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# On the compatibility of the adiabatic and rotating wave approximations for robust population transfer in qubits

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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 main result gives a precise quantification of the uncertainty interval of the resonance frequency for which the strategy works. We believe that this result, beside its mathematical interest, could be useful in experimental situations.

**Keywords:** spin dynamics, rotating wave approximation, adiabatic approximation

**AMS subject classification:** 35Q41, 81P15, 81Q15, 81Q50

## 1 Introduction

Consider a two-level system described by the Schrödinger equation

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

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  $\alpha$ . The solution of (1) (that depends on  $\alpha$  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  $\alpha$ ) 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  $\varepsilon > 0$  arbitrarily small, find a time  $T$  and an external field  $w : [0, T] \rightarrow \mathbb{R}$  such that*

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

*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 ([6, 11, 12, 13]). As far as we are aware, the problem is open in the case of real-valued functions.

For physicists the approach to overcome this problem consist in the following two steps ([15, 20, 21, 25]):

- use an external field oscillating at the resonance frequency 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  $\alpha$ . This second step substantially exploits the presence of a complex-valued external field and is called adiabatic approximation (AA, for short) [8, 14, 19, 22, 26]. Alternative robust methods are developed, for example, in [9, 24].

However the RWA may affect the precision of the adiabatic strategy, as it has been remarked in [10]. 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  $\alpha$ . 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  $\psi_{w_\varepsilon}$  and  $\psi_{w_\varepsilon^R}$  be the solutions of (2) with initial condition  $\psi_0 \in \mathbb{C}^2$  corresponding to the external fields  $w_\varepsilon$  and  $w_\varepsilon^R$ , 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  $\Delta'$  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 a system driven by two scalar functions  $u(t)$  and  $v(t) = \Delta'(t)/2$ . A more detailed 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, 7, 18]. Thus it is crucial to have a precise quantification of the error.

## 1.2 Adiabatic approximation

Since for  $\varepsilon$  small the solutions of system (2) corresponding to the external fields (3) and (4), starting from the same initial condition, are close, one is lead to work with functions of the type (4), that give rise after a change of variables and a change of time to system (6) in which two real-valued functions are present. Such a system can be easily driven by adiabatic pulses.

As an illustration, let us forget for a second that the system with two external fields comes from the RWA and let us start with the system (2) and the function (4) in which  $\varepsilon = 1$ . Let us consider the case in which the energy of the system is not known precisely. We are then considering the system

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

Let us choose the pulse  $w$  in the form

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

where, as before,  $u(\cdot)$  and  $\Delta(\cdot)$  are two real-valued smooth functions. 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. Let now  $v_0, v_1 \in \mathbb{R}$  be such that  $v_0 < \alpha_0$  and  $\alpha_1 < v_1$  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

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

the adiabatic theorem (see, e.g., [23]) 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  $\Psi$  of system (9) with initial condition  $(0, 1)$  and corresponding to the external field  $(u_\varepsilon, v_\varepsilon)$  satisfies  $|\Psi(T/\varepsilon) - (e^{i\theta}, 0)| \leq C\varepsilon$  for some  $\theta$ .*

Going back to equation (7), the external field 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  $\varepsilon$ . For more details, see [3].

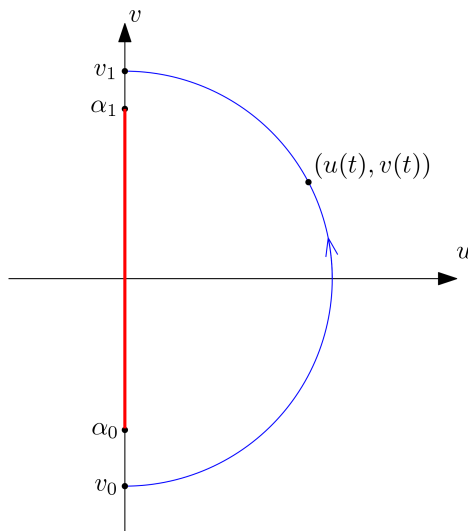


Figure 1: An adiabatic path as the one applied in Proposition 2.

### 1.3 Combination of RWA and AA and statement of the main 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. Let us denote by  $\varepsilon_1$  the small parameter that in the RWA was called  $\varepsilon$  and by  $\varepsilon_2$  what in the AA was called  $\varepsilon$ . A formal cascade of the two approaches yields a path 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  $\varepsilon_1$  and  $\varepsilon_2$  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  $\varepsilon_2$  (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  $\varepsilon_1$  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  $\varepsilon_1$  goes to zero.

As a consequence, this method can only work when  $\alpha = 0$ . Under this restriction, and for suitable relations between  $\varepsilon_1$  and  $\varepsilon_2$  as they both go to zero, the cascade of the two approximations can be proved to work (see [4]).

