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Ensemble qubit controllability with a single control via adiabatic and rotating wave approximations

Rémi Robin*,¹, Nicolas Augier², Ugo Boscain¹, and Mario Sigalotti¹

¹Laboratoire Jacques-Louis Lions, Sorbonne Université, Université de Paris, Inria, CNRS, France

²Inria, Université Côte d’Azur, INRAE, CNRS, Sorbonne Université, Sophia Antipolis, France

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Abstract

In the physics literature it is common to see the rotating wave approximation and the adiabatic approximation used “in cascade” to justify the use of chirped pulses for two-level quantum systems driven by one external field, in particular when the resonance frequency of the system is not known precisely.

Both approximations need relatively long time and are essentially based on averaging theory of dynamical systems. Unfortunately, the two approximations cannot be done independently since, in a sense, the two time scales interact. The purpose of this paper is to study how the cascade of the two approximations can be justified and how large becomes the final time as the fidelity goes to one, while preserving the robustness of the adiabatic strategy. Our first result, based on high-order averaging techniques, gives a precise quantification of the uncertainty interval of the resonance frequency for which the population inversion works. As a byproduct of this result, we prove that it is possible to control an ensemble of spin systems by a single real-valued control, providing a non-trivial extension of a celebrated result of ensemble controllability with two controls by Khaneja and Li.

Keywords: Averaging, control of quantum mechanical systems, spin dynamics, rotating wave approximation, adiabatic approximation

AMS subject classification: 81Q93, 34C29, 81Q15

1 Introduction

Consider a two-level system described by the Schrödinger equation

$$i\frac{d\psi}{dt} = \begin{pmatrix} E + \alpha & w(t) \\ w(t) & -E - \alpha \end{pmatrix} \psi. \quad (1)$$

*remi.robin@inria.fr

Here $w : [0, T] \rightarrow \mathbb{R}$ is a (sufficiently regular) function representing an external field, $E > 0$, and $\alpha \in [\alpha_0, \alpha_1]$ is an unknown parameter representing the fact that the *resonance frequency* of the system $2(E + \alpha)$ is not known precisely, but lies between $2(E + \alpha_0)$ and $2(E + \alpha_1)$. All along the paper we assume the condition

$$[\alpha_0, \alpha_1] \subset (-E, \infty), \quad 0 \in (\alpha_0, \alpha_1),$$

guaranteeing that the eigenvalues of the matrix in equation (1) are never zero, independently of the value of α . The solution of (1) (that depends on α and $w(\cdot)$) with initial condition $\psi_w^\alpha(0) = (0, 1)$ is the wave function $\psi_w^\alpha : [0, T] \rightarrow \mathbb{C}^2$.

One would like to find a function $w(\cdot)$ (the same for all values of α) such that, if at time zero the system is at the ground state $(0, 1)$ (i.e., it is in the eigenstate corresponding to the eigenvalue $-E - \alpha$), then at time T the system is close to a state of the form $(e^{i\theta}, 0)$ for some $\theta \in \mathbb{R}$. In mathematical terms this can be rephrased as follows.

P: For every $\varepsilon > 0$, find a time T and an external field $w : [0, T] \rightarrow \mathbb{R}$ such that

$$|\psi_w^\alpha(T) - (e^{i\theta}, 0)| < \varepsilon,$$

for every $\alpha \in [\alpha_0, \alpha_1]$ and for some $\theta \in \mathbb{R}$ (possibly depending on $\varepsilon, E, T, w, \alpha$).

In the mathematical literature it has been proved that problem **P** admits a solution when one replaces the real-valued function w by a complex-valued one, as in equation (2) below ([7, 12, 13, 14]). As far as we are aware, the problem is open in the case of real-valued functions. The result proved in this paper (Theorem 3) solves problem **P** in a more general framework, in which there is an additional parameter dispersion on the coupling between the control and the system (that is, $w(t)$ is replaced by $\delta w(t)$ for δ in a compact interval of $(0, +\infty)$).

Solving **P** is a key ingredient to prove ensemble controllability of (1) with more general initial and final conditions. This celebrated problem has been solved in the case where w is replaced by a complex-valued control in [13, 12] and [7].

The intuitive approach to tackle problem **P**, consists in the following two steps ([16, 21, 22, 26]):

- use an external field oscillating at the resonance frequency $2E$ and having a small and slowly varying amplitude and a slowly varying phase, to simulate by rotating wave approximation (RWA, for short) a system driven by a complex-valued function (in a sense, this “duplicates” the number of available external fields);
- use an adiabatic strategy based on chirped pulses (i.e., pulses whose frequency is slowly increasing from a value below $2(E + \alpha_0)$ to a value above $2(E + \alpha_1)$) to drive the system from an eigenstate to the other one independently of the value of α . This second step substantially exploits the presence of a complex-valued external field and is called adiabatic approximation (AA, for short) [9, 15, 20, 23, 27]. Alternative robust methods are developed, for example, in [10, 25].

However the RWA may affect the precision of the adiabatic strategy, as it has been remarked in [11]. In order to detail in which sense the “cascade” of the two approximations introduced above may break down, let us give some quantitative estimate.

1.1 Rotating wave approximation

Consider a two-level system of the form

$$i \frac{d\psi}{dt} = \begin{pmatrix} E & w(t) \\ w^*(t) & -E \end{pmatrix} \psi. \quad (2)$$

Here we assume that the resonance frequency of the system is known precisely, hence we have no α . The symbol w^* denotes the complex conjugate of w , which represents here a complex-valued external field. For every $\varepsilon > 0$, consider the external fields

$$w_\varepsilon(t) = 2\varepsilon u(\varepsilon t) \cos(2Et + \Delta(\varepsilon t)), \quad (3)$$

$$w_\varepsilon^R(t) = \varepsilon u(\varepsilon t) e^{-i(2Et + \Delta(\varepsilon t))}. \quad (4)$$

where $u(\cdot)$ and $\Delta(\cdot)$ are two real-valued smooth functions defined on $[0, T]$, $T > 0$. We have the following.

Proposition 1. *For $\varepsilon > 0$ let ψ_{w_ε} and $\psi_{w_\varepsilon^R}$ be the solutions of (2) with initial condition $\psi_0 \in \mathbb{C}^2$ corresponding to the external fields w_ε and w_ε^R , respectively. Then $\max_{t \in [0, T/\varepsilon]} |\psi_{w_\varepsilon}(t) - \psi_{w_\varepsilon^R}(t)|$ converges to 0 as $\varepsilon \rightarrow 0$.*

The proof of this fact is well known. If one applies the unitary change of variables

$$\psi_{w_\varepsilon}(t) = \begin{pmatrix} e^{-i(Et + \Delta(\varepsilon t)/2)} & 0 \\ 0 & e^{i(Et + \Delta(\varepsilon t)/2)} \end{pmatrix} \hat{\psi}_{w_\varepsilon}(t)$$

then $\hat{\psi}_{w_\varepsilon}(t)$ satisfies the Schrödinger equation

$$i \frac{d\hat{\psi}_{w_\varepsilon}}{dt} = \varepsilon \left[\begin{pmatrix} -\Delta'(\varepsilon t)/2 & u(\varepsilon t) \\ u(\varepsilon t) & \Delta'(\varepsilon t)/2 \end{pmatrix} + \begin{pmatrix} 0 & e^{i(4Et + 2\Delta(\varepsilon t))} u(\varepsilon t) \\ e^{-i(4Et + 2\Delta(\varepsilon t))} u(\varepsilon t) & 0 \end{pmatrix} \right] \hat{\psi}_{w_\varepsilon}.$$

Here Δ' indicates the derivative of the function $\Delta : [0, T] \rightarrow \mathbb{R}$. Now, defining $s = \varepsilon t$, varying in the interval $[0, T]$, and $\tilde{\psi}_{w_\varepsilon}(s) = \hat{\psi}_{w_\varepsilon}(t/\varepsilon)$ we obtain

$$i \frac{d\tilde{\psi}_{w_\varepsilon}}{ds} = \left[\begin{pmatrix} -\Delta'(s)/2 & u(s) \\ u(s) & \Delta'(s)/2 \end{pmatrix} + \underbrace{\begin{pmatrix} 0 & e^{i(4Es/\varepsilon + 2\Delta(s))} u(s) \\ e^{-i(4Es/\varepsilon + 2\Delta(s))} u(s) & 0 \end{pmatrix}}_{=: B(s, \varepsilon)} \right] \tilde{\psi}_{w_\varepsilon}. \quad (5)$$

The same change of variables on $\psi_{w_\varepsilon^R}$ gives rise to

$$i \frac{d\tilde{\psi}_{w_\varepsilon^R}}{ds} = \begin{pmatrix} -\Delta'(s)/2 & u(s) \\ u(s) & \Delta'(s)/2 \end{pmatrix} \tilde{\psi}_{w_\varepsilon^R}. \quad (6)$$

Equations (5) and (6) differ only for the term $B(s, \varepsilon)$. Since for every interval $[s_1, s_2] \subseteq [0, T]$ we have

$$\lim_{\varepsilon \rightarrow 0} \int_{s_1}^{s_2} B(s, \varepsilon) = 0$$

and B is uniformly bounded, we have that solutions of (5) converge uniformly in $[0, T]$ to solutions of (6) with the same initial condition. This is a classical averaging result that can

be found, for instance, in [1, Chapter 8]. Coming back to the original variables one obtains that $|\psi_{w_\varepsilon} - \psi_{w_\varepsilon^R}|$ converges uniformly to zero on the interval $[0, T/\varepsilon]$.

This simple argument is very useful. We started with a system driven by one scalar function w and we obtain at the limit a system driven by a complex-valued control or, equivalently, system (6) where the controls are the two scalar functions $u(t)$ and $v(t) = \Delta'(t)/2$. A more detailed quantitative analysis permits to conclude that on $[0, T/\varepsilon]$ we have

$$|\psi_{w_\varepsilon} - \psi_{w_\varepsilon^R}| = O(\varepsilon).$$

(See, for instance, [5, Appendix A] for a quantitative version of the averaging result mentioned above.) Higher order RWA can be obtained by considering higher-order averaging results.

In recent applications, it is sometimes necessary to use intense external fields. In these cases the RWA may become inaccurate, as pointed out in [2, 8, 19]. Thus it is crucial to have a precise quantification of the error.

1.2 Adiabatic approximation

We have seen in the previous section how to make the solutions of system (2) approximate those of system (2). We show here how such a system can be easily driven by adiabatic pulses.

Let us consider the case in which the energy of the system is not known precisely. We are then considering the system

$$i \frac{d\psi}{dt} = \begin{pmatrix} E + \alpha & w(t) \\ w^*(t) & -E - \alpha \end{pmatrix} \psi, \quad \text{where } \alpha \in [\alpha_1, \alpha_2]. \quad (7)$$

Let us choose the pulse w in the form

$$w(t) = u(t)e^{-i(2Et + \Delta(t))}, \quad (8)$$

where $u(\cdot)$ and $\Delta(\cdot)$ are two real-valued smooth functions. This choice of control corresponds to (4) in which ε has been set equal to 1. Applying the change of variables

$$\psi(t) = \begin{pmatrix} e^{-i(Et + \Delta(t)/2} & 0 \\ 0 & e^{i(Et + \Delta(t)/2)} \end{pmatrix} \Psi(t),$$

we obtain

$$i \frac{d\Psi}{ds} = \begin{pmatrix} \alpha - v(s) & u(s) \\ u(s) & -\alpha + v(s) \end{pmatrix} \Psi. \quad (9)$$

where $v(t) := \Delta'(t)/2$.

Notice that the eigenvalues of the matrix in equation (9), seen as functions of the pair (u, v) , coincide if and only if $u = 0$ and $v = \alpha$, where a conical eigenvalue intersection occurs. Fix now $v_0 < \alpha_0$ and $v_1 > \alpha_1$ and consider a smooth path $t \mapsto (u(t), v(t))$ lying in the half-plane $u > 0$ except for the initial and final points, where $u = 0$ (see Figure 1).

Define

$$u_\varepsilon(t) = u(\varepsilon t), \quad v_\varepsilon(t) = v(\varepsilon t).$$

Since the eigenvalues of the Hamiltonian in Equation (9) are

$$\pm \sqrt{(\alpha - v(s))^2 + u(s)^2} \neq 0,$$

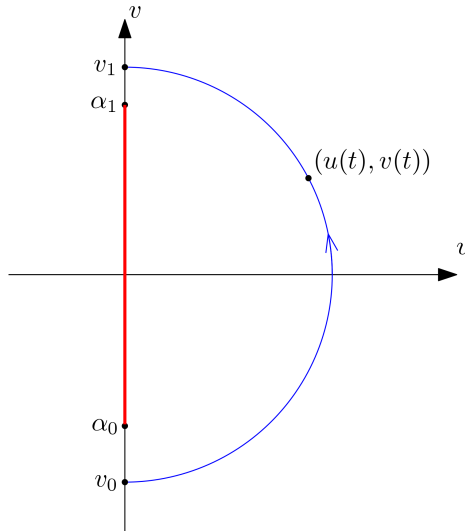


Figure 1: An adiabatic path as the one applied in Proposition 2.

the adiabatic theorem (see, e.g., [24]) ensures that, for $\varepsilon > 0$ small, the trajectory of (9) corresponding to $(u_\varepsilon, v_\varepsilon)$ and starting from $(0, 1)$ stays close to the eigenvector associated with the negative eigenvalue. More precisely, we have the following estimate.

