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Effective adiabatic control of a decoupled Hamiltonian obtained by rotating wave approximation

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Abstract

In this paper we study up to which extent we can apply adiabatic control strategies to a quantum control model obtained by rotating wave approximation. In particular, we show that, under suitable assumptions on the asymptotic regime between the parameters characterizing the rotating wave and the adiabatic approximations, the induced flow converges to the one obtained by considering the two approximations separately and by combining them formally in cascade. As a consequence, we propose explicit control laws which can be used to induce desired populations transfers, robustly with respect to parameter dispersions in the controlled Hamiltonian.

1 Introduction

A common and fruitful approach to study the controllability properties of a quantum system consists in replacing the controlled Hamiltonian $H(u)$ by an effective Hamiltonian $H_{\text{eff}}(\hat{u})$ with more degrees of freedom, in such a way that the dynamics induced by H_{eff} can be approximated arbitrarily well by the trajectories corresponding to H.

One of the most popular procedures to do so is based on the so-called *rotating wave approximation* and works as follows: up to a time-dependent change of coordinates (which consists in adopting a rotating coordinate frame driven by the drift Hamiltonian $H(0)$ corresponding to the control $u = 0$), and up to taking as control the superposition of monochromatic pulses in resonance with the spectral gaps of the system, we can split the resulting dynamics into those terms which oscillate fast and those which evolve relatively slowly. Then, if we assume that the control is applied on a time-interval of length T (much larger than the period of the oscillating terms) and is of amplitude of order $1/T$, then the effect of the oscillating terms can be neglected by an averaging argument and the effect of the remaining terms is of order 1 (see, e.g. [10, 11, 12, 18]). The increase in the amount of degrees of freedom of the effective Hamiltonian obtained in this way comes from the fact that the amplitude and phase of every monochromatic pulse applied as control in the original system play the role of independent controls in the resulting effective system. We say that the original Hamiltonian is *decoupled*, in the sense that it can be seen as the linear combination of Hamiltonians of smaller rank which can be controlled independently.

For a quantum control systems with several degrees of freedom, a popular control strategy is based on adiabatic approximation. If the controlled Hamiltonian varies slowly, a trajectory having as initial condition an eigenvector approximately follows the quasi-static curve corresponding to the eigenvectors of the non-autonomous Hamiltonian. The property of having several degrees of freedom in the controlled Hamiltonian allows to design loops in the space of controls whose corresponding adiabatic trajectories drive the system from an energy level to a different one [8, 17, 20, 21]. The advantage of the adiabatic control strategy (instead of, for instance, Rabi pulses) is that it is robust to parameter incertainties in the Hamiltonian. In particular, it can be used to drive ensembles of quantum systems [4, 14, 18, 21].

It is then tempting to adopt an adiabatic control strategy to the quantum system corresponding to the decoupled Hamiltonian obtained by the rotating wave approximation. The resulting control for the original system is a superposition of monochromatic

pulses whose amplitude and phase vary slowly. Actually, since the precision of both adiabatic and rotating wave approximations depend on the length of the time-interval on which the control is defined, the concatenation of the two strategies leads to a 'doubly slow' control. More precisely, the resulting control is defined on a interval of the type $[0, 1/(\epsilon_1\epsilon_2)]$, where the rotating wave approximation becomes more accurate as $\epsilon_1 \to 0$, while the adiabatic strategy converges to the desired target as $\epsilon_2 \to 0$. However, the convergence of the rotating wave approximation is guaranteed only when $\epsilon_2 > 0$ is fixed. The concatenation of the two time-scales approximations is then not guaranteed to hold, in general, as $(\epsilon_1, \epsilon_2) \to (0, 0)$.

In [5] we considered this question for two-level systems with a simple structure. In particular, seting $\epsilon_1 = \epsilon_2^\alpha$, we showed that the controls obtained by concatenating the two strategies do steer the system approximately close to the desired trajectories, at least when $\alpha > 1$.

Here we extend the results of [5] by considering more general quantum control systems. More precisely, we consider single-input control-affine systems (i.e., we take $H(u) = H_0 + uH_1$, with H_0 and H_1 self-adjoint $n \times n$ matrices), and we show how to identify the corresponding decoupled Hamiltonian corresponding to the rotating wave approximation. Then, we prove that, under the assumption that $\epsilon_1 = \epsilon_2^\alpha$ for some $\alpha > 1$, the trajectories of the original system corresponding to the pulses obtained by the formal cascade of the two approximations converge to the adiabatic trajectories of the decoupled Hamiltonian. The proof is based on adapted quantitative averaging results for unbounded oscillating vector fields on the unit group $U(n)$, in the spirit of [13, 15].

Under some simplifying assumption on the resonances of the system (which lead to simpler expressions of the decoupled Hamiltonian), we also give explicit expressions of the pulses leading to generalized (i.e., multilevel) chirped pulses and STIRAP trajectories of the decoupled Hamiltonian.

As we recalled above, one of the main reasons to adopt an adiabatic control strategy is that it guarantees precious robustness properties with respect to the parameters of the controlled Hamiltonian. Our results show that the control strategy that we propose is still robust with respect to the parameter dispersions in H_1, although this is not in general true for the parameter dispersions in the drift Hamiltonian H_0. The case of parameter dispersions in H_0 requires a different strategy and is discussed for two-level systems in [16].

The paper is organized as follows. In Section 2 we give the general expression of the decoupled Hamiltonian obtained by rotating wave approximation for single-input bilinear quantum systems. We also state the main result about the effectiveness of the concatenation of the adiabatic control of the decoupled Hamiltonian and the rotating wave approximation (Theorem 3), and we give the general expression of the corresponding pulses. Section 3 contains the proof of Theorem 3 and the averaging results used to obtained it. Finally, in Section 4, we apply the general construction to the case where the original Hamiltonian satisfy a suitable non-resonance simplifying property, and we identify some explicit adiabatic controls for the decoupled Hamiltonian that induce a complete population transfer between the energy levels of the drift Hamiltonian.

2 Decoupled Hamiltonian and its induced adiabatic evolution

Fix $n \in \mathbf{N}$ and let $H_0, H_1 \in i\mathfrak{u}(n)$, where $\mathfrak{u}(n)$ denotes the Lie algebra of $n \times n$ skew-adjoint matrices. Consider the system

$$i\frac{d\psi(t)}{dt} = (H_0 + u(t)H_1)\psi(t), \qquad \psi(t) \in \mathbf{C}^n, \quad (1)$$

where the control u takes values in $\mathbf{R}$. Up to a unitary change of variables, we can assume that $H_0 = \mathrm{diag}(E_j)_{j=1}^n$ with $E_1, \ldots, E_n \in \mathbf{R}$. Define

$$\Xi = \left\{ |E_j - E_k| \mid (j,k) \in \{1, \ldots, n\}^2,\ (H_1)_{j,k} \neq 0 \right\}$$

i.e., Ξ is the set of nonnegative spectral gaps of H_0 corresponding to a direct coupling by the controlled Hamiltonian H_1. Let us now use the spectral gaps in Ξ to identify a controlled Hamiltonian which corresponds to a decoupling of H_1. The effectivity of such a decoupling is illustrated in the next sections.

For $\sigma \in \Xi$, let $\mathcal{R}_\sigma \subset \{1, \ldots, n\}^2$ and $H_1^\sigma \in i\mathfrak{u}(n)$ be defined by

$$\mathcal{R}_\sigma = \{(j,k) \mid E_j - E_k = \sigma,\ (H_1)_{j,k} \neq 0\}, \quad (2)$$

$$(H_1^\sigma)_{j,k} = \begin{cases} (H_1)_{j,k} & \text{if } |E_j - E_k| = \sigma, \\ 0 & \text{otherwise.} \end{cases}$$

The idea of the decoupling is to consider that each of the matrices H_1^σ can be controlled autonomously. More precisely, define the *decoupled Hamiltonian* $H_\mathrm{d} : \mathbf{R}^n \times \mathbf{R}^\Xi \to i\mathfrak{u}(n)$ by

$$H_\mathrm{d}(\delta, w) = \sum_{j=1}^n \delta_j e_{jj} + \sum_{\sigma \in \Xi} w_\sigma H_1^\sigma, \quad (3)$$

where $\mathbf{R}^{\Xi}$ denotes the set of real vectors $(w_\sigma)_{\sigma\in\Xi}$, and, for every $j,k \in \{1,\dots,n\}$, e_{jk} is the $n\times n$ matrix whose (j,k)-coefficient is equal to 1 and the others are equal to 0.

