamma(t), \zeta)\| \leq \frac{2}{\rho t}, \quad \|R(\ell_k(t), \zeta)\| \leq \frac{2}{\rho t},$$

938 holding for every $\zeta \in \Gamma_\tau$ and $t \in I_\tau$. By applying (17) we get, for every $t \in I_\tau$ and
 939 $l \leq k - 1$,

$$940 \quad \frac{d^l}{dt^l} P_j(\gamma(t)) - \frac{d^l}{dt^l} P_j(\ell(t)) = -(2\pi i)^{-1} \oint_{\Gamma_\tau} \frac{d^l}{dt^l} \left[R(\ell_k(t), \zeta) (H(\ell_k(t)) - H(\gamma(t))) R(\gamma(t), \zeta) \right] d\zeta.$$

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

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946

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