Proposition 2. *There exists $C > 0$ such that, for every $\alpha \in [\alpha_0, \alpha_1]$ and every $\varepsilon > 0$, the solution Ψ of system (9) with initial condition $(0, 1)$ and corresponding to the control $(u_\varepsilon, v_\varepsilon)$ satisfies $|\Psi(T/\varepsilon) - (e^{i\theta}, 0)| \leq C\varepsilon$ for some $\theta \in \mathbb{R}$.*

Going back to equation (7), the control corresponding to $(u_\varepsilon, v_\varepsilon)$ is

$$w_\varepsilon(t) = u(\varepsilon t)e^{i(Et + \frac{\Delta(\varepsilon t)}{\varepsilon})}.$$

Such a law is called a (amplitude modulated) *chirped pulse*, since the range of frequency swept by the pulse is $\{2E + \Delta'(s) \mid s \in [0, T]\}$, which is independent of ε . For more details, see [3].

1.3 Combination of RWA and AA and statement of the population inversion result

What one would like to do is to consider the two approximations in cascade, in order to induce a transition from the state $(0, 1)$ to $(1, 0)$ (up to a phase) for an ensemble of systems parameterized by $\alpha \in [\alpha_0, \alpha_1]$ using a real-valued external field. The cascade of the two approximations is expected to behave well in many experimental setups, such as in NMR, due to the separation of timescales between the RWA and the AA. However, for intense external fields or in presence of large parametric dispersions, the outcome of the cascade is more challenging to predict and quantify precisely. Let us denote by ε_1 the small parameter that in the RWA was called ε and by ε_2 what in the AA was called ε . A formal cascade of the two approaches yields a control law of the form

$$w_{\varepsilon_1, \varepsilon_2}(t) = 2\varepsilon_1 u(\varepsilon_1 \varepsilon_2 t) \cos\left(2Et + \frac{\Delta(\varepsilon_1 \varepsilon_2 t)}{\varepsilon_2}\right),$$

where $u(\cdot)$ and $v(\cdot)$ are the same functions as those used in Proposition 2.

The hope is that the pulse $w_{\varepsilon_1, \varepsilon_2}$, for ε_1 and ε_2 small, induces approximately a transition from the state $(0, 1)$ to a state of the form $(e^{i\theta}, 0)$ in time $T/(\varepsilon_1 \varepsilon_2)$. The two approximations are, however, competing: when one decreases ε_2 (better AA), one needs the RWA to be true for a longer time as the final time is of order $1/(\varepsilon_1 \varepsilon_2)$. On the other hand, decreasing ε_1 deteriorates the performances of the AA:

1. The error on the adiabatic theorem depends of the gap between the eigenvalues, which goes to zero as $\varepsilon_1 \rightarrow 0$;
2. The range of frequencies swept by the pulse is $\{2E + \varepsilon_1 \Delta'(s) \mid s \in [0, T]\}$, that is, the allowed dispersion on the frequency is shrinking as ε_1 goes to zero.

As a consequence, this method can only work when $\alpha = 0$. Under this restriction, and for suitable relations between ε_1 and ε_2 as they both go to zero, the cascade of the two approximations can be proved to work (see [4, 6]).

Another possibility would be to fix ε_1 small and to hope that the limit as $\varepsilon_2 \rightarrow 0$ makes the RWA work as well. Nevertheless, the k -th order RWA is usually valid up to a time of order $\frac{1}{\varepsilon_1^k}$, whereas we would need the time to be of order $\frac{1}{\varepsilon_1 \varepsilon_2}$. In fact, without restriction on the allowed frequency, simulations show that convergence does not hold, as illustrated in Figure 2.

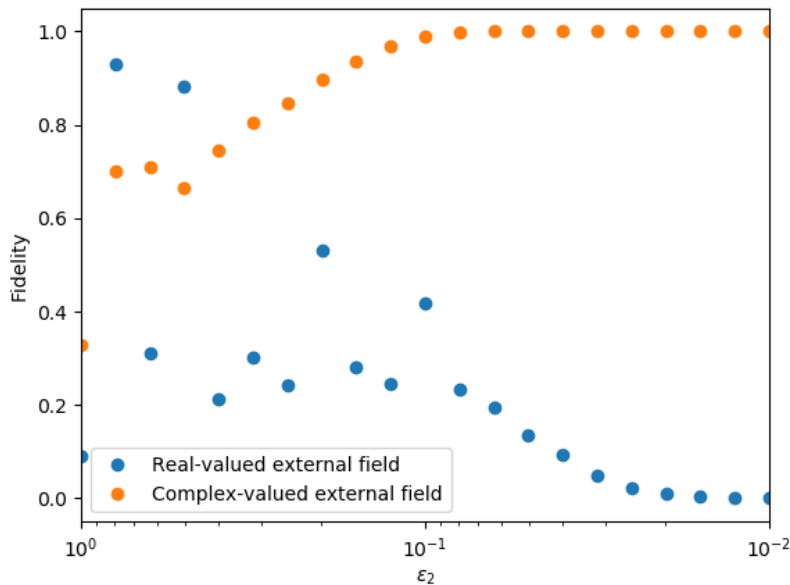


Figure 2: Comparison of the real-valued and complex-valued chirp scheme of the first point of Remark 5 with $E = 0.75$, $\alpha = 0.25$, $\varepsilon_1 = 1$, $v_0 = -0.5$, $v_1 = 0.5$. Notice that the assumptions of Theorem 3 are not satisfied.

An approach to tackle the issue of the shrinking interval of frequencies swept by the pulse

is to divide $\Delta(\varepsilon_1\varepsilon_2t)$ by $\varepsilon_1\varepsilon_2$ and not just by ε_2 . We claim that an external field of the type

$$w_{\varepsilon_1,\varepsilon_2}(t) = 2\varepsilon_1\delta u(\varepsilon_1\varepsilon_2t) \cos\left(2Et + \frac{\Delta(\varepsilon_1\varepsilon_2t)}{\varepsilon_1\varepsilon_2}\right), \quad (10)$$

where δ is a positive constant, can induce a transition for the robust population transfer problem, provided that the relative order between ε_1 and ε_2 satisfies some suitable constraint as both parameters go to zero and under some further assumptions on the range $[\alpha_0, \alpha_1]$. This is detailed in the following theorem.

Theorem 3. *Assume that $v_0 < 0 < v_1$ are such that $3(E + v_0) \geq E + v_1$. Fix $T > 0$ and $u, \Delta : [0, T] \rightarrow \mathbb{R}$ smooth (e.g., $u \in C^2$ and $\Delta \in C^3$) such that*

1. $(u(0), \Delta'(0)) = (0, 2v_0)$ and $(u(T), \Delta'(T)) = (0, 2v_1)$;
2. $\forall s \in (0, T), u(s) > 0$ and $\Delta''(s) \geq 0$.

Denote by $\psi_{\varepsilon_1,\varepsilon_2}^\alpha$ the solution of (1) with initial condition $\psi_{\varepsilon_1,\varepsilon_2}^\alpha(0) = (0, 1)$ and control $w_{\varepsilon_1,\varepsilon_2}$ as in (10). Then, for every $N_0 \in \mathbb{N}$, for every compact interval $I \subseteq (v_0, v_1)$, there exist $C_{N_0} > 0$ and $\eta > 0$ such that for every $\alpha \in I$ and every $(\varepsilon_1, \varepsilon_2) \in (0, \eta)^2$,

$$\left| \psi_{\varepsilon_1,\varepsilon_2}^\alpha\left(\frac{1}{\varepsilon_1\varepsilon_2}\right) - (e^{i\theta}, 0) \right| < C_{N_0} \max(\varepsilon_2/\varepsilon_1, \varepsilon_1^{N_0-1}/\varepsilon_2)$$

for some $\theta \in \mathbb{R}$. Moreover, the constant C_{N_0} can be taken locally uniform with respect to the parameter $\delta > 0$ appearing in (10).

Roughly speaking, $\varepsilon_2/\varepsilon_1$ is the AA error and $\varepsilon_1^{N_0-1}/\varepsilon_2$ the RWA error. We define the fidelity of a pulse as the quantity $\inf_\theta |\psi_{\varepsilon_1,\varepsilon_2}^\alpha(\frac{1}{\varepsilon_1\varepsilon_2}) - (e^{i\theta}, 0)|$ (also denoted $|\langle \psi_{\varepsilon_1,\varepsilon_2}^\alpha(\frac{1}{\varepsilon_1\varepsilon_2}) | e_1 \rangle|$). It is a natural measure of the transition rate induced by a pulse. Thus, by playing on the integer N_0 and on the order of magnitude between ε_1 and ε_2 , we can express the fidelity attained by the strategy above in terms of the duration of the pulse.

Corollary 4. *Taking $\varepsilon_1 = \varepsilon_2^{2/N_0}$ ($N_0 \geq 3$) leads to an error of the order $\mathcal{T}^{\frac{2/N_0-1}{1+2/N_0}}$, where $\mathcal{T} = 1/(\varepsilon_1\varepsilon_2)$ is the duration of the pulse $w_{\varepsilon_1,\varepsilon_2}$.*

Remark 5. • *As an example, one can apply Theorem 3 with $T = 1$, $\delta = 1$, $\Delta(s) = \frac{v_0-v_1}{\pi} \sin(\pi s) + (v_0 + v_1)s$ and $u(s) = 1 - \cos(2\pi s)$, $s \in [0, 1]$. More explicitly,*

$$w_{\varepsilon_1,\varepsilon_2}(t) = 2\varepsilon_1(1 - \cos(2\pi\varepsilon_1\varepsilon_2t)) \cos\left(2Et + \frac{(v_0 - v_1) \sin(\pi\varepsilon_1\varepsilon_2t)}{\pi\varepsilon_1\varepsilon_2} + (v_0 + v_1)t\right).$$

All the simulations in this paper use this pulse scheme and some compare to the complex-valued pulse

$$w_{\varepsilon_1,\varepsilon_2}^R(t) = \varepsilon_1(1 - \cos(2\pi\varepsilon_1\varepsilon_2t)) \exp\left(2iEt + i\frac{(v_0 - v_1) \sin(\pi\varepsilon_1\varepsilon_2t)}{\pi\varepsilon_1\varepsilon_2} + i(v_0 + v_1)t\right).$$

- *By taking N_0 large, one can get, for each $\eta > 0$, a fidelity close to one at order $\mathcal{T}^{-1+\eta}$, to compare with the standard $O(\mathcal{T}^{-1})$ of the adiabatic theorem.*

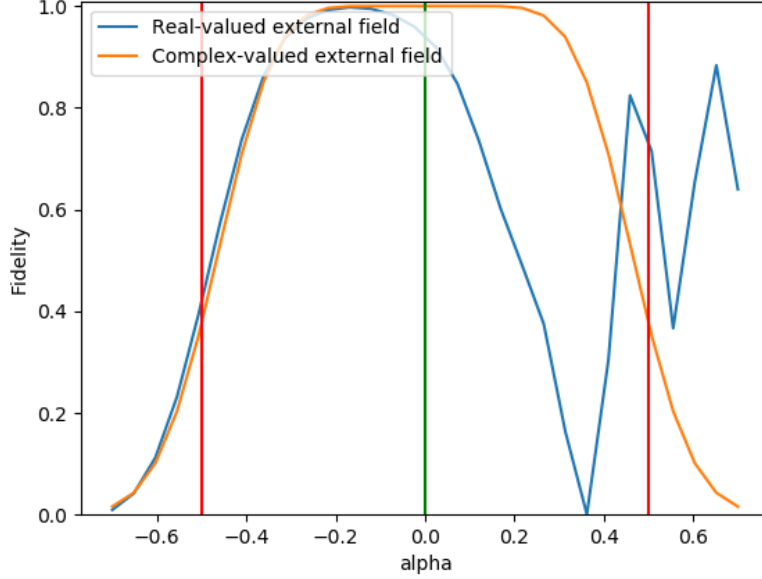


Figure 3: $E = 0.75$, $\alpha = 0.25$, $\varepsilon_1 = 1$, $\varepsilon_2 = 0.1$, $v_0 = -0.5$, $v_1 = 0.5$. Assumption $4E + 3\Delta'(s) - 2\alpha < 0$ is satisfied if and only if $\alpha < 0$.

- The assumption $3(E + v_0) \geq E + v_1$ ensures non-overlapping of some characteristic frequencies (cf. Lemma 25). It could be replaced by the weaker one: $4E + 3\Delta' - 2\alpha > 0$ for every $\alpha \in [\alpha_0, \alpha_1]$ and everywhere in $[0, T]$. Nevertheless, asking this condition to be valid for every compact subinterval $[\tilde{\alpha}_0, \tilde{\alpha}_1]$ of (v_0, v_1) is equivalent to the inequality $3(E + v_0) \geq E + v_1$.

Numerical simulations suggest that the inequality $4E + 3\Delta' - 2\alpha > 0$ is sharp in the following sense: if for a given α , $4E + 3\Delta'(s) - 2\alpha < 0$ for some $s \in [0, T]$, an inequality as in Theorem 3 seem not to hold. As an illustration, in Figure 3 we observe that for $\alpha \geq 0$ (condition $4E + 3\Delta' - 2\alpha > 0$ not satisfied), the accuracy of the RWA is worse than for $\alpha < 0$ (condition $4E + 3\Delta' - 2\alpha > 0$ satisfied).

Remark 6. Many questions concerning the combination of the RWA and AA remain open. In particular we do not know if a version of Theorem 3 holds with ε_1 fixed, small enough, and ε_2 going to 0.

Concerning systems with higher number of levels (possibly infinite), we expect the techniques developed in this paper to work. Nevertheless, such an extension seems not trivial.