2.1 Adiabatic evolution of the decoupled Hamiltonian

For every $k \in \{1,\dots,n\}$ consider a smooth function $\varphi_k : [0,1] \to \mathbf{R}$ such that $\varphi_k(0) = 0$. Consider, in addition, a family of smooth functions $v_\sigma : [0,1] \to \mathbf{R}$, $\sigma \in \Xi$, and, if $0 \notin \Xi$, set $v_0 \equiv 0$.

Assume, moreover, that

$$\begin{aligned} &\varphi_j - \varphi_k = \varphi_p - \varphi_q \\ &\text{if } \exists\, \sigma \in \Xi \text{ s.t. } (j,k),(p,q) \in \mathcal{R}_\sigma \text{ and } v_\sigma \neq 0, \end{aligned} \tag{4}$$

where by $v_\sigma \neq 0$ we mean that v_σ is not identically equal to zero. Concerning the solvability of the constraint (4), notice that, for every $\phi \in C^\infty([0,1],\mathbf{R})$ such that $\phi(0) = 0$, the choice $\varphi_k = \phi$ for every $k = 1,\dots,n$ satisfies (4). In general, there exists a linear subspace L of $\mathbf{R}^n$ of dimension at least one such that (4) is satisfied if and only if the vector valued function $\varphi = (\varphi_j)_{j=1}^n : [0,1] \to \mathbf{R}^n$ takes values in L.

Given $\varphi = (\varphi_j)_{j=1}^n : [0,1] \to L$ and $\sigma \in \Xi$ such that $v_\sigma \neq 0$, we define

$$\hat\varphi_\sigma = \varphi_j - \varphi_k, \qquad \text{for } (j,k) \in \mathcal{R}_\sigma.$$

Let $\alpha > 1$ and define

$$\begin{aligned} u_\epsilon(t) &= \epsilon v_0(\epsilon^{\alpha+1}t) \\ &+ 2\epsilon \sum_{\sigma\in\Xi\setminus\{0\}} v_\sigma(\epsilon^{\alpha+1}t)\cos\left(\sigma t + \frac{\hat\varphi_\sigma(\epsilon^{\alpha+1}t)}{\epsilon}\right). \end{aligned} \tag{4}$$

Denote $v = (v_\sigma)_{\sigma\in\Xi}$ and let $h_{\mathrm{d}} : [0,1] \to i\mathfrak{u}(n)$ be the non-autonomous Hamiltonian

$$h_{\mathrm{d}}(\tau) = H_{\mathrm{d}}(-\varphi'(\tau), v(\tau)), \qquad \tau \in [0,1]. \tag{5}$$

Before stating our main result on the approximation by solutions of system (1) of the adiabatic trajectories induced by the non-autonomous Hamiltonian h_{d}, let us introduce the following gap condition.

Definition 1. *For $h \in C^\infty([0,1], i\mathfrak{u}(n))$, let $\lambda_1,\dots,\lambda_n : [0,1] \to \mathbf{R}$ be smooth and such that $\{\lambda_1(\tau),\dots,\lambda_n(\tau)\}$ is the spectrum of $h(\tau)$ for every $\tau \in [0,1]$. We say that h satisfies a* gap condition *if there exists $C > 0$ such that*

$$\begin{aligned} &\forall j,\ell \in \{1,\dots,n\} \text{ s.t. } j \neq \ell, \\ &\forall \tau \in [0,1], \qquad |\lambda_j(\tau) - \lambda_\ell(\tau)| \geq C. \end{aligned} \tag{GAP}$$

Given a nonnegative integer κ, we say that h satisfies a κ-th order gap condition *if*

$$\begin{aligned} &\forall j,\ell \in \{1,\dots,n\} \text{ s.t. } j \neq \ell, \forall \tau \in [0,1], \\ &\begin{cases} \exists r \in \{0,\dots,\kappa\} & \text{s.t. } \frac{d^r(\lambda_\ell - \lambda_j)}{d\tau^r}(\tau) \neq 0, \\ \lambda_p(\tau) \neq \lambda_j(\tau) & \text{for } p \neq j,\ell. \end{cases} \end{aligned} \tag{κ-GAP}$$

Remark 2. *Notice that a 0-th order gap condition is nothing else that a gap condition. Concerning the regularity of eigenvalues, it is known if $h \mapsto h(\tau)$ is C^∞, and if the order of contact of any two unequal eigenvalues of h is finite, then all the eigenvalues and all the eigenvectors $h(\tau)$ can be chosen to be C^∞ with respect to τ [3, Theorem 7.6].*

Our main result is the following.

Theorem 3. *Set $\psi_0 \in \mathbf{C}^n$ and let $\psi_\epsilon(\cdot)$ be the solution of*

$$i\frac{d\psi_\epsilon(t)}{dt} = (H_0 + u_\epsilon(t)H_1)\,\psi_\epsilon(t), \qquad 0 \leq t \leq \frac{1}{\epsilon^{\alpha+1}},$$

with $\psi_\epsilon(0) = \psi_0$. Define $\hat\Psi_\epsilon$ as the solution of

$$\frac{d\hat\Psi_\epsilon(s)}{ds} = h_{\mathrm{d}}(\epsilon s)\hat\Psi_\epsilon(s), \qquad 0 \leq s \leq \frac{1}{\epsilon}, \tag{6}$$

with $\hat\Psi_\epsilon(0) = \psi_0$. Assume that h_{d} satisfies a κ-th order gap condition for some nonnegative integer κ. Then

$$\left\|\psi_\epsilon\left(\frac{\tau}{\epsilon^{\alpha+1}}\right) - V_\epsilon(\tau)\hat\Psi_\epsilon\left(\frac{\tau}{\epsilon}\right)\right\| < c\epsilon^{\min(\frac{1}{\kappa+1},\alpha-1)}$$

for $0 \leq \tau \leq 1$, where $V_\epsilon(\tau) = \operatorname{diag}\left(e^{-i(\frac{E_j\tau}{\epsilon^{\alpha+1}} + \frac{\varphi_j(\tau)}{\epsilon})}\right)_{j=1}^n$ and $c > 0$ is independent of $\tau \in [0,1]$ and $\epsilon > 0$.

The proof is postponed to the next section, where the required preliminary technical results are obtained.

3 Approximation results and proof of Theorem 3

In this section, we prove several averaging results leading to the proof of Theorem 3. Up to a suitable time-rescaling and change of coordinates, the proof is based on an adiabatic approximation where high-order oscillating terms are proved to be negligible.

3.1 Negligible high-order terms in adiabatic approximation

Consider $A \in C^\infty([0,1],\mathfrak{u}(n))$. The adiabatic evolution corresponding to A is described by the equation

$$\frac{d\hat{X}_\epsilon(s)}{ds} = A(\epsilon s)\hat{X}_\epsilon(s), \quad 0 \le s \le \frac{1}{\epsilon}. \tag{7}$$

Our goal is to understand under which conditions on a perturbation term $(B_\epsilon(\cdot))_{\epsilon>0}$ the flows of (7) and

$$\frac{dX_\epsilon(s)}{ds} = \left(A(\epsilon s) + B_\epsilon(\epsilon s)\right) X_\epsilon(s), \quad 0 \le s \le \frac{1}{\epsilon}, \tag{8}$$

are arbitrarily close, as $\epsilon \to 0$.