Another possibility would be to fix  $\varepsilon_1$  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.

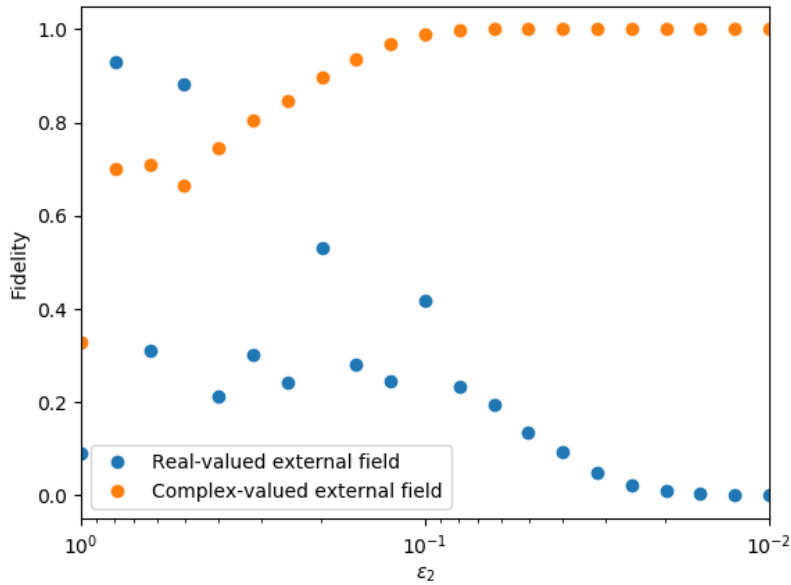


Figure 2: Comparison of the real-valued and complex-valued chirp scheme of the first point of Remark 5 with  $E = 0.75$ ,  $\alpha = 0.25$ ,  $\varepsilon_1 = 1$ ,  $v_0 = -0.5$ ,  $v_1 = 0.5$ . Notice that the assumptions of Theorem 3 are not satisfied.

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  $\varepsilon_2$ . We claim that an external field of the type

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

can induce a transition for the robust population transfer problem, provided that the limits  $\varepsilon_1, \varepsilon_2 \rightarrow 0$  are made in a suitable way and under some further assumptions on the range  $[\alpha_0, \alpha_1]$ . This is detailed in the following theorem, which is the main result of our paper.

**Theorem 3.** *Assume that  $v_0 < 0 < v_1$  are such that  $3(E + v_0) \geq E + v_1$ . Choose  $T$  and  $u, \Delta : [0, T] \rightarrow \mathbb{R}$  smooth enough (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 external field  $w_{\varepsilon_1, \varepsilon_2}$  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  $\delta > 0$  such that for every  $\alpha \in I$  and every  $(\varepsilon_1, \varepsilon_2) \in (0, \delta)^2$ , there exists  $\theta$  such that  $|\psi_{\varepsilon_1, \varepsilon_2}^\alpha(\frac{1}{\varepsilon_1\varepsilon_2}) - (e^{i\theta}, 0)| < C_{N_0} \max(\varepsilon_2/\varepsilon_1, \varepsilon_1^{N_0-1}/\varepsilon_2)$ .

Roughly speaking,  $\varepsilon_2/\varepsilon_1$  is the AA error and  $\varepsilon_1^{N_0-1}/\varepsilon_2$  the RWA error. By playing on the integer  $N_0$  and on the order of magnitude between  $\varepsilon_1$  and  $\varepsilon_2$ , 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.** • *For example, one can use  $T = 1$ ,  $\Delta(s) = \frac{v_0-v_1}{\pi} \sin(\pi s) + (v_0 + v_1)s$  and  $u(s) = 1 - \cos(\pi s)$ ,  $s \in [0, 1]$ , as pulse in Theorem 3. More explicitly,*

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

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

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

- *By taking  $N_0$  large, one can get, for each  $\eta > 0$ , a transition rate of the order  $\mathcal{T}^{-1+\eta}$ , to compare with the standard  $O(\mathcal{T}^{-1})$  of the adiabatic theorem.*
- *The assumption  $3(E + v_0) \geq E + v_1$  can be replaced by the weaker one: for a given  $I \subset (v_0, v_1)$  compact,  $4E + 3\Delta'(s) - 2\alpha > 0$ , for every  $\alpha$  in  $I$  and every  $s$  in  $[0, T]$ . Nevertheless, asking this condition to be valid on every compact interval of  $(v_0, v_1)$  is equivalent to  $3(E + v_0) \geq E + v_1$ . This assumption ensures non-overlapping of some characteristic frequencies (cf. Lemma 18).*

The condition  $3(E + v_0) \geq E + v_1$  linking the frequency of the system with its dispersion is the main contribution of the paper. Numerical simulations suggest that it is sharp in the following sense: if for a given  $\alpha$ ,  $4E + 3\Delta'(s) - 2\alpha < 0$ , an inequality as in Theorem 3 seem not to hold. As an illustration, in Figure 3 we observe that for  $\alpha \geq 0$  (condition  $4E + 3\Delta'(s) - 2\alpha < 0$  not satisfied), the accuracy of the RWA is worse than for  $\alpha < 0$  (condition  $4E + 3\Delta'(s) - 2\alpha < 0$  satisfied).