We postpone the proof of Theorem 3 to Section 3. This proof is technical and is sketched in Sections 3.1 and 3.2 (see also Remark 34).

2 Application to the ensemble control problem

We denote by $\sigma_x, \sigma_y, \sigma_z$ the Pauli matrices given by

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (11)$$

and by SU_2 the special unitary group of degree 2. We recall that its Lie algebra \mathfrak{su}_2 is generated by $i\sigma_x, i\sigma_y$, and $i\sigma_z$.

There is a natural distance on SU_2 induced by the norm of endomorphism on \mathbb{C}^2 , which we denote $\|\cdot\|$. Let $v_0 < 0 < v_1$ and $0 < \delta_m \leq \delta_M$. Let $\mathcal{D} = [v_0, v_1] \times [\delta_m, \delta_M]$ be the compact set of the dispersion parameters and endow $\mathcal{F} := C^0(\mathcal{D}, SU_2)$ with the usual distance $d_{\mathcal{F}}(f, g) := \max_{d \in \mathcal{D}} \|f(d) - g(d)\|$.

Li and Khaneja proved in [13] the following ensemble operator controllability result.

Theorem 7 (Li–Khaneja, 2009). *For any control bound $K > 0$, any target distribution $M_F \in \mathcal{F}$, and any $\varepsilon > 0$, there exist some $T > 0$ and controls $u, v \in L^\infty([0, T], [-K, K])$ such that the solution of the equation*

$$i \frac{d}{dt} M(\alpha, \delta, t) = ((E + \alpha)\sigma_z + \delta u(t)\sigma_x + \delta v(t)\sigma_y)M(\alpha, \delta, t), \quad M(\alpha, \delta, 0) = I_2, \quad \forall (\alpha, \delta) \in \mathcal{D} \quad (12)$$

satisfies $d_{\mathcal{F}}(M(\cdot, \cdot, T), M_F(\cdot, \cdot)) < \varepsilon$.

Remark 8. • *The result was originally stated on SO_3 for the Bloch sphere, the extension to SU_2 stated in Theorem 12 is straightforward.*

- *This is a very strong ensemble controllability result, as it tackles the controllability of the semigroups.*

We extend here this result to the problem of a qubit driven by a single real control, thus replacing Equation (12) by

$$i \frac{d}{dt} M(\alpha, \delta, t) = ((E + \alpha)\sigma_z + \delta u(t)\sigma_x)M(\alpha, \delta, t), \quad M(\alpha, \delta, 0) = I_2, \quad \forall (\alpha, \delta) \in \mathcal{D}. \quad (13)$$

One of the key ingredients of the proof of Theorem 7 is the existence of an adiabatic pulse inducing a propagator $U \in \mathcal{F}$ such that $\max_{d \in \mathcal{D}} \min_{\theta \in [0, 2\pi]} \|U(d)(0, 1)^T - (e^{i\theta}, 0)^T\|$ is arbitrarily small.

Theorem 3 ensures the following corollary.

Corollary 9. *Suppose that $3(E + v_0) > E + v_1$. Then, for any $K > 0$ and any $\varepsilon > 0$, there exist $T > 0$ and a control $u \in L^\infty([0, T], [-K, K])$ such that the solution of Equation (13) satisfies $\max_{(\alpha, \delta) \in \mathcal{D}} \min_{\theta \in [0, 2\pi]} \|M(\alpha, \delta, T)(0, 1)^T - (e^{i\theta}, 0)^T\| < \varepsilon$.*

Based on Corollary 9, we will prove the following result, which generalizes Theorem 7 under the extra assumption on the α -dispersion.

Theorem 10. *Suppose that $3(E + v_0) > E + v_1$. Let $\varepsilon > 0$, $M_F \in \mathcal{F}$, and $K > 0$. Then there exist $T > 0$ and $u \in L^\infty([0, T], [-K, K])$ such that the solution of Equation (13) satisfies $d_{\mathcal{F}}(M(\cdot, \cdot, T), M_F(\cdot, \cdot)) < \varepsilon$.*

The proof, sketched below, is an adaptation of the arguments used in [13]. Let $\mathcal{R} = \{M(\cdot, \cdot, T) \mid T > 0, M \text{ is a solution of (13) for some } u \in L^\infty([0, T], [-K, K])\}$. It is clear that \mathcal{R} and its closure $\bar{\mathcal{R}}$ are semigroups of \mathcal{F} . We have to prove that $\bar{\mathcal{R}} = \mathcal{F}$.

Lemma 11. *For all t in \mathbb{R} , $(\alpha, \delta) \mapsto e^{-t(E+\alpha)i\sigma_z}$ is in $\bar{\mathcal{R}}$.*

Proof. Using a null control in (13) during a time $t \geq 0$, we get $(\alpha, \delta) \mapsto e^{-t(E+\alpha)i\sigma_z}$ belongs to \mathcal{R} .

Let us prove that the result also holds for $t < 0$. Set an arbitrary $\varepsilon > 0$. By Corollary 9, there exists $U^\varepsilon \in \mathcal{R}$ such that

$$\max_{d \in \mathcal{D}} \min_{\theta \in [0, 2\pi]} \|U^\varepsilon(d)(0, 1)^T - (e^{i\theta}, 0)^T\| < \varepsilon.$$

Using Euler angle decomposition, there exist three functions $a_\varepsilon, b_\varepsilon, c_\varepsilon$ from \mathcal{D} to $[0, 2\pi]$ (not necessarily continuous) such that $U^\varepsilon(d) = e^{a_\varepsilon(d)i\sigma_z} e^{b_\varepsilon(d)i\sigma_x} e^{c_\varepsilon(d)i\sigma_z}$ for every $d \in \mathcal{D}$. In particular, $\max_{d \in \mathcal{D}} |b_\varepsilon(d) - \pi|$ is of order ε , so that $\sup_{d \in \mathcal{D}} \|U^\varepsilon(d) - \tilde{U}^\varepsilon(d)\|$ is also of order ε , where $\tilde{U}^\varepsilon(d) := e^{a_\varepsilon(d)i\sigma_z} e^{\pi i\sigma_x} e^{c_\varepsilon(d)i\sigma_z}$. For all $t > 0$, we have that $(\alpha, \delta) \mapsto e^{-t(E+\alpha)i\sigma_z}$ is in $\bar{\mathcal{R}}$, by using the control $u \equiv 0$. Using the relation $e^{-\pi i\sigma_x} e^{r i\sigma_z} e^{\pi i\sigma_x} = e^{-r i\sigma_z}$, $r \in \mathbb{R}$, we deduce that

$$\begin{aligned} \tilde{U}^\varepsilon(d) e^{-t(E+\alpha)i\sigma_z} \tilde{U}^\varepsilon(d) &= e^{a_\varepsilon(d)i\sigma_z} e^{-\pi i\sigma_x} e^{c_\varepsilon(d)i\sigma_z} e^{-t(E+\alpha)i\sigma_z} e^{a_\varepsilon(d)i\sigma_z} e^{\pi i\sigma_x} e^{c_\varepsilon(d)i\sigma_z} \\ &= e^{t(E+\alpha)i\sigma_z}, \end{aligned}$$

for every $d = (\alpha, \delta)$ in \mathcal{D} . This shows that $(\alpha, \delta) \mapsto e^{t(E+\alpha)i\sigma_z}$ is at distance of order ε from an element of \mathcal{R} , concluding the proof. \square

Lemma 12. *Let $u \in \mathbb{R}$. Then $(\alpha, \delta) \mapsto e^{u\delta i\sigma_x}$ is in $\bar{\mathcal{R}}$.*

Proof. Consider first the case $|u| \leq K$. Setting $V_n(\alpha, \delta) = e^{-(E+\alpha)i\sigma_z + u\delta i\sigma_x}/n$, one can easily check that the sequence $((\alpha, \delta) \mapsto (V_n(\alpha, \delta) e^{t(E+\alpha)i\sigma_z/n})^n)_{n \in \mathbb{N}}$ is in $\bar{\mathcal{R}}$ and converges to $(\alpha, \delta) \mapsto e^{u\delta i\sigma_x}$ in \mathcal{F} . This concludes the case $|u| \leq K$. We deduce the general case using the fact that $\bar{\mathcal{R}}$ is a semigroup. \square

Let

$$\mathfrak{g} = \{X \in \mathcal{C}^0(\mathcal{D}, \mathfrak{su}_2) \mid \forall t \in \mathbb{R}, e^{tX} \in \bar{\mathcal{R}}\}. \quad (14)$$

Thus $(\alpha, \delta) \mapsto \delta i\sigma_x$ and $(\alpha, \delta) \mapsto (E + \alpha)i\sigma_z$ belong to \mathfrak{g} . The space $\mathcal{C}^0(\mathcal{D}, \mathfrak{su}_2)$ has a natural addition, product, and Lie bracket. Moreover, it has the structure of Banach algebra using as norm the sup norm, denoted by $|\cdot|_\infty$. Before concluding the proof of Theorem 10, let us to show that \mathfrak{g} is a Lie algebra by proving that it is stable by addition and Lie bracket.

Lemma 13. *The set \mathfrak{g} defined in (14) is stable under addition and Lie brackets:*

$$[\mathfrak{g}, \mathfrak{g}] \subset \mathfrak{g}, \quad \mathfrak{g} + \mathfrak{g} \subset \mathfrak{g}.$$

Proof. Pick $X, Y \in \mathfrak{g}$. Let us first prove that $e^{t[X, Y]} \in \bar{\mathcal{R}}$ for every $t \in \mathbb{R}$. To this purpose, consider $U(s) = e^{sX} e^{sY} e^{-sX} e^{-sY}$, $s \in [0, 1]$. Then there exists a constant $C > 0$ depending only on $|X|_\infty$ and $|Y|_\infty$ such that $d_{\mathcal{F}}(U(\sqrt{s}), e^{s[X, Y]}) \leq Cs^{3/2}$ for every $s \in [0, 1]$. Using the

fact that the application $x \mapsto x^n$ is $(n-1)$ -Lipschitz on the unit ball of any Banach algebra, we get

$$d_{\mathcal{F}}(U(\sqrt{s/n})^n, e^{s[X,Y]}) \leq C(s/n)^{3/2}(n-1) \leq Cs^{3/2}n^{-1/2}, \quad s \in [0, 1].$$

As a consequence, $e^{s[X,Y]} \in \bar{\mathcal{R}}$ for every $s \in [0, 1]$. Applying the same reasoning to $-X$ instead of X , we get that $e^{s[X,Y]} \in \bar{\mathcal{R}}$ for every $s \in [-1, 1]$. We conclude the proof of the stability under Lei bracket by using the semigroup structure of $\bar{\mathcal{R}}$.

Concerning the stability under addition, set $V(s) = e^{sX}e^{sY}$ and notice that $V(s) \in \bar{\mathcal{R}}$ for every $s \in \mathbb{R}$. Noticing that $V(t/n)^n \xrightarrow[n \rightarrow \infty]{d_{\mathcal{F}}} e^{t(X+Y)}$, we deduce that $e^{t(X+Y)} \in \bar{\mathcal{R}}$ for every $t \in \mathbb{R}$. \square

Denote by $\text{ad}_X(Y) = [X, Y]$ the adjoint representation both in \mathfrak{su}_2 and in $\mathcal{C}^0(\mathcal{D}, \mathfrak{su}_2)$. We recall the Pauli matrices commutation laws

$$[i\sigma_x, i\sigma_y] = -i\sigma_z, \quad [i\sigma_y, i\sigma_z] = -i\sigma_x, \quad [i\sigma_z, i\sigma_x] = -i\sigma_y.$$

After some straightforward computations, one gets

$$\begin{aligned} \text{ad}_{\delta i\sigma_x}^{2l}(\text{ad}_{(E+\alpha)i\sigma_z}^{2k+1}(\delta i\sigma_x)) &= (-1)^{l+k}(E+\alpha)^{2k+1}\delta^{2l+1}i\sigma_y, \\ \text{ad}_{\delta i\sigma_x}^{2l+1}(\text{ad}_{(E+\alpha)i\sigma_z}^{2k+1}(\delta i\sigma_x)) &= (-1)^{l+k}(E+\alpha)^{2k+1}\delta^{2l+2}i\sigma_z, \\ \text{ad}_{(E+\alpha)i\sigma_z}^{2l}\text{ad}_{\delta i\sigma_x}^{2k+1}(\text{ad}_{(E+\alpha)i\sigma_z}^{2k+1}(\delta i\sigma_x)) &= (-1)^{l+k+1}(E+\alpha)^{2k+2}\delta^{2l+1}i\sigma_x. \end{aligned}$$

Thus for any $n, m \in \mathbb{N}$, and any sequence $(b_{k,l})_{k,l}$ of real numbers, we have

$$\begin{aligned} \sum_{k=0}^m \sum_{l=0}^n b_{k,l} \delta^{2k+2} (E+\alpha)^{2l+1} i\sigma_x &\in \mathfrak{g}, \\ \sum_{k=0}^m \sum_{l=0}^n c_{k,l} \delta^{2k+1} (E+\alpha)^{2l+1} i\sigma_y &\in \mathfrak{g}, \\ \sum_{k=0}^m \sum_{l=0}^n d_{k,l} \delta^{2k+1} (E+\alpha)^{2l+2} i\sigma_z &\in \mathfrak{g}. \end{aligned}$$

By the Stone–Weierstrass theorem, for any continuous function $f \in C(\mathcal{D}, \mathbb{R})$ we can approximate $\frac{f(d)}{(E+\alpha)\delta^2}$ uniformly on \mathcal{D} by polynomials of the form $\sum_{k=0}^m \sum_{l=0}^n b_{k,l} \delta^{2k} (E+\alpha)^{2l}$. This proves that $f(d)i\sigma_x \in \mathfrak{g}$. With a similar argument, we get $f(d)i\sigma_{\star} \in \mathfrak{g}$ for $\star = x, y, z$.