Definition 4. *Given $\alpha > 1$, denote by $S(\alpha)$ the set of families $(B_\epsilon)_{\epsilon>0}$ of functions in $C^\infty([0,1],\mathfrak{u}(n))$ such that*

- *for every $j \in \{1,\dots,n\}$, there exist $\beta_{jj} \in \mathbf{R}\setminus\{0\}$ and $v_{jj}, h_{jj} \in C^\infty([0,1],\mathbf{R})$ such that $(B_\epsilon(\tau))_{jj} = iv_{jj}(\tau)\cos(\frac{\beta_{jj}\tau}{\epsilon^{\alpha+1}} + \frac{h_{jj}(\tau)}{\epsilon})$ and every $\tau \in [0,1]$,*
- *for every $1 \le j < k \le n$ there exist $\beta_{jk} \in \mathbf{R}\setminus\{0\}$ and $v_{jk}, h_{jk} \in C^\infty([0,1],\mathbf{R})$ such that $(B_\epsilon(\tau))_{jk} = iv_{jk}(\tau)e^{i(\frac{\beta_{jk}\tau}{\epsilon^{\alpha+1}} + \frac{h_{jk}(\tau)}{\epsilon})}$ for every $\tau \in [0,1]$.*

Theorem 5. *Consider $A \in C^\infty([0,1],\mathfrak{u}(n))$ and a finite sum $(B_\epsilon)_{\epsilon>0}$ of elements belonging to $S(\alpha)$ with $\alpha > 1$. Assume that $A(\cdot)$ satisfies a κ-th order gap condition for some nonnegative integer κ. Fix $X_0 \in \mathbf{C}^n$. Let $\hat{X}_\epsilon$ and X_ϵ be the solutions of, respectively, (7) and (8) with $\hat{X}_\epsilon(0) = X_0$ and $X_\epsilon(0) = X_0$. Then there exists $c > 0$ such that $\|\hat{X}_\epsilon(s) - X_\epsilon(s)\| \le c\epsilon^{\min(\frac{1}{\kappa+1},\alpha-1)}$ for every $s \in [0,1/\epsilon]$ and $\epsilon > 0$.*

Before proving Theorem 5, let us show how it can be used to deduce Theorem 3.

Proof of Theorem 3. Let us introduce the notation $\hat{\Xi}$ for $\Xi \cup (-\Xi)$, and, for $\sigma \in \hat{\Xi}$, let $\hat{H}_1^\sigma$ be the matrix such that $(\hat{H}_1^\sigma)_{j,k} = (H_1)_{j,k}$ if $E_j - E_k = \sigma$ and 0 otherwise. Moreover, for $\sigma \in \hat{\Xi}$ such that $v_{|\sigma|} \neq 0$ and j,k such that $E_j - E_k = \sigma$ and $(H_1)_{j,k} \neq 0$, set

$$\chi_\sigma(\tau) = \frac{\sigma\tau}{\epsilon^{\alpha+1}} + \frac{\varphi_j(\tau) - \varphi_k(\tau)}{\epsilon}, \qquad \sigma \in \hat{\Xi},$$

and notice that $\chi_{-\sigma}(\tau) = -\chi_\sigma(\tau)$.

Define $\Psi_\epsilon(\tau) = V_\epsilon^*(\tau)\psi_\epsilon(\tau/\epsilon^{\alpha+1})$, $\tau \in [0,1]$, and notice that $\Psi_\epsilon(0) = \psi_0$, since $\varphi(0) = 0$. Since diagonal matrices commute, we easily get that Ψ_ϵ satisfies

$$i\frac{d\Psi_\epsilon(\tau)}{d\tau} = -\frac{1}{\epsilon}\mathrm{diag}(\varphi'(\tau))\Psi_\epsilon(\tau) + C_\epsilon(\tau)\Psi_\epsilon(\tau), \tag{9}$$

where for $\tau \in [0,1]$,

$$\begin{aligned} C_\epsilon(\tau) =& \frac{u_\epsilon(\tau/\epsilon^{\alpha+1})}{\epsilon^{\alpha+1}} V_\epsilon^*(\tau) H_1 V_\epsilon(\tau) \\ =& \frac{u_\epsilon(\tau/\epsilon^{\alpha+1})}{\epsilon^{\alpha+1}} \sum_{\sigma\in\hat{\Xi}} e^{i\chi_\sigma(\tau)}\hat{H}_1^\sigma. \end{aligned}$$

Notice now that

$$\frac{u_\epsilon(\tau/\epsilon^{\alpha+1})}{\epsilon^{\alpha+1}} = \frac{v_0(\tau)}{\epsilon} + \frac{1}{\epsilon}\sum_{\sigma\in\Xi\setminus\{0\}} v_\sigma(\tau)(e^{i\chi_\sigma(\tau)} + e^{-i\chi_\sigma(\tau)}).$$

In order to rewrite system (9) in the form $\frac{d\Psi_\epsilon(\tau)}{d\tau} = \frac{1}{\epsilon}\left(A(\tau) + B_\epsilon(\tau)\right)\Psi_\epsilon(\tau)$, define

$$\begin{aligned} A(\tau) =& i\mathrm{diag}(\varphi'(\tau)) \\ &- i\left(v_0(\tau)\hat{H}_1^0 + \sum_{\sigma\in\Xi\setminus\{0\}} v_\sigma(\tau)(\hat{H}_1^\sigma + \hat{H}_1^{-\sigma})\right) \\ =& i\mathrm{diag}(\varphi'(\tau)) + \sum_{\sigma\in\Xi} v_\sigma(\tau)H_1^\sigma = -ih_{\mathrm{d}}(\tau), \end{aligned}$$

and

$$\begin{aligned} B_\epsilon(\tau) =& -iv_0(\tau)\sum_{\sigma\in\hat{\Xi}\setminus\{0\}} e^{i\chi_\sigma(\tau)}\hat{H}_1^\sigma \\ &- i\sum_{\sigma\in\Xi\setminus\{0\}} v_\sigma(\tau)(e^{2i\chi_\sigma(\tau)}\hat{H}_1^\sigma + e^{-2i\chi_\sigma(\tau)}\hat{H}_1^{-\sigma}) \\ &- i\sum_{\sigma\in\Xi\setminus\{0\}} v_\sigma(\tau)\sum_{\hat{\sigma}\in\Xi\setminus\{\pm\sigma\}}\Big(e^{i(\chi_{\hat{\sigma}}(\tau)+\chi_\sigma(\tau))}\hat{H}_1^{\hat{\sigma}} \\ &+ e^{i(-\chi_{\hat{\sigma}}(\tau)+\chi_\sigma(\tau))}\hat{H}_1^{-\hat{\sigma}}\Big). \end{aligned}$$

One easily checks that $(B_\epsilon)_{\epsilon>0}$ is a finite sum of elements of $S(\alpha)$. By applying Theorem 5, we get that $\|\Psi_\epsilon(\tau) - \hat{\Psi}_\epsilon(\tau)\| < c\epsilon^{\min(\frac{1}{\kappa+1},\alpha-1)}$ for every $\tau \in [0,1]$ for some $c > 0$ independent of $\tau \in [0,1]$ and $\epsilon > 0$.

3.2 Proof of Theorem 5

The results in this section have been presented, in a preliminary version, in [5]. The proof of Theorem 5 is split in three steps. In the first of such steps, we consider an oscillating (possibly unbounded) perturbation term on a bounded time-interval and we give a condition ensuring its negligibility in terms of the asymptotic behavior of its iterated integrals.

Proposition 6. *Let D and $(M_\epsilon)_{\epsilon>0}$ be in $C^\infty([0,1],\mathfrak{u}(n))$. Assume that $\int_0^\tau M_\epsilon(\vartheta)d\vartheta = O(\epsilon)$ and that there exists $\eta > 0$ such that*

$$\int_0^\tau |M_\epsilon(\vartheta)|\left|\int_0^\vartheta M_\epsilon(\theta)d\theta\right| d\vartheta = O(\epsilon^\eta),$$

both estimates being uniform with respect to $\tau \in [0,1]$. *Denote the flow of the equation* $\frac{dx(\tau)}{d\tau} = D(\tau)x(\tau)$ *by* $P_\tau \in \mathrm{U}(n)$ *and the flow of the equation* $\frac{dx(\tau)}{d\tau} = (D(\tau) + M_\epsilon(\tau))x(\tau)$ *by* $P^\epsilon_\tau \in \mathrm{U}(n)$. *Then* $P^\epsilon_\tau = P_\tau + O(\epsilon^{\min(\eta,1)})$, *uniformly with respect to* $\tau \in [0,1]$.