Finally, let $\rho > 0$ be such that $(a_1, a_2, a_3) \mapsto e^{a_1 i\sigma_x + a_2 i\sigma_y + a_3 i\sigma_z}$ is a diffeomorphism between a neighborhood of 0 in \mathbb{R}^3 and the ball of radius ρ centered at I_2 in SU_2 . Then for every $M_F \in \mathcal{F}$ such that $d_{\mathcal{F}}(M_F, I_2) < \rho$ there exist $f_1, f_2, f_3 \in \mathcal{C}^0(\mathcal{D}, \mathbb{R})$ such that $M_F(d) = e^{f_1(d)i\sigma_x + f_2(d)i\sigma_y + f_3(d)i\sigma_z}$. Thus $M_F \in \bar{\mathcal{R}}$. Since $\bar{\mathcal{R}}$ is a semigroup, we deduce that $\bar{\mathcal{R}}$ is both open and closed in \mathcal{F} , yielding that $\bar{\mathcal{R}} = \mathcal{F}$. This concludes the proof of Theorem 10.

3 Proof of Theorem 3

3.1 A first change of variables

Let $w_{\varepsilon_1, \varepsilon_2}$ be as in (10). In order to recast the equation

$$i \frac{d}{dt} \psi = H\psi = ((E+\alpha)\sigma_z + w_{\varepsilon_1, \varepsilon_2} \sigma_x) \psi$$

in the interaction frame, set

$$\psi_I(t) = e^{i(E+\alpha)\sigma_z t} \psi(t), \quad E_1(t) = 2\alpha t - \frac{\Delta(\varepsilon_1 \varepsilon_2 t)}{\varepsilon_1 \varepsilon_2}, \quad E_2(t) = 4Et + 2\alpha t + \frac{\Delta(\varepsilon_1 \varepsilon_2 t)}{\varepsilon_1 \varepsilon_2},$$

and notice that

$$i \frac{d}{dt} \psi_I = H_I \psi_I,$$

where

$$\begin{aligned} H_I(t) &= -(E + \alpha)\sigma_z + e^{i(E+\alpha)\sigma_z t} H(t) e^{-i(E+\alpha)\sigma_z t} \\ &= \varepsilon_1 u(\varepsilon_1 \varepsilon_2 t) \begin{pmatrix} 0 & e^{iE_1(t)} + e^{iE_2(t)} \\ e^{-iE_1(t)} + e^{-iE_2(t)} & 0 \end{pmatrix}. \end{aligned}$$

We will assume without loss of generality that $T = 1$. For $E \in \mathbb{R}$, define

$$A(E) = \begin{pmatrix} 0 & e^{iE} \\ e^{-iE} & 0 \end{pmatrix}, \quad B(E) = \begin{pmatrix} 0 & -ie^{iE} \\ ie^{-iE} & 0 \end{pmatrix}. \quad (15)$$

In terms of these new notations, we can rewrite $H_I(t) = \varepsilon_1 u(\varepsilon_1 \varepsilon_2 t) A(E_1(t)) + \varepsilon_1 u(\varepsilon_1 \varepsilon_2 t) A(E_2(t))$, $t \in [0, \frac{1}{\varepsilon_1 \varepsilon_2}]$.

In the usual first order RWA setting, one neglects the term containing the factor $A(E_2)$, which is highly oscillating compared to the first one. A standard method to justify this, is to use a change of variables close to the identity (see, e.g., [17] and [18]). Inspired by this, we introduce the notation

$$f_1(t) = \frac{d}{dt} E_1(t), \quad f_2(t) = \frac{d}{dt} E_2(t), \quad (16)$$

and we apply the unitary change of variables

$$\tilde{\psi}_I(t) = \exp\left(i\varepsilon_1 \frac{u(\varepsilon_1 \varepsilon_2 t)}{f_2(t)} B(E_2(t))\right) \psi_I(t). \quad (17)$$

The dynamics of $\tilde{\psi}_I$ are characterized by the Hamiltonian

$$\begin{aligned} \tilde{H}_I(t) &= i \frac{d}{dt} \left(\cos\left(\varepsilon_1 \frac{u(\varepsilon_1 \varepsilon_2 t)}{f_2(t)}\right) I + i \sin\left(\varepsilon_1 \frac{u(\varepsilon_1 \varepsilon_2 t)}{f_2(t)}\right) B(E_2(t)) \right) \\ &\quad \left(\cos\left(\varepsilon_1 \frac{u(\varepsilon_1 \varepsilon_2 t)}{f_2(t)}\right) I - i \sin\left(\varepsilon_1 \frac{u(\varepsilon_1 \varepsilon_2 t)}{f_2(t)}\right) B(E_2(t)) \right) \\ &\quad + \left(\cos\left(\varepsilon_1 \frac{u(\varepsilon_1 \varepsilon_2 t)}{f_2(t)}\right) I + i \sin\left(\varepsilon_1 \frac{u(\varepsilon_1 \varepsilon_2 t)}{f_2(t)}\right) B(E_2(t)) \right) H_I \\ &\quad \left(\cos\left(\varepsilon_1 \frac{u(\varepsilon_1 \varepsilon_2 t)}{f_2(t)}\right) I - i \sin\left(\varepsilon_1 \frac{u(\varepsilon_1 \varepsilon_2 t)}{f_2(t)}\right) B(E_2(t)) \right). \end{aligned}$$

Notice that the first term can be rewritten as $-\varepsilon_1 u(\varepsilon_1 \varepsilon_2 t) A(E_2(t)) + O(\varepsilon_1^2)$, so that $\tilde{H}_I(t) = \varepsilon_1 A(E_1(t)) + O(\varepsilon_1^2 + \varepsilon_1^2 \varepsilon_2)$, where the notation $O(\cdot)$ is defined as follows.

Definition 14. Let R be a $(\varepsilon_1, \varepsilon_2)$ -parameterized function in the following sense: for every $\varepsilon_1, \varepsilon_2 > 0$, $R_{\varepsilon_1, \varepsilon_2}$ is a real-valued function defined on the interval $[0, \frac{1}{\varepsilon_1 \varepsilon_2}]$. We say that $R = O(g(\varepsilon_1, \varepsilon_2))$ with $g : \mathbb{R}_+^2 \rightarrow \mathbb{R}_+$ if there exist $\delta, C > 0$ such that for every $(\varepsilon_1, \varepsilon_2) \in (0, \delta)^2$ and $t \in [0, \frac{1}{\varepsilon_1 \varepsilon_2}]$, we have $|R_{\varepsilon_1, \varepsilon_2}(t)| \leq Cg(\varepsilon_1, \varepsilon_2)$.

Remark 15. • We have $|\psi_I - \tilde{\psi}_I| = O(\varepsilon_1)$. Moreover, from the hypotheses of Theorem 3, we have $u(0) = u(1) = 0$, thus $\psi_I(0) = \tilde{\psi}_I(0)$ and $\tilde{\psi}_I(\frac{1}{\varepsilon_1\varepsilon_2}) = \psi_I(\frac{1}{\varepsilon_1\varepsilon_2})$.

- Let ψ_{rwa} be the solution of the Schrödinger equation with initial condition $\psi_I(0)$ and Hamiltonian $\varepsilon_1 u(\varepsilon_1\varepsilon_2 t)A(E_1(t))$. Then it turns out that $|\psi_{\text{rwa}}(\frac{1}{\varepsilon_1\varepsilon_2}) - \tilde{\psi}_I(\frac{1}{\varepsilon_1\varepsilon_2})| = O(\varepsilon_1/\varepsilon_2)$ (see Lemma 29). To prove convergence as $(\varepsilon_1, \varepsilon_2) \rightarrow 0$ in a suitable asymptotic regime, it would thus be enough to show that the dynamics of $\varepsilon_1 u(\varepsilon_1\varepsilon_2 t)A(E_1(t))$ induce a transition between $(0, 1)$ and $(1, 0)$ up to a phase, in the regime $\varepsilon_1 \ll \varepsilon_2$. Nevertheless this is not the case (recall that ‘standard’ adiabatic theorem cannot be applied since ε_1 is not fixed) as illustrated in Figure 4.

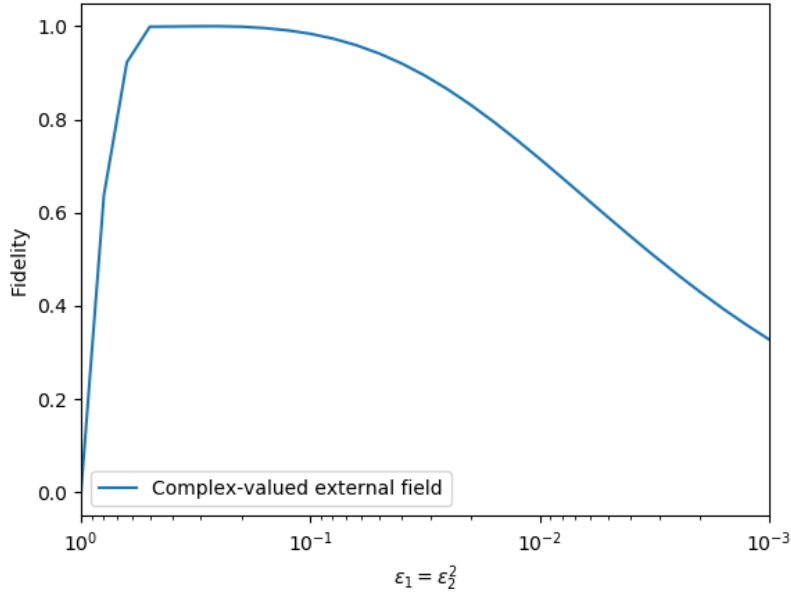


Figure 4: Taking $v_0 = -0.5$, $v_1 = 0.5$, $E = 0$, and $\alpha = 0$, we observe that the fidelity does not converge to 1 as $(\varepsilon_1, \varepsilon_2) \rightarrow 0$ in the regime $\varepsilon_1 \ll \varepsilon_2$. The plot corresponds to the choice $\varepsilon_1 = \varepsilon_2^2$.

3.2 Idea of the proof

We aim at providing correction terms to the Hamiltonian $\varepsilon_1 u(\varepsilon_1\varepsilon_2 t)A(E_1(t))$, in order to improve the order of the averaging approximation. For this we will repeat a procedure similar to the one introduced in Equation (17). At each step the expression of the obtained effective Hamiltonian is more complicated but provides a more accurate estimate of the final state. Then it will be possible to apply adiabatic theory to prove transition for the effective Hamiltonian. More precisely, we will prove the following theorem.

Theorem 16. Let $\alpha \in (v_0, v_1)$ and assume that $E + \alpha > 0$ and $4E - 3\Delta'(s) > 2\alpha$ for every $s \in [0, 1]$. Then, for every $N_0 \in \mathbb{N}$ there exists a Hamiltonian H_{RWA} of the form

$$H_{\text{RWA}}(t) = \varepsilon_1 h_1(\varepsilon_1\varepsilon_2 t)A(E_1(t)) + \varepsilon_1^2 h_2(\varepsilon_1\varepsilon_2 t)B(E_2(t)) + \varepsilon_1^2 h_3(\varepsilon_1\varepsilon_2 t)\sigma_z, \quad (18)$$

with h_1, h_2, h_3 polynomials in $(\varepsilon_1, \varepsilon_2)$ with coefficients in $\mathcal{C}^\infty([0, 1], \mathbb{R})$, such that the solution ψ_{RWA} of the Cauchy problem

$$i \frac{d}{dt} \psi_{\text{RWA}} = H_{\text{RWA}} \psi_{\text{RWA}}, \quad \psi_{\text{RWA}}(0) = \psi_1(0),$$

satisfies $|\psi_{\text{RWA}}(\frac{1}{\varepsilon_1 \varepsilon_2}) - \psi_1(\frac{1}{\varepsilon_1 \varepsilon_2})| = O(\varepsilon_1^2 \varepsilon_2 + \varepsilon_1^{N_0-1} / \varepsilon_2)$. More precisely, there exist $h_{j,p,q} \in \mathcal{C}^\infty([0, 1], \mathbb{R})$, for $j = 1, 2, 3$, $p = 0, \dots, N_0$, and $q = 0, 1$, such that

1. $h_1 = u + \sum_{p=1}^{N_0} \sum_{q=0}^1 \varepsilon_1^p \varepsilon_2^q h_{1,p,q}$ with $h_{1,p,0}(0) = h_{1,p,0}(1) = 0$,
2. $h_2 = \sum_{p=0}^{N_0} \sum_{q=0}^1 \varepsilon_1^p \varepsilon_2^q h_{2,p,q}$ with $h_{2,p,0}(0) = h_{2,p,0}(1) = 0$,
3. $h_3 = \sum_{p=0}^{N_0} \sum_{q=0}^1 \varepsilon_1^p \varepsilon_2^q h_{3,p,q}$ with $h_{3,p,0}(0) = h_{3,p,0}(1) = 0$.

After that, we will prove that H_{RWA} induces a transition between eigenstates with an error of order $O(\varepsilon_2/\varepsilon_1)$, which will be enough to prove Theorem 3.

3.3 The rotating wave approximation

Definition 17. Define the algebra \mathcal{S} of slow functions as the set of all $(\varepsilon_1, \varepsilon_2)$ -parameterized functions f (in the sense of Definition 14) such that for every $t \in [0, \frac{1}{\varepsilon_1 \varepsilon_2}]$, $f_{\varepsilon_1, \varepsilon_2}(t) = g(\varepsilon_1 \varepsilon_2 t)$ for some smooth $g : [0, 1] \rightarrow \mathbb{R}$ independent of $(\varepsilon_1, \varepsilon_2)$. The quantity $\sup_{t \in [0, \frac{1}{\varepsilon_1 \varepsilon_2}]} |f_{\varepsilon_1, \varepsilon_2}(t)|$ is independent of $(\varepsilon_1, \varepsilon_2)$ and provides a norm, endowing \mathcal{S} with the structure of Banach algebra.

Remark 18. • The functions f_1 and f_2 defined in (16) are slow.

- \mathcal{S} is isometric to the Banach algebra $\mathcal{C}^\infty([0, 1], \mathbb{R})$.
- Given $f \in \mathcal{S}$, its t -derivative \dot{f} defined by $\dot{f}_{\varepsilon_1, \varepsilon_2}(t) = \frac{d}{dt} f_{\varepsilon_1, \varepsilon_2}(t)$ is such that $\frac{1}{\varepsilon_1 \varepsilon_2} \dot{f} \in \mathcal{S}$.

For every $j \in \mathbb{Z}$, let us introduce the notations

$$\begin{aligned} \Lambda_j &= (j+1)E_1 - jE_2, & \tilde{\phi}_j &= jE_1 - jE_2, \\ \lambda_j &= (j+1)f_1 - jf_2, & \phi_j &= jf_1 - jf_2. \end{aligned} \tag{19}$$

Definition 19. Define the set

$$G = \{\pm Z(\Lambda_p), \pm \cos(\Phi_p)\sigma_z, \pm \sin(\Phi_p)\sigma_z \mid Z \in \{A, B\}, p \in \mathbb{Z}\}.$$

We say that an element of G is oscillating if its associated integer p is different from 0.

Lemma 20. G has the following stability properties:

1. $\forall p \in \mathbb{Z}, \forall X \in G$, $\cos(\Phi_p)X$ and $\sin(\Phi_p)X$ are in $\text{span}_{\mathbb{R}} G$;
2. $\forall X, Y \in G$, $i[X, Y] \in \text{span}_{\mathbb{R}} G$;
3. $\forall X, Y \in G$, $XYX \in \text{span}_{\mathbb{R}} G$.

Proof. The first point is a consequence of the fact that $\{\Phi_p \mid p \in \mathbb{Z}\}$ is a group for the addition. Thus, for every $p, q \in \mathbb{Z}$,

$$2 \cos(\Lambda_p) \cos(\Phi_q) \sigma_z = \cos(\Phi_p + \Phi_q) \sigma_z + \cos(\Phi_p - \Phi_q) \sigma_z \in \text{span}_{\mathbb{R}} G.$$

Moreover, $2 \cos(\Phi_p) A(\Lambda_q) = A(\Lambda_{q+p}) + A(\Lambda_{q-p}) \in \text{span}_{\mathbb{R}} G$. The remaining cases can be checked similarly.

For the second point, for every $E, E', E'' \in \mathbb{R}$,

$$\begin{aligned} i[A(E), A(E')] &= -2 \sin(E - E') \sigma_z, \\ i[A(E), \cos(E') \sigma_z] &= 2 \cos(E') B(E) = B(E + E') + B(E - E'), \\ i[\cos(E') \sigma_z, \cos(E'') \sigma_z] &= 0. \end{aligned}$$

Using the fact that, for every $p \in \mathbb{Z}$, $A(\Lambda_p - \pi/2) = B(\Lambda_p)$, we obtain that $i[A(\Lambda_p), G] \in \text{span}_{\mathbb{R}} G$. Similar results can easily be obtained for $B(\Lambda_p)$, $\cos(\Phi_p) \sigma_z$, and $\sin(\Phi_p) \sigma_z$.

The last point relies on the relations

$$\begin{aligned} A(E)A(E')A(E) &= A(2E - E'), \\ \cos(E')A(E)\sigma_z A(E) &= -\cos(E')\sigma_z, \\ 2 \cos^2(E')\sigma_z A(E)\sigma_z &= A(E) + \frac{1}{2}(A(E + 2E') + A(E - 2E')), \\ 2 \cos^2(E') \cos(E'')\sigma_z^3 &= \left(\cos(E'') + \frac{1}{2}(\cos(2E' + E'') + \cos(2E' - E'')) \right) \sigma_z. \end{aligned}$$

□

Definition 21. Define the vector space \mathcal{E} as the set of entire series in $(\varepsilon_1, \varepsilon_2)$ with coefficients in the set $\text{span}_{\mathcal{S}} G$, i.e.,

$$\left\{ \sum_{j,k \geq 0} \varepsilon_1^j \varepsilon_2^k \sum_{g \in H_{j,k}} s_g g \mid H_{j,k} \subset G \text{ finite, } s_g \in \mathcal{S}, \right. \\ \left. \sum_{j,k \geq 0} \varepsilon_1^j \varepsilon_2^k \sum_{g \in H_{j,k}} |s_g| < \infty \text{ for } (\varepsilon_1, \varepsilon_2) \text{ small enough} \right\}.$$

3.3.1 The elimination procedure

In order to generalize (17), we introduce the operation of elimination of an oscillating term of a coefficient of \mathcal{E} .

Definition 22. Define the operation $\text{Pr} : G \rightarrow G$ by the relations $\text{Pr}(\pm A(\Lambda_p)) = \pm B(\Lambda_p)$, $\text{Pr}(\pm B(\Lambda_p)) = \mp A(\Lambda_p)$, $\text{Pr}(\pm \cos(\Phi_p) \sigma_z) = \pm \sin(\Phi_p) \sigma_z$, and $\text{Pr}(\pm \sin(\Phi_p) \sigma_z) = \mp \cos(\Phi_p) \sigma_z$.

Definition 23. Let $H \in \mathcal{E}$ and $Z(E)$ be an oscillating term of G ($E = \Lambda_p$ if $Z \in \{A, B\}$ or $E = \Phi_p$ if $Z(E) \in \{\cos(E) \sigma_z, \sin(E) \sigma_z\}$). Suppose that $f = \dot{E}$ (which is necessarily slow) is nowhere vanishing. Fix $j \geq 1$, $k \geq 0$, $s \in \mathcal{S}$ and let $c = \varepsilon_1^j \varepsilon_2^k s$. The operation of elimination of $cZ(E)$ from H is defined as

$$\begin{aligned} \text{El}(c, Z(E))(H) &= i \frac{d}{dt} \left[\exp \left(i(c/f) \text{Pr}(Z)(E) \right) \right] \exp \left(-i(c/f) \text{Pr}(Z)(E) \right) \\ &\quad + \exp \left(i(c/f) \text{Pr}(Z)(E) \right) H \exp \left(-i(c/f) \text{Pr}(Z)(E) \right), \quad (20) \\ \tilde{\text{El}}(c, Z(E))(\psi) &= \exp \left(ic/f \text{Pr}(Z)(E) \right) \psi. \end{aligned}$$

In fact, the elimination procedure is the generalization of the change of variables in Equation (17). It transforms the Hamiltonian dynamics $i\frac{d}{dt}\psi = H\psi$ into the dynamics $i\frac{d}{dt}\eta = \text{El}(c, Z(E))(H)\eta$, where $\eta = \widetilde{\text{El}}(c, Z(E))\psi$. The term *elimination* is motivated by the following lemma, stating that the procedure described above generates in the transformed Hamiltonian only terms of degree higher than $\varepsilon_1^j\varepsilon_2^k$.

Lemma 24. *Take $H, Z(E), j, k, c$ as in Definition 23. Then $\text{El}(c, Z(E))(H) \in \mathcal{E}$. Besides, if $H = O(\varepsilon_1)$ then $\text{El}(c, Z(E))(H + cZ(E)) = H + O(\varepsilon_1^{j+1}\varepsilon_2^k)$.*

Proof. First recall that for each matrix M such that $M^2 = I$ and each $c \in \mathbb{R}$, $\exp(icM) = \cos(c)I + i\sin(c)M$. As $A(E)^2 = B(E)^2 = \sigma_z^2 = I$, we can give an explicit expression for $\text{El}(c, Z(E))(H)$.

Let us start from the case $Z(E) = A(\Lambda_p)$, for which we have

$$\text{El}(c, A(\Lambda_p))(H) = J_1 + J_2 + J_3, \quad (21)$$

where

$$\begin{aligned} J_1 &= i\frac{d}{dt}(c/f)\left(-\sin(c/f)I + i\cos(c/f)B(\Lambda_p)\right)\left(\cos(c/f)I - i\sin(c/f)B(\Lambda_p)\right) \\ &= -\frac{d}{dt}(c/f)B(\Lambda_p), \\ J_2 &= -\sin(c/f)\frac{d}{dt}B(\Lambda_p)\left(\cos(c/f)I - i\sin(c/f)B(\Lambda_p)\right) \\ &= -f\sin(c/f)A(\Lambda_p)\left(\cos(c/f)I - i\sin(c/f)B(\Lambda_p)\right), \\ J_3 &= \left(\cos(c/f)I + i\sin(c/f)B(\Lambda_p)\right)H\left(\cos(c/f)I - i\sin(c/f)B(\Lambda_p)\right). \end{aligned}$$

The term J_1 is obviously an element of \mathcal{E} . Besides, $\cos(c/f)$ and $\sin(c/f)$ are entire series in $\varepsilon_1, \varepsilon_2$ with coefficients in \mathcal{S} . Thus,

$$J_2 = -f\sin(c/f)\cos(c/f)A(\Lambda_p) - f\sin^2(c/f)\sigma_z$$

is also an element of \mathcal{E} . The last term to be considered is

$$J_3 = \cos^2(c/f)H + \cos(c/f)\sin(c/f)i[B(\Lambda_p), H] + \sin^2(c/f)B(\Lambda_p)HB(\Lambda_p).$$

Thanks to Lemma 20, J_3 is then the sum of elements of \mathcal{E} .

Let us now assume that $H = O(\varepsilon_1)$ and focus on the order of each term (in the case $Z(E) = A(\Lambda_p)$). We notice that $J_1 = O(\varepsilon_1^{j+1}\varepsilon_2^{k+1})$ as $\frac{d}{dt}(s/f) = O(\varepsilon_1\varepsilon_2)$ and $J_2 = -cA(\Lambda_p) + O(\varepsilon_1^{j+1}\varepsilon_2^k)$. Finally, $J_3 = H + (c/f)i[B(\Lambda_p), H] + O(\varepsilon_1^{j+1}\varepsilon_2^k)$. As $H = O(\varepsilon_1)$, we get $(c/f)i[B(\Lambda_p), H] = O(\varepsilon_1^{j+1}\varepsilon_2^k)$. Thus

$$\text{El}(c, Z(E))(H + cZ(E)) = -cZ(E) + H + cZ(E) + O(\varepsilon_1^{j+1}\varepsilon_2^k).$$

The same computations as above work for the case $Z(E) = B(\Lambda_p)$.

In the case $Z(E) = \cos(\Phi_p)\sigma_z$ we have

$$\text{El}(c, \cos(\Phi_p)\sigma_z)(H) = J_1 + J_2 + J_3, \quad (22)$$

where

$$\begin{aligned} J_1 &= -\frac{d}{dt}(c/f) \sin(\Phi_p) \sigma_z, \\ J_2 &= -c \cos(\Phi_p) \sigma_z, \\ J_3 &= (\cos(c/f \sin(\Phi_p))I + i \sin(c/f \sin(\Phi_p))\sigma_z)H(\cos(c/f \sin(\Phi_p))I - i \sin(c/f \sin(\Phi_p))\sigma_z). \end{aligned}$$

Note that $\sin(c/f \sin(\Phi_p))$ and $\cos(c/f \sin(\Phi_p))$ can be developed as entire series in $\varepsilon_1, \varepsilon_2$ with coefficients in $\mathcal{S} \cos(\Phi_q)$ and $\mathcal{S} \sin(\Phi_q)$ for $q \in \mathbb{Z}$. Lemma 20 ensures that $\text{El}(c, \cos(\Phi_p)\sigma_z)(H)$ is an element of \mathcal{E} . The computations of the order of the terms when $H = O(\varepsilon_1)$ are similar to those made above, and one can apply the same reasoning to $\text{El}(c, \sin(\Phi_p)\sigma_z)(H)$. \square

A key assumption of Lemma 24 above is that f is nowhere vanishing. The following result ensures that this is the case for all frequencies of the oscillating terms in G .

Lemma 25. *Let $j \in \mathbb{Z}$ be nonzero. Then the functions λ_j and ϕ_j , defined as in (19), are nowhere vanishing in $[0, \frac{1}{\varepsilon_1 \varepsilon_2}]$.*

Proof. Let us first prove that

$$2f_1(t) < f_2(t), \quad \forall t \in \left[0, \frac{1}{\varepsilon_1 \varepsilon_2}\right], \quad (23)$$

where we recall that f_1, f_2 are defined in (16). Indeed,

$$2f_1(t) - f_2(t) = 2\alpha - 4E - 2\Delta'(\varepsilon_1 \varepsilon_2 t) - \Delta'(\varepsilon_1 \varepsilon_2 t) < 2v_1 - 4E - 6v_0,$$

where we used the inequality $\alpha < v_1$ and the fact that, according to the hypotheses of Theorem 3, Δ' is increasing from $2v_0$ to $2v_1$. The inequality $2v_1 - 4E - 6v_0 = 2(E + v_1) - 6(E + v_0) \leq 0$, corresponding to the assumption $3(E + v_0) \geq E + v_1$ of Theorem 3, concludes the proof of (23).