Proof. Let $K > 0$ be such that $|\int_0^\tau M_\epsilon(\vartheta)d\vartheta| < K\epsilon$ for every $\tau \in [0,1]$ and denote by Q^ϵ_τ the flow associated with M_ϵ. Hence, $Q^\epsilon_\tau = \mathrm{Id} + \int_0^\tau M_\epsilon(\vartheta)Q^\epsilon_\vartheta d\vartheta$. By integration by parts, $Q^\epsilon_\tau = \mathrm{Id} + \left(\int_0^\tau M_\epsilon(\vartheta)d\vartheta\right) Q^\epsilon_\tau - \int_0^\tau \left(\int_0^\vartheta M_\epsilon(\theta)d\theta\right) M_\epsilon(\vartheta)Q^\epsilon_\vartheta d\vartheta$. Moreover, Q^ϵ_τ is bounded uniformly with respect to (τ,ϵ), since it evolves in $\mathrm{U}(n)$. Hence, $|Q^\epsilon_\tau - \mathrm{Id}| \le C_1\epsilon + C_2\epsilon^\eta$, where C_1, C_2 are positive constants which do not depend on (τ,ϵ). We deduce that $Q^\epsilon_\tau = \mathrm{Id} + O(\epsilon^{\min(\eta,1)})$, uniformly with respect to $\tau \in [0,1]$. By the variations formula (see, e.g., [2, Section 2.7]), $P^\epsilon_\tau = Q^\epsilon_\tau W^\epsilon_\tau$, where $W^\epsilon_\tau \in \mathrm{U}(n)$ is the flow of the equation $\frac{dx(\tau)}{d\tau} = (Q^\epsilon_\tau)^{-1}D(\tau)Q^\epsilon_\tau x(\tau)$. By the previous estimate, we have $(Q^\epsilon_\tau)^{-1}D(\tau)Q^\epsilon_\tau = D(\tau) + O(\epsilon^{\min(\eta,1)})$ uniformly with respect to $\tau \in [0,1]$. By an easy application of Gronwall's Lemma, we get that $W^\epsilon_\tau = P_\tau + O(\epsilon^{\min(\eta,1)})$ and we can conclude. □

The second step of the proof of Theorem 5 consists in the following lemma, which will be used to apply Proposition 6 to a suitable reformulation of Equation (8).

Lemma 7. *Let* $\alpha > 1$ *and* $(B_\epsilon)_{\epsilon>0}$ *be a finite sum of elements in* $S(\alpha)$. *Fix* $P \in C^\infty([0,1],\mathrm{U}(n))$ *and* $\Gamma = \mathrm{diag}(\Gamma_j)_{j=1}^n$ *with* $\Gamma_j \in C^\infty([0,1],\mathbf{R})$, $j = 1,\dots,n$. *For every* $\epsilon > 0$ *and* $\tau \in [0,1]$, *define*

$$M(P,\Gamma,\epsilon)(\tau) = e^{i\frac{\Gamma(\tau)}{\epsilon}}P^*(\tau)B_\epsilon(\tau)P(\tau)e^{-i\frac{\Gamma(\tau)}{\epsilon}}. \quad (10)$$

Then

$$\int_0^\tau M(P,\Gamma,\epsilon)(\vartheta)d\vartheta = O(\epsilon^\alpha) \quad (11)$$

and

$$\int_0^\tau |M(P,\Gamma,\epsilon)(\vartheta)| \left|\int_0^\vartheta M(P,\Gamma,\epsilon)(\theta)d\theta\right| d\vartheta = O(\epsilon^{\alpha-1}),$$

both estimates being uniform with respect to $\tau \in [0,1]$.

Proof. First notice that, since $B_\epsilon(\tau) = O(1/\epsilon)$, then $M(P,\Gamma,\epsilon)(\tau) = O(1/\epsilon)$, both estimates being uniform with respect to $\tau \in [0,1]$. Hence, it is enough to prove (11). By linearity, it is enough to prove that, for every $j,k \in \{1,\dots,n\}$, every $\beta \in \mathbf{R}\setminus\{0\}$, and every $v,h \in C^\infty([0,1],\mathbf{R})$, the matrix $C_\epsilon(\tau) = \frac{1}{\epsilon}v(\tau)e^{i(\frac{\beta\tau}{\epsilon^{\alpha+1}} + \frac{h(\tau)}{\epsilon})}e_{jk}$ satisfies

$$\int_0^\tau e^{i\frac{\Gamma(\vartheta)}{\epsilon}}P^*(\vartheta)C_\epsilon(\vartheta)P(\vartheta)e^{-i\frac{\Gamma(\vartheta)}{\epsilon}}d\vartheta = O(\epsilon^{\alpha+1}).$$

Denoting $p_{\ell m}(\tau) = (P(\tau))_{\ell,m}$ for every $\ell,m \in \{1,\dots,n\}$, we have that

$$e^{i\frac{\Gamma(\tau)}{\epsilon}}P^*(\tau)C_\epsilon(\tau)P(\tau)e^{-i\frac{\Gamma(\tau)}{\epsilon}} = \frac{v(\tau)}{\epsilon}e^{i(\frac{\beta\tau}{\epsilon^{\alpha+1}} + \frac{h(\tau)}{\epsilon})}\sum_{\ell,m=1}^n \overline{p_{j\ell}(\tau)}p_{km}(\tau)e^{\frac{i}{\epsilon}(\Gamma_\ell(\tau)-\Gamma_m(\tau))}e_{\ell m}.$$

We conclude the proof by showing that, for every $a \in C^\infty([0,1],\mathbf{R})$, we have

$$\int_0^\tau a(\vartheta)e^{i(\frac{\beta\vartheta}{\epsilon^{\alpha+1}} + \frac{h(\vartheta)}{\epsilon})}d\vartheta = O(\epsilon^{\alpha+1}), \quad (12)$$

uniformly with respect to $\tau \in [0,1]$. Integrating by parts, for every $\tau \in [0,1]$,

$$\begin{aligned}
&\int_0^\tau a(\vartheta)e^{i(\frac{\beta\vartheta}{\epsilon^{\alpha+1}} + \frac{h(\vartheta)}{\epsilon})}d\vartheta \\
&= i\frac{\epsilon^{\alpha+1}}{\beta}\int_0^\tau e^{i\frac{\beta\vartheta}{\epsilon^{\alpha+1}}}\left(a'(\vartheta) + i\frac{h'(\vartheta)}{\epsilon}a(\vartheta)\right)e^{i\frac{h(\vartheta)}{\epsilon}}d\vartheta \\
&+ \left[-i\frac{\epsilon^{\alpha+1}}{\beta}e^{i\frac{\beta\vartheta}{\epsilon^{\alpha+1}}}a(\vartheta)e^{i\frac{h(\vartheta)}{\epsilon}}\right]_0^\tau \\
&= -\frac{\epsilon^\alpha}{\beta}\int_0^\tau h'(\vartheta)a(\vartheta)e^{i(\frac{\beta\vartheta}{\epsilon^{\alpha+1}} + \frac{h(\vartheta)}{\epsilon})}d\vartheta + O(\epsilon^{\alpha+1}).
\end{aligned}$$

Iterating the integration by parts on the integral term $\lceil\frac{1}{\alpha}\rceil$ more times, we obtain (12). □

Let us now prove Theorem 5. This is done by providing an explicit expression of the adiabatic evolution of (7). We actually prove in the next proposition that, under the assumptions of Theorem 5, the leading term of the flow of (8) does not depend on $(B_\epsilon)_{\epsilon>0}$. Since equation (7) corresponds to the case $B_\epsilon \equiv 0$ for every $\epsilon > 0$, one deduces Theorem 5 simply by triangular inequality.