Moreover,

$$f_2(t) = 4E + 2\alpha + \Delta'(t) \geq 4(E + v_0) \geq \frac{4(E + v_1)}{3} > 0, \quad \forall t \in \left[0, \frac{1}{\varepsilon_1 \varepsilon_2}\right].$$

In particular, $f_1 - f_2 = -4E - 2\Delta' \leq -4(E + v_0) < 0$. This implies that ϕ_j never vanishes for $j \neq 0$. Finally, for $j > 0$, $\lambda_j = (j + 1)f_1 - jf_2 = (j - 1)(f_1 - f_2) + 2f_1 - f_2 < 0$, and, similarly, $\lambda_j = (j + 1)(f_1 - f_2) + f_2 > 0$ for $j < 0$. \square

3.3.2 Algorithm description

We can now introduce an algorithm to simplify the Hamiltonian H_1 . The cleaning operation $\text{cl}_{\bar{p}}(p_0, q_0)$, with $p_0 \leq \bar{p}$, consists in eliminating from H_1 all oscillating terms of degree $\varepsilon_1^p \varepsilon_2^q$ for

$$\begin{cases} p \leq \bar{p} \\ q < q_0 \end{cases} \quad \text{and} \quad \begin{cases} p \leq p_0 \\ q = q_0 \end{cases}$$

in lexicographic order on (p, q) .

The algorithm is constructed by induction, as follows:

- $\text{cl}_p(0, 0) = H_1$;
- for $0 \leq p' < p$, $\text{cl}_p(p' + 1, q)$ is obtained from $\text{cl}_p(p', q)$ by eliminating one by one all its oscillating terms of degree $(p' + 1, q)$, using Lemma 24;
- $\text{cl}_p(0, q + 1) = \text{cl}_p(p, q)$. Notice that, by construction, there is no term of degree $(0, q + 1)$ in $\text{cl}_p(p, q)$.

Associated with the transformed Hamiltonian $\text{cl}_{p_0}(p, q)$, we define $\tilde{\text{cl}}_{p_0}(p, q)$ the variable obtained iteratively from ψ_1 by applying, at every use of Lemma 24, the corresponding transformation $\tilde{\text{El}}$.

Remark 26. *According to Lemma 24, each elimination procedure produces only terms of higher degree, thus the algorithm yielding $\text{cl}_{p_0}(p, q)$ ends after a finite number of steps.*

When we apply the algorithm, we first deal with monomials of the type $\varepsilon_1^p \varepsilon_2^0$, $p \geq 1$. The following lemma provides a useful property concerning their corresponding coefficients.

Lemma 27. *Define $\mathcal{S}_0 = \{s \in \mathcal{S} \mid s(0) = s(\frac{1}{\varepsilon_1 \varepsilon_2}) = 0\}$. Given $p, p', q \in \mathbb{N}$ with $p' \leq p$, consider the decomposition $\text{cl}_p(p', q) = H_1 + \varepsilon_2 H_2$, where H_1 is an entire series in ε_1 with coefficient in $\text{span}_{\mathcal{S}} G$ and $H_2 \in \mathcal{E}$ (H_1 collects all the monomials of the type $\varepsilon_1^n \varepsilon_2^0$). Then the coefficients of H_1 are in $\text{span}_{\mathcal{S}_0} G$.*

Proof. Let us first consider the case $q = 0$. Then $H = H_1 + \varepsilon_2 H_2$ and we want to eliminate an element $cZ(E)$ with $c = \varepsilon_1^{p+1} s$ and $s \in \mathcal{S}_0$ using Formula (20). Notice that

$$-\frac{d}{dt}(c/f)\text{Pr}(Z)(E) \quad \text{and} \quad \exp\left(i(c/f)\text{Pr}(Z)(E)\right)\varepsilon_2 H_2 \exp\left(-i(c/f)\text{Pr}(Z)(E)\right)$$

only consist of monomials of the type $\varepsilon_1^n \varepsilon_2^m$ with $m \geq 1$.

On the other hand, the terms J_1 and J_2 in Equations (21) and (22) (and the corresponding ones for $Z(E) = B(E)$ and $Z(E) = \sin(E)\sigma_z$) are clearly in $\text{span}_{\mathcal{S}_0} G$. Besides, the coefficients of

$$\exp\left(i(c/f)\text{Pr}(Z)(E)\right)H_1 \exp\left(-i(c/f)\text{Pr}(Z)(E)\right)$$

also stay in $\text{span}_{\mathcal{S}_0} G$, as \mathcal{S}_0 is a subalgebra.

In the case $q \neq 0$, the elimination of a term of degree (p, q) with $q \geq 1$ does not impact the monomials of the type $\varepsilon_1^n \varepsilon_2^0$, according to Lemma 24. \square

Let G_0 be the set of non-oscillating elements of G .

Lemma 28. *Assume that (23) holds. Then we have*

$$\text{cl}_{N_0}(N_0, 1) = \varepsilon_1 H_{N_0} + \varepsilon_1^{N_0+1} H_{r, N_0} + \varepsilon_1^2 \varepsilon_2 H'_{N_0} + \varepsilon_1^{N_0+1} \varepsilon_2 H'_{N_0, r} + \varepsilon_1^3 \varepsilon_2^2 H''_r,$$

where

1. H_{N_0} is a polynomial of degree $N_0 - 1$ in ε_1 with coefficients in $\text{span}_{\mathcal{S}_0} G_0$,
2. H'_{N_0} is a polynomial of degree $N_0 - 2$ in ε_1 with coefficients in $\text{span}_{\mathcal{S}} G_0$,
3. H_{r, N_0} is an entire series in ε_1 with coefficients in $\text{span}_{\mathcal{S}_0} G$,

4. H'_{r,N_0} is an entire series in ε_1 with coefficients in $\text{span}_S G$,

5. H''_r is an entire series in $\varepsilon_1, \varepsilon_2$ with coefficients in $\text{span}_S G$.

Proof. Points 1 and 3 follow from Lemma 27, while points 2, 4, and 5 follow from Lemma 24. \square

Noticing that, in particular, $\text{cl}_{N_0}(N_0, 1) = \varepsilon_1 H_{N_0} + \varepsilon_1^2 \varepsilon_2 H'_{N_0} + O(\varepsilon_1^3 \varepsilon_2^2 + \varepsilon_1^{N_0})$, we introduce the truncation $H_{\text{RWA}} = \varepsilon_1 H_{N_0} + \varepsilon_1^2 \varepsilon_2 H'_{N_0}$ of $\text{cl}_{N_0}(N_0, 1)$ and we denote by ψ_{RWA} the solution of

$$i \frac{d}{dt} \psi_{\text{RWA}} = H_{\text{RWA}} \psi_{\text{RWA}}, \quad \psi_{\text{RWA}}(0) = \psi_{N_0}(0), \quad (24)$$

where $\psi_{N_0} = \widetilde{\text{cl}}_{N_0}(N_0, 1)$. Notice that, even if we are using the same notation ψ_{RWA} , we are considering here a RWA of higher-order than the one discussed in Remark 15.

Lemma 29. *We have the following estimates:*

1. $|\psi_{N_0}(\frac{1}{\varepsilon_1 \varepsilon_2}) - \psi_I(\frac{1}{\varepsilon_1 \varepsilon_2})| = O(\varepsilon_1^2 \varepsilon_2)$;
2. $|\psi_{N_0}(\frac{1}{\varepsilon_1 \varepsilon_2}) - \psi_{\text{RWA}}(\frac{1}{\varepsilon_1 \varepsilon_2})| = O(\varepsilon_1^2 \varepsilon_2 + \varepsilon_1^{N_0-1}/\varepsilon_2)$.

Proof. By Lemma 27, all the changes of variable used for obtaining $\text{cl}_{N_0}(N_0, 0)$ from H_I are of the form $\widetilde{\text{El}}(c, Z(E))(\psi)$ with $c = \varepsilon_1^p s$, $s \in \mathcal{S}_0$. Thus $\psi_I(0) = \widetilde{\text{cl}}(N_0, 0)(0)$ and $\psi_I(\frac{1}{\varepsilon_1 \varepsilon_2}) = \widetilde{\text{cl}}_{N_0}(N_0, 0)(\frac{1}{\varepsilon_1 \varepsilon_2})$. Such changes of variable preserve the state at the initial and final time. After that we applied finitely many changes of variable of the form $\psi \mapsto \exp(i\varepsilon_1^p \varepsilon_2^q s Z(E))\psi$ with $p \geq 2$ and $q = 1$. Thus

$$\sup_{t \in [0, \frac{1}{\varepsilon_1 \varepsilon_2}]} |\widetilde{\text{cl}}_{N_0}(N_0, 0)(t) - \psi_{N_0}(t)| = O(\varepsilon_1^2 \varepsilon_2), \quad (25)$$

which concludes the proof of the first estimate.

Notice that

$$\begin{aligned} \frac{d}{dt} |\psi_{N_0} - \psi_{\text{RWA}}|^2 &= 2 \text{Re} \, i \langle \psi_{N_0} - \psi_{\text{RWA}} | \text{cl}_{N_0}(N_0, 1) \psi_{N_0} - H_{\text{RWA}} \psi_{\text{RWA}} \rangle \\ &= 2 \text{Re} \, i \langle \psi_{N_0} - \psi_{\text{RWA}} | H_{\text{RWA}} (\psi_{N_0} - \psi_{\text{RWA}}) \rangle \\ &\quad + i \langle \psi_{N_0} - \psi_{\text{RWA}} | (\text{cl}_{N_0}(N_0, 1) - H_{\text{RWA}}) \psi_{N_0} \rangle \\ &\leq |\psi_{N_0} - \psi_{\text{RWA}}| O(\varepsilon_1^3 \varepsilon_2^2 + \varepsilon_1^{N_0}). \end{aligned}$$

Thus,

$$2 \frac{d}{dt} |\psi_{N_0} - \psi_{\text{RWA}}| \leq O(\varepsilon_1^3 \varepsilon_2^2 + \varepsilon_1^{N_0}),$$

and we conclude by integrating over $[0, \frac{1}{\varepsilon_1 \varepsilon_2}]$. \square

This concludes the proof of Theorem 16.

3.4 Two scales adiabatic approximation

The goal of this part is to prove the following lemma:

Lemma 30. *There exists $\delta > 0$ such that the solution ψ_{RWA} of (24) satisfies $|\psi_{\text{RWA}}(\frac{1}{\varepsilon_1\varepsilon_2}) - (e^{i\theta}, 0)| \leq M\varepsilon_2/\varepsilon_1$ for some $\theta \in \mathbb{R}$ (possibly depending on $\varepsilon_1, \varepsilon_2, \alpha$) for $(\varepsilon_1, \varepsilon_2) \in (0, \delta)^2$.*

With a slight abuse of notation, let us say in this section that a $(\varepsilon_1, \varepsilon_2)$ -parametric function f is a $O(g(\varepsilon_1, \varepsilon_2))$ (respectively, a $\Omega(g(\varepsilon_1, \varepsilon_2))$) if there exist $M, \delta > 0$ such that

$$\forall \varepsilon_1, \varepsilon_2 \in (0, \delta)^2, \forall s \in [0, 1], |f_{\varepsilon_1, \varepsilon_2}(s)| \leq Mg(\varepsilon_1, \varepsilon_2) \text{ (respectively, } |f_{\varepsilon_1, \varepsilon_2}(s)| \geq Mg(\varepsilon_1, \varepsilon_2)). \quad (26)$$

Recall that

$$H_{\text{RWA}}(t) = \varepsilon_1 h_1(\varepsilon_1 \varepsilon_2 t) A(E_1(t)) + \varepsilon_1^2 h_2(\varepsilon_1 \varepsilon_2 t) B(E_2(t)) + \varepsilon_1^2 h_3(\varepsilon_1 \varepsilon_2 t) \sigma_z,$$

with $h_1, h_2,$ and h_3 given by Theorem 16. We introduce the unitary change of variables $\psi_{\text{slow}}(t) = U(t)\psi_{\text{RWA}}(t)$ with

$$U(t) = \begin{pmatrix} e^{i(\alpha t - \frac{\Delta(\varepsilon_1 \varepsilon_2 t)}{2\varepsilon_1 \varepsilon_2})} & 0 \\ 0 & e^{-i(\alpha t - \frac{\Delta(\varepsilon_1 \varepsilon_2 t)}{2\varepsilon_1 \varepsilon_2})} \end{pmatrix}.$$

The notation ψ_{slow} is motivated by the fact that the Hamiltonian corresponding to its evolution is slow in the sense that it only depends on the *slow variable* $s = \varepsilon_1 \varepsilon_2 t$, also known as *macroscopic* or *reduced time*. More precisely, $i \frac{d}{dt} \psi_{\text{slow}}(t) = H_{\text{slow}}(\varepsilon_1 \varepsilon_2 t) \psi_{\text{slow}}(t)$, where

$$H_{\text{slow}}(s) = \varepsilon_1 h_1(s) \sigma_x + \varepsilon_1^2 h_2(s) \sigma_y + \left(\alpha - \frac{\Delta'(s)}{2} + \varepsilon_1^2 h_3(s) \right) \sigma_z. \quad (27)$$

We cannot directly apply a ‘standard adiabatic theorem’ to describe the evolution of ψ_{slow} because the adiabatic path depends on $(\varepsilon_1, \varepsilon_2)$.

The eigenvalues of $H_{\text{slow}}(s)$ are

$$\pm \omega_{\varepsilon_1, \varepsilon_2}(s) = \pm \sqrt{(\varepsilon_1 h_1(s))^2 + (\varepsilon_1^2 h_2(s))^2 + (\alpha - \Delta'(s)/2 + \varepsilon_1^2 h_3(s))^2}, \quad s \in [0, 1].$$

Using a Taylor series development, we have $\omega_{\varepsilon_1, \varepsilon_2} = \Omega(\varepsilon_1)$. Thus, for $(\varepsilon_1, \varepsilon_2)$ small enough, $\omega_{\varepsilon_1, \varepsilon_2}$ does not vanish. As a consequence, we can introduce the spectral projector $P_{\varepsilon_1, \varepsilon_2}(s)$ of $H_{\text{slow}}(s)$ on the negative eigenvalue. Consider $\gamma_{\varepsilon_1, \varepsilon_2} : [0, 1] \rightarrow S^2$ such that $H_{\text{slow}}(s) = \omega_{\varepsilon_1, \varepsilon_2}(s) \gamma_{\varepsilon_1, \varepsilon_2}(s) \cdot \vec{\sigma}$ where $\vec{a} \cdot \vec{\sigma} = a_1 \sigma_x + a_2 \sigma_y + a_3 \sigma_z$. We want to approximate $P_{\varepsilon_1, \varepsilon_2}$ and its derivatives by the spectral projector on the negative eigenvalue for the simplified Hamiltonian $\tilde{H}_{\text{slow}} = \varepsilon_1 u \sigma_x + (\alpha - \Delta'/2) \sigma_z$ and its derivatives.

Lemma 31. *Let $-\tilde{\omega}_{\varepsilon_1}(s)$ be the negative eigenvalue of the Hamiltonian $\tilde{H}_{\text{slow}}(s) = \varepsilon_1 u(s) \sigma_x + (\alpha - \Delta'(s)/2) \sigma_z$ and $\tilde{P}_{\varepsilon_1}(s)$ be the spectral projector on $-\tilde{\omega}_{\varepsilon_1}(s)$, $s \in [0, 1]$. Then*

- $|P_{\varepsilon_1, \varepsilon_2} - \tilde{P}_{\varepsilon_1}| = O(\varepsilon_1)$,
- $|\frac{d}{ds} P_{\varepsilon_1, \varepsilon_2} - \frac{d}{ds} \tilde{P}_{\varepsilon_1}| = O(1)$,
- $|\frac{d^2}{ds^2} P_{\varepsilon_1, \varepsilon_2} - \frac{d^2}{ds^2} \tilde{P}_{\varepsilon_1}| = O(1/\varepsilon_1)$.

Proof. First, remark that for every nonnegative integer ν

$$\frac{d^\nu}{ds^\nu} H_{\text{slow}}(s) = \frac{d^\nu}{ds^\nu} \tilde{H}_{\text{slow}}(s) + \frac{d^\nu}{ds^\nu} R(\varepsilon_1, \varepsilon_2, s), \quad (28)$$

where $\frac{d^\nu}{ds^\nu} R(\varepsilon_1, \varepsilon_2, s) = O(\varepsilon_1^2)$.

For $H \in i\mathfrak{su}_2 \setminus \{0\}$, define the orthogonal projector $P(H)$ as the projector on the negative eigenvalue of H . The map P is C^∞ and positively homogeneous of degree 0 on $i\mathfrak{su}_2 \setminus \{0\}$.

For every $r > 0$, let B_r be the Euclidean ball of center 0 and radius r in $\mathcal{M}_2(\mathbb{C})$. Denote by \mathcal{K} the compact set $i\mathfrak{su}_2 \cap \partial B_1$. The differential dP is positively homogeneous of degree -1 , since

$$\forall H, h \in i\mathfrak{su}_2, dP_H(h) = dP_{\frac{H}{|H|}} \left(\frac{h}{|H|} \right).$$

As a consequence, for $H \in \mathfrak{su}_2 \setminus B_r$, $|dP_H| \leq \frac{\sup_{L \in \mathcal{K}} |dP_L|}{r}$. Thus, there exists a universal constant $C > 0$ such that P is $\frac{C}{r}$ -Lipschitz continuous on $i\mathfrak{su}_2 \setminus B_r$.

Moreover, consider $r(\varepsilon_1, \varepsilon_2) := \inf_{s \in [0, 1]} \omega_{\varepsilon_1, \varepsilon_2}(s)/2 = \Omega(\varepsilon_1)$. As $H_{\text{slow}} - \tilde{H}_{\text{slow}} = O(\varepsilon_1^2)$, for $\varepsilon_1, \varepsilon_2$ small enough we can assume that the segment $[H_{\text{slow}}(s), \tilde{H}_{\text{slow}}(s)] \cap B_{r(\varepsilon_1, \varepsilon_2)}$ is the empty set for every $s \in [0, 1]$. Then, applying P to the equality (28) for $\nu = 0$, we obtain

$$|P_{\varepsilon_1, \varepsilon_2}(s) - \tilde{P}_{\varepsilon_1}(s)| \leq \frac{C}{r(\varepsilon_1, \varepsilon_2)} |R(\varepsilon_1, \varepsilon_2, s)| \leq M' \varepsilon_1, \quad \forall s \in [0, 1].$$

For the second point, we have $\frac{d}{ds} P_{\varepsilon_1, \varepsilon_2}(s) = dP_{H_{\text{slow}}(s)} \left(\frac{d}{ds} H_{\text{slow}}(s) \right)$. As dP is positively homogeneous of degree -1 , $d^2 P$ is positively homogeneous of degree -2 . Thus $H \mapsto dP_H$ is $\frac{C'}{r^2}$ -Lipschitz continuous on $i\mathfrak{su}_2 \setminus B_r$ with $C' = \sup_{L \in \mathcal{K}} |d^2 P_L|$. Thus, for $\varepsilon_1, \varepsilon_2$ small enough,

$$\left| dP_{H_{\text{slow}}} \left(\frac{d}{ds} H_{\text{slow}} \right) - dP_{\tilde{H}_{\text{slow}}} \left(\frac{d}{ds} H_{\text{slow}} \right) \right| \leq \frac{C'}{r(\varepsilon_1, \varepsilon_2)^2} |H_{\text{slow}} - \tilde{H}_{\text{slow}}|,$$

and

$$\left| dP_{\tilde{H}_{\text{slow}}} \left(\frac{d}{ds} H_{\text{slow}} \right) - dP_{\tilde{H}_{\text{slow}}} \left(\frac{d}{ds} \tilde{H}_{\text{slow}} \right) \right| \leq \frac{C}{r(\varepsilon_1, \varepsilon_2)} \left| \frac{d}{ds} H_{\text{slow}} - \frac{d}{ds} \tilde{H}_{\text{slow}} \right|.$$

Thus we get

$$dP_{H_{\text{slow}}} \left(\frac{d}{ds} H_{\text{slow}} \right) = dP_{\tilde{H}_{\text{slow}}} \left(\frac{d}{ds} \tilde{H}_{\text{slow}} \right) + O(1).$$

The third point is obtained by the same kind of argument. \square

Remark 32. The Hamiltonian $\tilde{H}_{\text{slow}}(s) = \varepsilon_1 u(s) \sigma_x + (\alpha - \Delta'(s)/2) \sigma_z$ is given by the first order RWA. The fact that ε_1 appears in front of the pulse is obviously of utter importance for the estimation of the RWA error but also means that the ‘adiabatic path’ is shrinking to the conical eigenvalue intersection. In fact, it is worse than just the shrinking of the spectral gap, as the derivative of the spectral projector is blowing up near the conical intersection (see Figures 5 and 6).

Define $\tilde{\gamma}_{\varepsilon_1}(s)$, $s \in [0, 1]$, by the relation $\tilde{H}_{\text{slow}}(s) = \tilde{\omega}_{\varepsilon_1}(s) \tilde{\gamma}_{\varepsilon_1}(s) \cdot \vec{\sigma}$ and denote by $(\tilde{\theta}, \tilde{\phi})$ the spherical coordinates of $\tilde{\gamma}_{\varepsilon_1}$. Hence $X = \sin(\tilde{\theta}/2) e_1 - e^{i\tilde{\phi}} \cos(\tilde{\theta}/2) e_2$ is an eigenvector of $\tilde{H}_{\text{slow}}(s)$ associated with the negative eigenvalue and

$$\tilde{P}_{\varepsilon_1} = \begin{pmatrix} \sin^2(\tilde{\theta}/2) & -e^{-i\tilde{\phi}} \sin(\tilde{\theta}/2) \cos(\tilde{\theta}/2) \\ -e^{i\tilde{\phi}} \sin(\tilde{\theta}/2) \cos(\tilde{\theta}/2) & \cos^2(\tilde{\theta}/2) \end{pmatrix}. \quad (29)$$

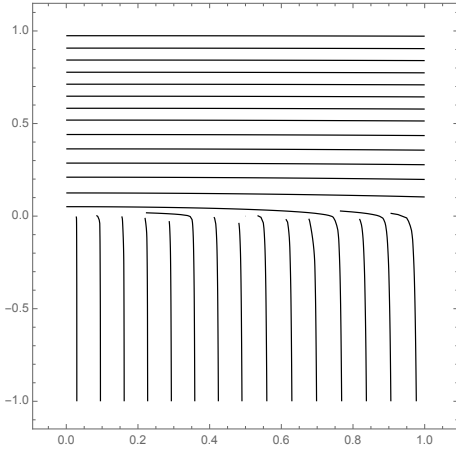


Figure 5: Eigendirection corresponding to the negative eigenvalue of \tilde{H}_{slow} as a function of $(u, \Delta') \in \mathbb{R}^2$, for $\varepsilon_1 = 0.01$ and $\alpha = 0$.

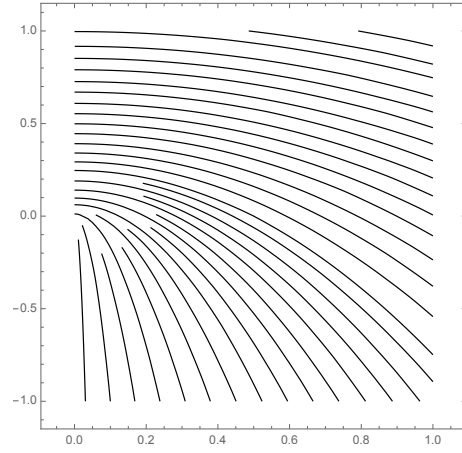


Figure 6: Eigendirection corresponding to the negative eigenvalue of \tilde{H}_{slow} as a function of $(u, \Delta') \in \mathbb{R}^2$, for $\varepsilon_1 = 1$ and $\alpha = 0$.

Lemma 33. *Under the assumptions of Theorem 3, we have:*

1. $|P_{\varepsilon_1, \varepsilon_2}(0) - P_{e_1}| = O(\varepsilon_1^2 \varepsilon_2)$ and $|P_{\varepsilon_1, \varepsilon_2}(1) - P_{e_2}| = O(\varepsilon_1^2 \varepsilon_2)$, where P_{e_i} is the orthogonal projector on $\mathbb{C}e_i$;
2. $\int_0^1 |(\frac{d}{ds} P_{\varepsilon_1, \varepsilon_2})(s)|^2 ds = O(1/\varepsilon_1)$;
3. $\int_0^1 |(\frac{d^2}{ds^2} P_{\varepsilon_1, \varepsilon_2})(s)| ds = O(1/\varepsilon_1)$;
4. $\int_0^1 |\frac{1}{\omega_{\varepsilon_1, \varepsilon_2}(s)^2} \frac{d}{ds} P_{\varepsilon_1, \varepsilon_2}(s)| |\frac{d}{ds} H_{\text{slow}}(s)| ds = O(1/\varepsilon_1^2)$.

Proof. Point 1 is a simple consequence of points 1, 2 and 3 in Theorem 16.

Concerning the other three points, thanks to Lemma 31 we are left to prove the corresponding estimates for $\tilde{P}_{\varepsilon_1, \varepsilon_2}$ and \tilde{H}_{slow} . We recall that $\tilde{\theta}(s) = \arccos\left((\alpha - \Delta'(s)/2)/\tilde{\omega}_{\varepsilon_1}(s)\right)$. We can bound the transverse velocity of $\tilde{\gamma}_{\varepsilon_1}(s)$ by its total velocity

$$|\tilde{\omega}_{\varepsilon_1}(s) \frac{d}{ds} \tilde{\theta}(s)| \leq \sqrt{(\varepsilon_1 \frac{d}{ds} u(s))^2 + (\Delta''(s)/2)^2} = O(1),$$

thus $\frac{d}{ds} \tilde{\theta} = O(1/\varepsilon_1)$.