Proposition 8. *Consider* $A \in C^\infty([0,1],\mathfrak{u}(n))$ *and let* $(B_\epsilon)_{\epsilon>0}$ *be a finite sum of elements in* $S(\alpha)$ *with* $\alpha > 1$. *Assume that* $iA(\cdot)$ *satisfies a* κ*-th order gap condition for some non-negative integer* κ. *Select* $\lambda_j \in C^\infty([0,1],\mathbf{R})$, $j = 1,\dots,n$, *and* $P \in C^\infty([0,1],\mathrm{U}(n))$ *such that, for* $j = 1,\dots,n$ *and* $\tau \in [0,1]$, $\lambda_j(\tau)$ *and the* j*-th column of* $P(\tau)$ *are, respectively, an eigenvalue of* $iA(\tau)$ *and a corresponding eigenvector. Define* $\Lambda(\tau) = \mathrm{diag}(\lambda_j(\tau))_{j=1}^n$, $\tau \in [0,1]$. *Fix* $X_0 \in \mathbf{C}^n$. *Let*

X_ϵ be the solution of $\frac{dX_\epsilon(s)}{ds} = (A(\epsilon s) + B_\epsilon(\epsilon s))X_\epsilon(s)$ such that $X_\epsilon(0) = X_0$. Set $\Upsilon_\epsilon(\tau) = P(\tau)\exp\left(-\frac{i}{\epsilon}\int_0^\tau \Lambda(\vartheta)d\vartheta\right)\exp\left(\int_0^\tau D(\vartheta)d\vartheta\right)P^*(0)$, where D is equal to the diagonal part of $\frac{dP^*}{d\tau}P$. Then

$$\|X_\epsilon(\tau/\epsilon) - \Upsilon_\epsilon(\tau)X_0\| < c\epsilon^{\min(\frac{1}{\kappa+1},\alpha-1)}$$

for some $c > 0$ independent of $\tau \in [0,1]$ and $\epsilon > 0$.

Proof. Define $\Gamma(\tau) = \int_0^\tau \Lambda(s)ds$ and $Y_\epsilon(\tau) = \exp\left(\frac{i}{\epsilon}\Gamma(\tau)\right)P^*(\tau)X_\epsilon(\tau/\epsilon)$. Then Y_ϵ satisfies

$$\frac{dY_\epsilon(\tau)}{d\tau} = (D_\epsilon(\tau) + M(P,\Gamma,\epsilon)(\tau))\,Y_\epsilon(\tau), \qquad (13)$$

where $M(P,\Gamma,\epsilon)$ is defined as in (10) and

$$D_\epsilon(\tau) = \exp\left(\frac{i}{\epsilon}\Gamma(\tau)\right)\frac{dP^*}{d\tau}(\tau)P(\tau)\exp\left(-\frac{i}{\epsilon}\Gamma(\tau)\right).$$

Denote by P_τ^ϵ and W_τ^ϵ the flows of the equations $\frac{dx(\tau)}{d\tau} = M(P,\Gamma,\epsilon)(\tau)x(\tau)$ and $\frac{dx(\tau)}{d\tau} = (P_\tau^\epsilon)^{-1}D_\epsilon(\tau)P_\tau^\epsilon x(\tau)$, respectively. By the variations formula, the flow of equation (13) is equal to $Q_\tau^\epsilon = P_\tau^\epsilon W_\tau^\epsilon$. By Proposition 6 and Lemma 7, we have $P_\tau^\epsilon = \mathrm{Id} + O(\epsilon^{\alpha-1})$. Hence $(P_\tau^\epsilon)^{-1}D_\epsilon(\tau)P_\tau^\epsilon = D_\epsilon(\tau) + O(\epsilon^{\alpha-1})$.

Using the κ-th order gap condition satisfied by $iA(\cdot)$, we have the estimate $\int_0^\tau D_\epsilon(\vartheta)d\vartheta = \int_0^\tau D(\vartheta)d\vartheta + O(\epsilon^{\frac{1}{\kappa+1}})$, uniformly with respect to $\tau \in [0,1]$. Indeed, each coefficient of $D_\epsilon(\tau)$ can be written as $(D_\epsilon(\tau))_{jl} = q_{jl}(\tau)e^{\frac{i}{\epsilon}\int_0^\tau(\lambda_j(\vartheta)-\lambda_l(\vartheta))d\vartheta}$, where q_{jl} is in $C^\infty([0,1],\mathbf{R})$, and the conclusion follows by, e.g., [6, Corollary A.6].

Moreover, since D_ϵ is bounded with respect to ϵ, we can conclude by standard averaging theory (see, e.g., [6, Theorem A.1] for a closely related formulation) that

$$W_\tau^\epsilon = \exp\left(\int_0^\tau D(\vartheta)d\vartheta\right) + O(\epsilon^{\min(\frac{1}{\kappa+1},\alpha-1)}).$$

It follows that

$$\begin{aligned} Q_\tau^\epsilon &= \left(\mathrm{Id} + O(\epsilon^{\alpha-1})\right) \\ &\quad\times\left(\exp\left(\int_0^\tau D(\vartheta)d\vartheta\right) + O(\epsilon^{\min(\frac{1}{\kappa+1},\alpha-1)})\right) \\ &= \exp\left(\int_0^\tau D(\vartheta)d\vartheta\right) + O(\epsilon^{\min(\frac{1}{\kappa+1},\alpha-1)}), \end{aligned}$$

concluding the proof of the proposition. □

3.3 The ensemble case

Theorem 3 can be extended to the ensemble control setting in which a parametric dispersion affects the Hamiltonian H_1. The key argument allowing for such an extension is that the estimates obtained in Section 3.2 can be made uniform with respect to the dispersion parameter. This is because the underlying averaging estimates (we refer in particular to [6, Corollary A.6] used in the proof of Proposition 8) can be replaced by uniform parametric estimates such as those in [6, Corollary A.8].

Let K be a compact subset of $\mathbf{R}^N$, for some $N \in \mathbf{N}$, and assume that $K \ni \delta \mapsto H_{1,\delta} \in i\mathrm{u}(n)$ is a continuous map. Let H_0 be as in Section 2 and extend the definition of Ξ by setting

$$\Xi = \{|E_j - E_k| \mid 1 \le j,k \le n,\ \exists\delta \in K \text{ s.t. } (H_{1,\delta})_{j,k} \neq 0\}.$$

With every $\delta \in K$ we can associate the decoupled Hamiltonians $H_{\mathrm{d},\delta}$ and $h_{\mathrm{d},\delta}$, and we notice that the control u_ϵ does not depend on δ. (To be precise, one should assume condition (4) to hold for every $(j,k),(p,q)$ such that $E_j - E_k = E_p - E_q$ and $(H_{1,\delta})_{j,k} \neq 0 \neq (H_{1,\delta})_{p,q}$ for some $\delta \in K$.) Then we have the following.

Theorem 9. *Set $\psi_0 \in \mathbf{C}^n$ and let $\psi_\epsilon^\delta(\cdot)$ be the solution of*

$$i\frac{d\psi_\epsilon^\delta(t)}{dt} = (H_0 + u_\epsilon(t)H_{1,\delta})\,\psi_\epsilon^\delta(t), \qquad 0 \le t \le \frac{1}{\epsilon^{\alpha+1}},$$

with $\psi_\epsilon^\delta(0) = \psi_0$. Define $\hat\Psi_\epsilon^\delta$ as the solution of

$$\frac{d\hat\Psi_\epsilon^\delta(s)}{ds} = h_{\mathrm{d},\delta}(\epsilon s)\hat\Psi_\epsilon^\delta(s), \qquad 0 \le s \le \frac{1}{\epsilon}, \qquad (14)$$

with $\hat\Psi_\epsilon^\delta(0) = \psi_0$. Assume that for every $\delta \in K$ the non-autonomous Hamiltonian $h_{\mathrm{d},\delta}$ satisfies a κ-th order gap condition for some nonnegative integer κ independent of δ. Then

$$\left\|\psi_\epsilon^\delta\left(\frac{\tau}{\epsilon^{\alpha+1}}\right) - V_\epsilon(\tau)\hat\Psi_\epsilon^\delta\left(\frac{\tau}{\epsilon}\right)\right\| < c\epsilon^{\min(\frac{1}{\kappa+1},\alpha-1)}$$

for $0 \le \tau \le 1$, where $V_\epsilon(\tau) = \mathrm{diag}\left(e^{-i(\frac{E_j\tau}{\epsilon^{\alpha+1}} + \frac{\varphi_j(\tau)}{\epsilon})}\right)_{j=1}^n$ and $c > 0$ is independent of $\tau \in [0,1]$, $\delta \in K$, and $\epsilon > 0$.