Using formula (29), it is clear that $|\frac{d}{ds} \tilde{P}_{\varepsilon_1}(s)| \lesssim |\frac{d}{ds} \tilde{\theta}|$ and $|\frac{d^2}{ds^2} \tilde{P}_{\varepsilon_1}(s)| \lesssim |\frac{d}{ds} \tilde{\theta}|^2 + |\frac{d^2}{ds^2} \tilde{\theta}|$, where \lesssim stands for inequality up to an universal multiplicative constant. As $\Delta'' \geq 0$, $\tilde{\theta}$ is increasing and

$$\int_0^1 \left| \frac{d}{ds} \tilde{\theta}(s) \right|^2 ds \leq \sup_{s \in [0,1]} \left| \frac{d}{ds} \tilde{\theta}(s) \right| \int_0^1 \left| \frac{d}{ds} \tilde{\theta}(s) \right| ds \leq \pi \sup_{s \in [0,1]} \left| \frac{d}{ds} \tilde{\theta}(s) \right| = O(1/\varepsilon_1).$$

Moreover, bounding the transverse acceleration of $\tilde{\gamma}_{\varepsilon_1}(s)$ by its total acceleration, we have

$$\left| 2 \frac{d}{ds} \tilde{\omega}_{\varepsilon_1}(s) \frac{d}{ds} \tilde{\theta}(s) - \tilde{\omega}_{\varepsilon_1}(s) \frac{d^2}{ds^2} \tilde{\theta}(s) \right| \leq \sqrt{(\varepsilon_1 \frac{d^2}{ds^2} u(s))^2 + (\Delta'''(s)/2)^2} = O(1).$$

As $\frac{d}{ds}\tilde{\omega}_{\varepsilon_1}(s) \leq \sqrt{(\varepsilon_1 \frac{d}{ds}u(s))^2 + (\Delta''(s)/2)^2} = O(1)$, we have

$$\int_0^1 \left| \frac{d}{ds}\tilde{\omega}_{\varepsilon_1}(s) \frac{d}{ds}\tilde{\theta}(s) \right| = O(1),$$

leading to

$$\int_0^1 \left| \frac{d^2}{ds^2}\tilde{\omega}_{\varepsilon_1}(s) \right| ds = O(1/\varepsilon_1).$$

Concerning point 4, notice the integral $\int_0^1 \left| \frac{1}{\omega_{\varepsilon_1, \varepsilon_2}(s)^2} \frac{d}{ds}P_{\varepsilon_1, \varepsilon_2}(s) \right| \left| \frac{d}{ds}H_{\text{slow}}(s) \right| ds$ can be upper bounded, up to a multiplicative constant, by

$$\int_0^1 \left(\frac{1}{\tilde{\omega}_{\varepsilon_1}(s)^2} \left| \frac{d}{ds}\tilde{\omega}_{\varepsilon_1}(s) \right| \left| \frac{d}{ds}\tilde{\theta}(s) \right| + \frac{1}{\tilde{\omega}_{\varepsilon_1}(s)} \left(\frac{d}{ds}\tilde{\theta}(s) \right)^2 \right) ds,$$

which is of order $1/\varepsilon_1^2$. □

To conclude the proof of Lemma 30, we deduce from [24, Corollary 2.3] the adiabatic estimate

$$\begin{aligned} \left| \psi_{\varepsilon_1, \varepsilon_2}^\alpha \left(\frac{1}{\varepsilon_1 \varepsilon_2} \right) - (e^{i\theta}, 0) \right| &\leq \varepsilon_1 \varepsilon_2 \left[\frac{\left| \frac{d}{ds}P_{\varepsilon_1, \varepsilon_2}(1) \right|}{\omega_{\varepsilon_1, \varepsilon_2}(1)} + \frac{\left| \frac{d}{ds}P_{\varepsilon_1, \varepsilon_2}(0) \right|}{\omega_{\varepsilon_1, \varepsilon_2}(0)} \right. \\ &\quad \left. + \int_0^1 \left(\frac{2 \left| \frac{d}{ds}P_{\varepsilon_1, \varepsilon_2}(s) \right|^2}{\omega_{\varepsilon_1, \varepsilon_2}(s)} + \frac{\left| \frac{d^2}{ds^2}P_{\varepsilon_1, \varepsilon_2}(s) \right|}{\omega_{\varepsilon_1, \varepsilon_2}(s)} + \frac{\left| \frac{d}{ds}P_{\varepsilon_1, \varepsilon_2}(s) \right| \left| \frac{d}{ds}H_{\text{slow}}(s) \right|}{2\omega_{\varepsilon_1, \varepsilon_2}(s)^2} \right) ds \right], \end{aligned}$$

for some $\theta \in \mathbb{R}$. Finally, Lemma 30 together with Theorem 16 conclude the proof of Theorem 3 for a given α and δ . To get uniformity on the range of α , notice that the algorithm does not depend on α elsewhere than in the expression of E_1 and E_2 (see (16)). For the adiabatic part, if we restrict α to a compact interval $I \subset (v_0, v_1)$, the estimates of Lemma 33 can be taken uniform with respect to α . The uniformity with respect to δ is straightforward.

Remark 34. *Now that we have detailed the whole proof, we want to stress some of its key points.*

1. *The changes of variables applied iteratively in order to eliminate the oscillating terms of the Hamiltonian induce a very small error (of order $\varepsilon_2 \varepsilon_1^2$) on the initial and the final state (Lemma 29), whereas the error is of order ε_1 if one look at the entire trajectory.*
2. *The frequencies which appear during the algorithm are of very special type ($pf_1 - pf_2$ and $(p+1)f_1 - pf_2$ for p integer) allowing us to perform as many changes of variables as we need and to give a simple condition implying that all such frequencies are nonzero.*
3. *Each change of variables yields a more complicated Hamiltonian. Fortunately, when we study the adiabatic dynamics of such an Hamiltonian, we can neglect all the terms except for those appearing in the first order RWA.*
4. *The first order RWA induces a population transfer in the limit $\varepsilon_2 \ll \varepsilon_1$.*

4 Numerical simulations

We present in this section some numerical simulations illustrating the results stated in Theorem 3. In all simulations we use the chirp scheme presented in Remark 5 with $E = 1$, $v_0 = -0.5$, and $v_1 = 0.5$.

Figure 7 shows the behavior of the distance from the target state as a function of $\varepsilon_1, \varepsilon_2$ represented in log scale. The AA error appears clearly, reflecting the fact that one needs $\varepsilon_2 \ll \varepsilon_1$ in order to have a fidelity close to 1. The figure also shows that the strategy has better performances than those anticipated theoretically in Theorem 3.

Figure 8 shows the fidelity as a function of α , while ε_1 and ε_2 (and hence \mathcal{T}) are fixed.

Figure 9 shows the fidelity as a function of the reduced time for three values of α , while ε_1 and ε_2 (and hence \mathcal{T}) are fixed. We clearly see that the RWA produces large oscillations (of magnitude of order ε_1), which become much smaller at the endpoints, as described in Remark 34, point 3.

Finally, Figure 10 illustrates the conflict between the AA and RWA. At $\mathcal{T} = 0.05$ fixed, for smaller ε_1 we observe that the RWA is more accurate as the thick line (1st order RWA) is closer to the highly oscillating one (the trajectory $\psi_{\varepsilon_1, \varepsilon_2}^0$). Nevertheless as ε_1 decreases, the ratio $\varepsilon_2/\varepsilon_1$ increases and the AA becomes less accurate.

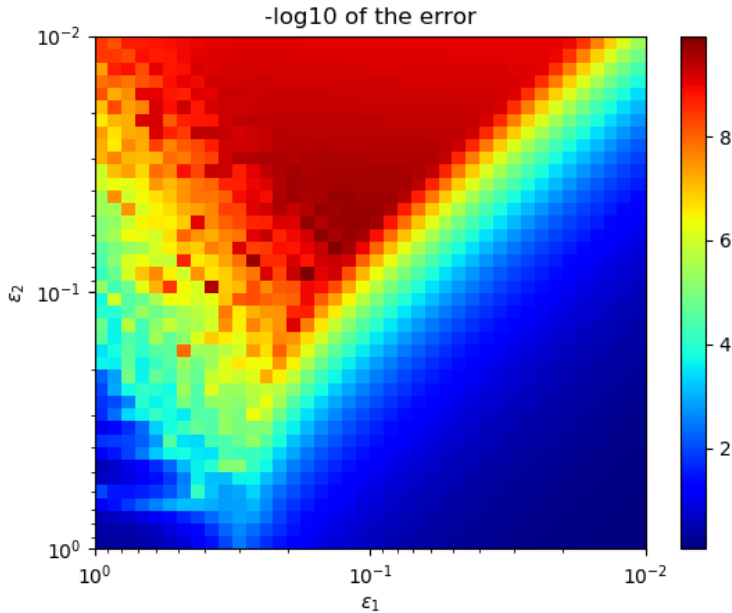


Figure 7: Log of the distance from $\psi_{\varepsilon_1, \varepsilon_2}^0(\frac{1}{\varepsilon_1 \varepsilon_2})$ to the orbit of $(1, 0)$.

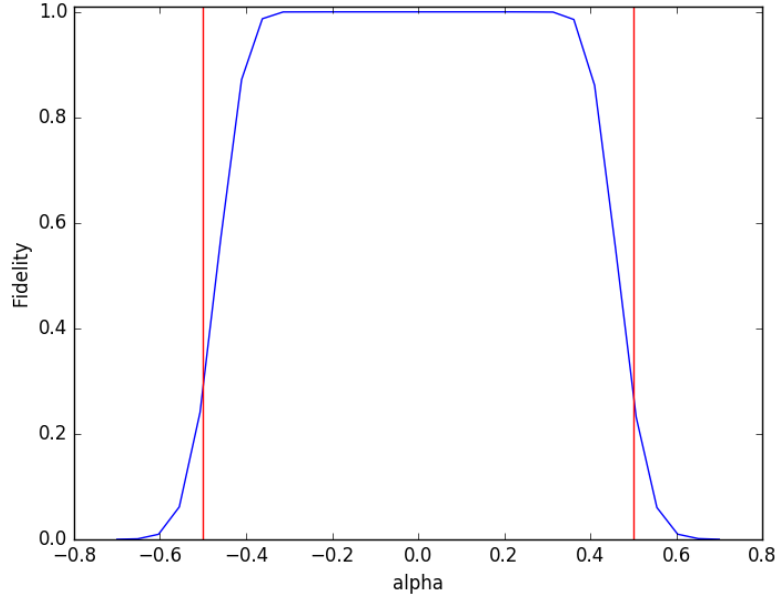


Figure 8: Population transfer as a function of α for $E = 1$, $\varepsilon_1 = 0.5$ and $\varepsilon_2 = 0.1$.

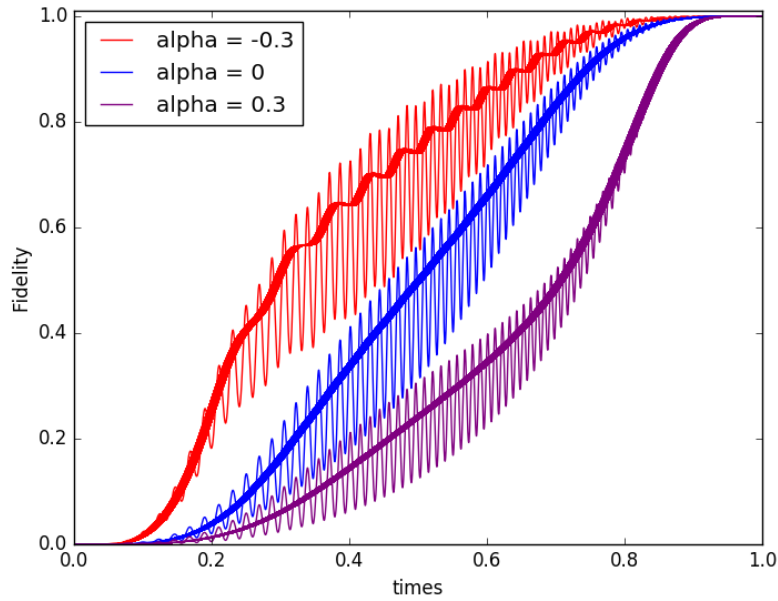


Figure 9: $\varepsilon_1 = 0.5$, $\varepsilon_2 = 0.1$ and $\alpha = 0$. In thick line are the trajectories corresponding to the equivalent 1st order RWA system.

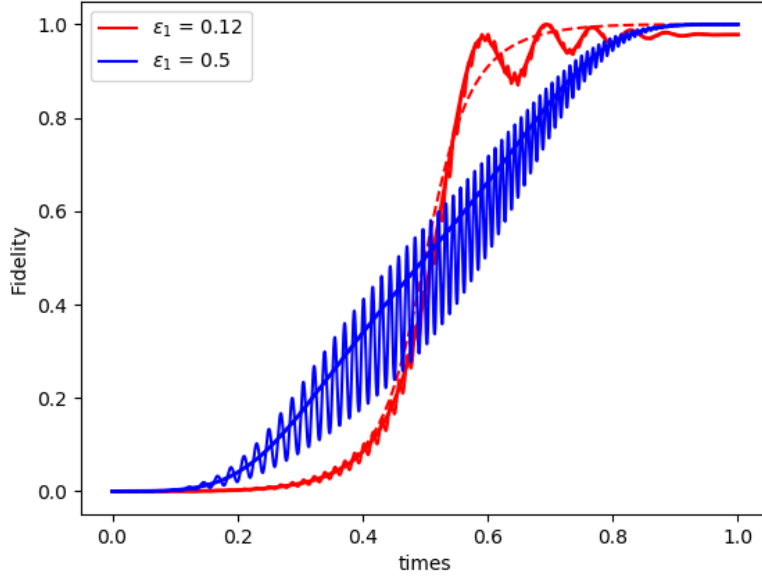


Figure 10: $\varepsilon_1\varepsilon_2 = 0.05$, $\alpha = 0$. In thick line are the trajectories corresponding to the equivalent 1st order RWA system and in dotted line the theoretical AA trajectories.

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