4 Control strategies

We present in this section some control strategies obtained by applying the general construction introduced in the previous sections, using different choices of the functional control parameters v and φ (cf. (5)).

4.1 Decoupled Hamiltonian for a non-resonant coupling

Let H_0 and H_1 be as in Section 2.

Definition 10. *Given $j, l \in \{1, \dots, n\}$, we say that H_1 non-resonantly couples the levels j and l if there exist $j_1, \dots, j_k \in \{1, \dots, n\}$ such that $j_1 = j$, $j_k = l$, and, for every $r = 1, \dots, k-1$, $(H_1)_{j_r, j_{r+1}} \neq 0$ and $\mathcal{R}_{|E_{j_r} - E_{j_{r+1}}|}$ is equal either to $\{(j_r, j_{r+1})\}$ or to $\{(j_{r+1}, j_r)\}$ (where $\mathcal{R}$ is defined as in (2)).*

Let us assume that H_1 non-resonantly couples two levels. Up to permutation, we can assume that $j = 1$, $l = m$, and $j_k = k$ for $k = 1, \dots, m$. Set $\sigma_j = |E_j - E_{j+1}|$ for $j = 1, \dots, m-1$. Notice that, in terms of the constraint (4) entering in the definition of the decoupling control u_ϵ, the non-resonant coupling condition implies that the functions $\hat{\varphi}_{\sigma_j}$, $j = 1, \dots, m-1$, can be chosen freely (up to the relation $\hat{\varphi}_{\sigma_j}(0) = 0$). Consider then $\alpha > 1$ and $v_1, \dots, v_{m-1}$ in $C^\infty([0,1], \mathbf{R})$, and define

$$u_\epsilon(t) = 2\epsilon \sum_{j=1}^{m-1} \frac{v_j(\epsilon^{\alpha+1} t)}{(H_1)_{j,j+1}} \cos\left(|E_j - E_{j+1}| t + \frac{\hat{\varphi}_j(\epsilon^{\alpha+1} t)}{\epsilon} \right),$$

for every $t \in [0, \frac{1}{\epsilon^{\alpha+1}}]$. For simplicity of notations, let $v = (v_j)_{j=1}^{m-1}$ and $\varphi = (\varphi_j)_{j=1}^{m}$, where $\varphi_1, \dots, \varphi_m \in C^\infty([0,1], \mathbf{R})$ satisfy $\mathrm{sign}(E_j - E_{j+1})(\varphi_j - \varphi_{j+1}) = \hat{\varphi}_j$.

In analogy with (3) and (5), define $H_{\mathrm{d}} : \mathbf{R}^m \times \mathbf{R}^{m-1} \to i\mathfrak{u}(n)$ and $h_{\mathrm{d}} : [0,1] \to i\mathfrak{u}(n)$ by

$$H_{\mathrm{d}}(\delta, w) = \begin{pmatrix} \delta_1 & w_1 & 0 & \cdots & \cdots & \cdots & 0 \\ w_1 & \delta_2 & w_2 & \ddots & \ddots & \ddots & \vdots \\ 0 & w_2 & \delta_3 & w_3 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & w_{m-2} & \delta_{m-1} & w_{m-1} & 0 \\ \vdots & \ddots & \ddots & \ddots & w_{m-1} & \delta_m & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & 0 \end{pmatrix},$$

and $h_{\mathrm{d}}(\tau) = H_{\mathrm{d}}(-\varphi'(\tau), v(\tau))$, where the zeros in the last line and in the last column of $H_{\mathrm{d}}(\delta, w)$ are null matrices of suitable dimensions. Notice that, with respect to the notations of Section 2, we are setting here $v_0 \equiv 0$.

4.2 Decoupled multilevel chirp pulse

Consider $u, \phi \in C^\infty([0,1], \mathbf{R})$ to be chosen later. Assume that $v_j = u$ for every $j \in \{1, \dots, m-1\}$ and that $\varphi_j = j\phi$ for $j \in \{1, \dots, m\}$. Hence, $h_{\mathrm{d}}(\tau) = H_{\mathrm{C}}(-\varphi'(\tau), u(\tau))$, where

$$H_{\mathrm{C}}(\rho, w) = \begin{pmatrix} \rho & w & 0 & \cdots & \cdots & \cdots & 0 \\ w & 2\rho & w & \ddots & \ddots & \ddots & \vdots \\ 0 & w & 3\rho & w & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & w & (m-1)\rho & w & 0 \\ \vdots & \ddots & \ddots & \ddots & w & m\rho & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & 0 \end{pmatrix}.$$

Recall the following result of linear algebra, that can be found, for instance, in [14].

Lemma 11. *Let A be the real-valued tridiagonal $n \times n$ matrix*

$$A = \begin{pmatrix} a_1 & c_1 & 0 & 0 & 0 & \dots \\ c_1 & a_2 & c_2 & 0 & 0 & \dots \\ 0 & c_2 & a_3 & c_3 & 0 & \dots \\ 0 & 0 & c_3 & a_4 & c_4 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & a_n \end{pmatrix}.$$

If $c_k \neq 0$ for every $k \in \{1, \dots, n-1\}$, then the eigenvalues of A are simple.

It follows from Lemma 11 that the only eigenvalue intersection of top-left $m \times m$ submatrix of $H_C(\rho, w)$ is located at $\rho = w = 0$.

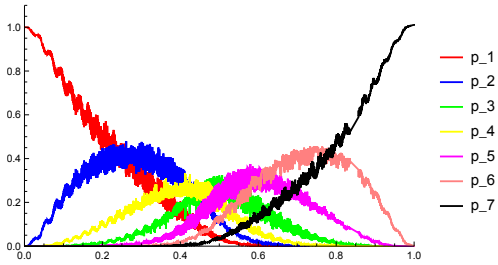
Denote by $e_1, \dots, e_n$ the canonical basis of $\mathbf{C}^n$. By Theorem 3, we have the following result.

Proposition 12. *Let $u, \phi \in C^\infty([0,1], \mathbf{R})$ be such that $u(0) = u(1) = 0$, $\phi(0) = 0$, $\phi'(0)\phi'(1) < 0$, and $u(\tau) \neq 0$ for $\tau \in (0,1)$. For every $\epsilon > 0$, let $\psi_\epsilon : [0, \frac{1}{\epsilon^{\alpha+1}}] \to \mathbf{C}^n$ be the solution of (1) with initial condition e_1 associated with the control u_ϵ. Then, there exists $C > 0$ independent of ϵ such that $\|\psi_\epsilon(\frac{1}{\epsilon^{\alpha+1}}) - e^{i\theta_\epsilon} e_m\| \leq C\epsilon^{\min(1, \alpha-1)}$ for some $\theta_\epsilon \in \mathbf{R}$.*

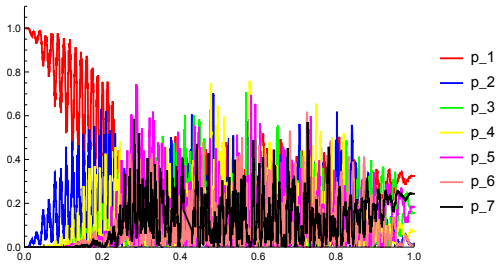
4.2.1 Simulations

Consider, for $\tau \in [0,1]$, $\phi(\tau) = -\frac{2}{\pi}\sin(\pi\tau)$ and $u(\tau) = 4\sin(\pi\tau)$, and define $H_0 = \mathrm{diag}(E_j)_{j=1}^7$. Let H_1 be the 7×7 symmetric matrix such that for every $1 \leq j \leq k \leq 7$, $(H_1)_{j,k} = 1$ if $k = j+1$ and 0 otherwise. Let $\psi_\epsilon : [0, \frac{1}{\epsilon^{\alpha+1}}] \to \mathbf{C}^n$ be the solution of (1) with initial condition e_1 associated with the control u_ϵ as in Proposition 12. Define for $j \in \{1, \dots, 7\}$, the *population in level j* as $p_j(\tau) = |\langle \psi_\epsilon(\frac{\tau}{\epsilon^{\alpha+1}}), e_j \rangle|^2$ for $\tau \in [0,1]$.

We have plotted on Figure 1(a) the population levels of ψ_ϵ in the case $\alpha = 1.2$, with $E_1 = 0$, $E_2 = 1$, $E_3 = 2.5$, $E_4 = 3$, $E_5 = 2.2$, $E_6 = 5$, $E_7 = 7$. The case where $\alpha = 0.8$ (violating the hypothesis $\alpha > 1$), while the other parameters are the same, is illustrated in Figure 1(b).



(a) $\alpha = 1.2$



(b) $\alpha = 0.8$

Figure 1: Evolution of the populations $(p_j(\tau))_{j=1}^7$ as functions of the renormalized time $\tau = \epsilon^{\alpha+1}t$, for $\epsilon = 10^{-2}$ and $\alpha = 1.2$ (1(a)), $\alpha = 0.8$ (1(b)).

Remark 13. *Applying Theorem 9 instead of Theorem 3, we can recover a version of Proposition 12 allowing for parametric dispersion in the controlled Hamiltonian H_1 of the form $H_{1,\delta} = \delta H_1$, with $\delta \in [\delta_0, \delta_1]$ for some $0 < \delta_0 < \delta_1$. Indeed, the property of non-resonantly coupling two levels is independent of δ and u_ϵ depends on δ only through a positive constant multiplicative factor. Hence the control u in Proposition 12 is also modified through a positive constant multiplicative factor, while ϕ does not depend on δ. Proposition 12 provides then an explicit robust control strategy reflecting the ensemble controllability result obtained by Chambrion in [9, Proposition 1], where it is mentioned that an ensemble control strategy is difficult to implement because of the "poor efficiency of tracking strategies via Lie brackets".*

4.3 Decoupled multilevel STIRAP

In order to reduce the populations in the intermediate levels along the controlled motion (see, for instance [19]), it is interesting to introduce another control strategy, which generalizes the well-known Stimulated Raman Adiabatic Passage (STIRAP). We are going to see that the proposed strategy is different depending on the parity of the integer m defined in Section 4.1.

Let $(d_j)_{j=1}^m \subset \mathbf{R}$ be increasing and consider $u_1, u_2 \in C^\infty([0,1], \mathbf{R})$ to be chosen later. For $j \in \{1, \dots, m-1\}$, let $v_j = u_1$ if j is odd, and $v_j = u_2$ if j is even. By choosing $\varphi_j(\tau) = -d_j\tau$ for $j \in \{1, \dots, m\}$ and $\tau \in [0,1]$, we have that $h_{\mathrm{d}}(\tau) = H_{\mathrm{S}}(u_1(\tau), u_2(\tau))$, where

$$H_{\mathrm{S}}(w_1, w_2) = \begin{pmatrix} d_1 & w_1 & 0 & \cdots & \cdots & \cdots & 0 \\ w_1 & d_2 & w_2 & \ddots & \ddots & \ddots & \vdots \\ 0 & w_2 & d_3 & w_1 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & w_1 & d_{m-1} & w_2 & 0 \\ \vdots & \ddots & \ddots & \ddots & w_2 & d_m & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & 0 & 0 \end{pmatrix}. \tag{15}$$

(The expression of H_{S} in (15) corresponds to the case where m is odd, the roles of w_1 and w_2 in the last lines of the matrix being inverted if m is even).

Denote by $\lambda_1(w_1, w_2) \leq \cdots \leq \lambda_m(w_1, w_2)$ the eigenvalues of the top-left $m \times m$ submatrix of $H_S(w_1, w_2)$. As a consequence of Lemma 11, the only eigenvalue intersections between λ_j and λ_{j+1}, $j \in \{1, \dots, m-1\}$, are located either on the axis $w_1 = 0$ or on the axis $w_2 = 0$.

Depending on the parity of m, one of the following two lemmas can be applied. The lemmas can be deduced from [1, Section II].

Lemma 14 (m odd)**.** *Assume that m is odd. Then there exist two finite positive sequences $(w_{2,k})_{k=1}^{\frac{m-1}{2}}$ and $(w_{1,k})_{k=\frac{m+1}{2}}^{m-1}$, which are respectively increasing and decreasing, such that*
- *for $k \in \{1, \dots, \frac{m-1}{2}\}$, $w_2 \mapsto \lambda_k(0, w_2)$ and $w_2 \mapsto \lambda_{k+1}(0, w_2)$ have a transverse intersection at $w_{2,k}$;*
- *for $k \in \{\frac{m+1}{2}, \dots, m-1\}$, $w_1 \mapsto \lambda_k(w_1, 0)$ and $w_1 \mapsto \lambda_{k+1}(w_1, 0)$ have a transverse intersection at $w_{1,k}$.*

Moreover, $\lambda_{k+1}(0, w_2)$ does not intersect $\lambda_k(0, w_2)$ nor $\lambda_{k+2}(0, w_2)$ for $w_2 \in (w_{2,k}, w_{2,k+1})$, and $\lambda_{k+1}(w_1, 0)$ does not intersect $\lambda_k(w_1, 0)$ nor $\lambda_{k+2}(w_1, 0)$ for $w_1 \in (w_{1,k+1}, w_{1,k})$.

Lemma 15 (m even)**.** *Assume that m is even. Then there exist two finite positive sequences $(w_{2,k})_{k=1}^{\frac{m}{2}-1}$, $(w_{1,k})_{k=\frac{m}{2}}^{m-2}$, which are, respectively, increasing and decreasing, such that*
- *for $k \in \{1, \dots, \frac{m}{2} - 1\}$, $w_2 \mapsto \lambda_k(0, w_2)$ and $w_2 \mapsto \lambda_{k+1}(0, w_2)$ have a transverse intersection at $w_{2,k}$;*
- *for $k \in \{\frac{m}{2}, \dots, m-2\}$, $w_1 \mapsto \lambda_k(w_1, 0)$ and $w_1 \mapsto \lambda_{k+1}(w_1, 0)$ have a transverse intersection at $w_{1,k}$.*

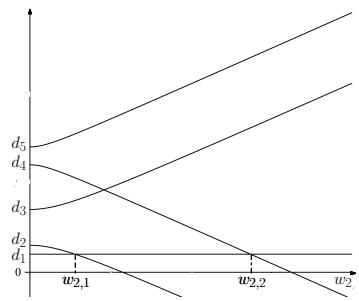
Moreover, $\lambda_{k+1}(0, w_2)$ does not intersect $\lambda_k(0, w_2)$ nor $\lambda_{k+2}(0, w_2)$ for $w_2 \in (w_{2,k}, w_{2,k+1})$, and $\lambda_{k+1}(w_1, 0)$

does not intersect $\lambda_k(w_1, 0)$ *nor* $\lambda_{k+2}(w_1, 0)$ *for* $w_1 \in (w_{1,k+1}, w_{1,k})$. *Furthermore, there exists* $w_2^\star > 0$ *such that* $w_2 \mapsto \lambda_{m-1}(0, w_2)$ *and* $w_2 \mapsto \lambda_m(0, w_2)$ *have a transverse intersection at* $w_2^\star$ *and*

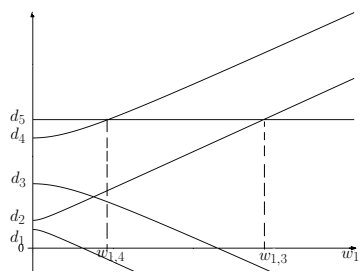
- $\lambda_{m-1}(0, w_2)$ *does not intersect* $\lambda_{m-2}(0, w_2)$ *nor* $\lambda_m(0, w_2)$ *for* $w_2 \in (0, w_2^\star)$*;*
- $\lambda_m(0, w_2)$ *does not intersect* $\lambda_{m-1}(0, w_2)$ *for* $w_2 \in (w_2^\star, +\infty)$.

Finally, $\lambda_m(w_1, 0)$ *does not intersect* $\lambda_{m-1}(w_1, 0)$ *for* $w_1 \in [0, +\infty)$.

In order to illustrate Lemmas 14 and 15, we have plotted in Figures 2 and 3 the spectrum of H_{S} for $m = 5$ and $m = 6$ on the axes $w_1 = 0$ and $w_2 = 0$.



(a) The eigenvalues of $H_{\mathrm{S}}(0, w_2)$ for $m = 5$.

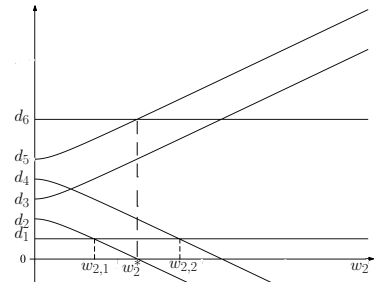


(b) The eigenvalues of $H_{\mathrm{S}}(w_1, 0)$ for $m = 5$.

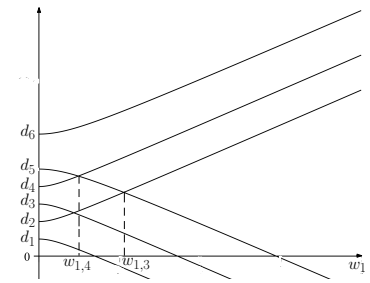
Figure 2:

Remark 16. *The eigenvalue intersections* $\lambda_k(w_1, w_2) = \lambda_{k+1}(w_1, w_2)$ *described in Lemmas 14 and 15 are not necessarily conical, even if they all are transverse in the directions that we are interested in (the horizontal or the vertical axis of the plane* (w_1, w_2)*). It is interesting to notice that numerical simulations show the presence of both conical and semi-conical eigenvalue intersections, using the terminology of [6, 7, 8].*

We deduce from Theorem 3 and Lemma 14 the following proposition.



(a) The eigenvalues of $H_{\mathrm{S}}(0, w_2)$ for $m = 6$.



(b) The eigenvalues of $H_{\mathrm{S}}(w_1, 0)$ for $m = 6$.

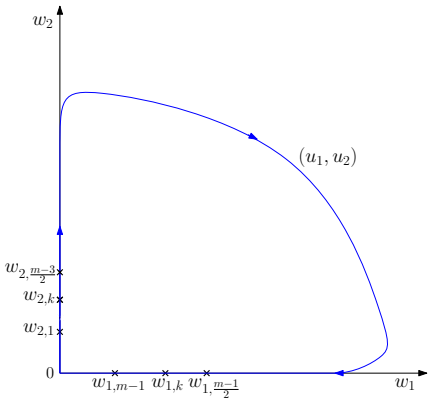
Figure 3:

Proposition 17 (m odd)**.** *Let* (u_1, u_2) *satisfy the following properties: there exist* $0 < \tau_1 < \tau_2 < 1$ *such that* $u_1|_{[0,\tau_1]} \equiv 0$, $u_2|_{[\tau_2,1]} \equiv 0$, $u_1(\tau), u_2(\tau) > 0$ *for* $\tau \in (\tau_1, \tau_2)$, u_2 *is increasing on* $[0, \tau_1]$ *from* 0 *to a value larger than* $w_{2,\frac{m-1}{2}}$, u_1 *is decreasing on* $[\tau_2, 1]$ *from a value larger than* $w_{1,\frac{m+1}{2}}$ *to* 0 *(see Figure 4(a)). For every* $\epsilon > 0$, *let* $\psi_\epsilon : [0, \frac{1}{\epsilon^{\alpha+1}}] \to \mathbf{C}^n$ *be the solution of* (1) *with initial condition* e_1 *associated with the control* u_ϵ. *Then, there exists* $C > 0$ *independent of* ϵ *such that* $\|\psi_\epsilon(\frac{1}{\epsilon^{\alpha+1}}) - e^{i\theta_\epsilon} e_m\| \leq C\epsilon^{\min(\frac{1}{2}, \alpha-1)}$ *for some* $\theta_\epsilon \in \mathbf{R}$.

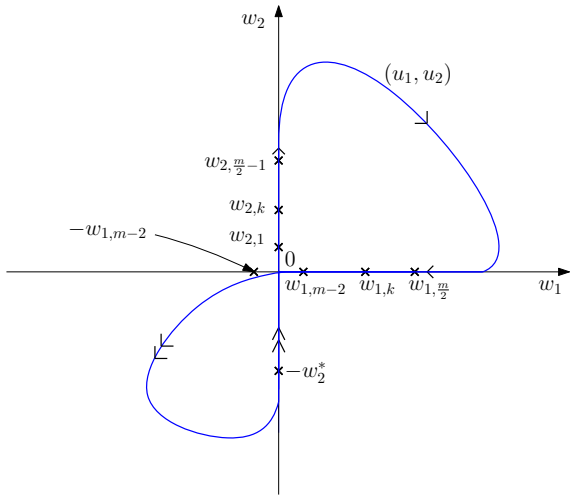
Remark 18 (m even)**.** *In the case where* m *is even we can state a result similar to Proposition 17 by considering a control loop* (u_1, u_2) *as in Figure 4(b). The corresponding solution* ψ_ϵ *makes an approximate transition (up to phases) from* e_1 *to* e_{m-1} *during the interval of time corresponding to the half-loop in the first quadrant and then it makes an approximate transition from* e_{m-1} *to* e_m *when following the half-loop in the third quadrant.*

4.3.1 Simulations

Define H_0 and H_1 as in Section 4.2.1. Let (u_1, u_2) be chosen as in Proposition 17. Let $\psi_\epsilon : [0, \frac{1}{\epsilon^{\alpha+1}}] \to \mathbf{C}^n$ be the solution of (1) with initial condition e_1 asso-



(a) Control path (u_1, u_2) in the plane (w_1, w_2) for m odd.



(b) Control path (u_1, u_2) in the plane (w_1, w_2) for m even.

Figure 4:

ciated with the control u_ϵ. We have plotted on Figure 5 the population levels $p_j(\tau) = |\langle \psi_\epsilon(\frac{\tau}{\epsilon^{\alpha+1}}), e_j\rangle|^2$, $j = 1, \dots, 7$, in the case $\alpha = 1.2$, with $E_1 = 0$, $E_2 = 1$, $E_3 = 2.5$, $E_4 = 3$, $E_5 = 2.2$, $E_6 = 5$, $E_7 = 7$.

Remark 19. *In analogy with Remark 13, we can extend Proposition 17 to the case where H_1 is replaced by $H_{1,\delta} = \delta H_1$, with $\delta \in [\delta_0, \delta_1]$, $0 < \delta_0 < \delta_1$.*

Remark 20. *We have focused in this and in the previous section on the control between eigenstates of the drift Hamiltonian H_0. As proposed in [8] (see also [22]) broken adiabatic paths (with discontinuous first order derivatives at conical intersections) can be used to induce superpositions between eigenstates. One could reason similarly for semi-conical intersections, using discontinuous second order derivatives and exploiting [6, Proposition 17]. The control strategy presented here can therefore be adapted to approximate, using oscillating controls, an adiabatic trajectory leading from an eigenstate of H_0 to a superposition of eigenstates with prescribed population levels.*

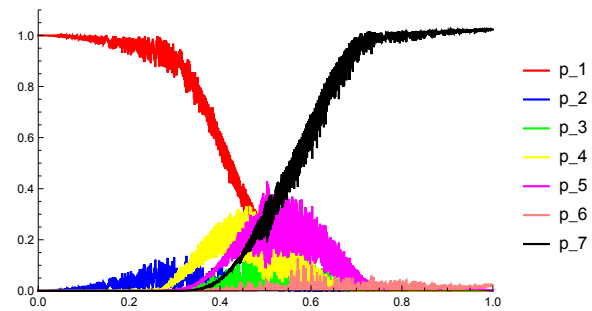


Figure 5: Evolution of the different populations $(p_j(\tau))_{j=1}^7$ as functions of the renormalized time $\tau = \epsilon t \in [0, 1]$, for $\alpha = 1.2$ and $\epsilon = 10^{-2}$.

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