**Remark 6.** *Many questions remain open considering the use of the RWA and AA. In particular we do not know if a version of Theorem 3 holds with  $\varepsilon_1$  fixed, small enough, and  $\varepsilon_2$  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.*

## 2 Proof of Theorem 3

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

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



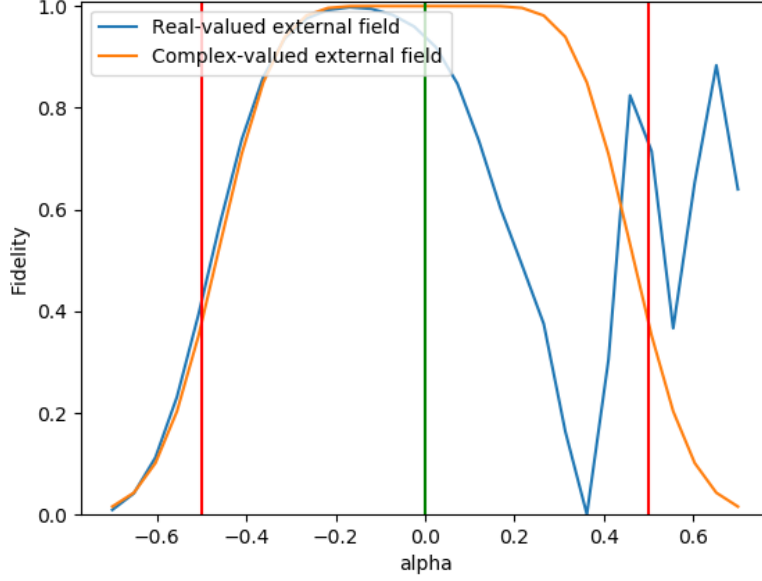


Figure 3:  $E = 0.75$ ,  $\alpha = 0.25$ ,  $\varepsilon_1 = 1$ ,  $\varepsilon_2 = 0.1$ ,  $v_0 = -0.5$ ,  $v_1 = 0.5$ . Assumption  $4E + 3\Delta'(s) - 2\alpha < 0$  is satisfied if and only if  $\alpha < 0$ .

in the interaction frame, set  $\psi_1(t) = e^{i(E+\alpha)\sigma_z t}\psi(t)$  and notice that

$$i\frac{d}{dt}\psi_1 = H_1\psi_1,$$

where

$$\begin{aligned} H_1(t) &= -(E + \alpha)\sigma_z + e^{i(E+\alpha)\sigma_z t} H(t) e^{-i(E+\alpha)\sigma_z t} \\ &= \varepsilon_1 u(\varepsilon_1 \varepsilon_2 t) \begin{pmatrix} 0 & e^{i(2\alpha t - \frac{\Delta(\varepsilon_1 \varepsilon_2 t)}{\varepsilon_1 \varepsilon_2})} + e^{i(4E + 2\alpha t + \frac{\Delta(\varepsilon_1 \varepsilon_2 t)}{\varepsilon_1 \varepsilon_2})} \\ e^{-i(2\alpha t - \frac{\Delta(\varepsilon_1 \varepsilon_2 t)}{\varepsilon_1 \varepsilon_2})} + e^{-i(4E + 2\alpha t + \frac{\Delta(\varepsilon_1 \varepsilon_2 t)}{\varepsilon_1 \varepsilon_2})} & 0 \end{pmatrix}. \end{aligned}$$

We will assume without loss of generality that  $T = 1$ . For readability, define, for every  $t \in [0, \frac{1}{\varepsilon_1 \varepsilon_2}]$ ,

$$E_1(t) = 2\alpha t - \frac{\Delta(\varepsilon_1 \varepsilon_2 t)}{\varepsilon_1 \varepsilon_2}, \quad f_1(t) = \frac{d}{dt} E_1(t), \quad (11)$$

$$E_2(t) = 4Et + 2\alpha t + \frac{\Delta(\varepsilon_1 \varepsilon_2 t)}{\varepsilon_1 \varepsilon_2}, \quad f_2(t) = \frac{d}{dt} E_2(t), \quad (12)$$

without mentioning explicitly the dependence on  $(\alpha, \varepsilon_1, \varepsilon_2)$ . For  $E \in \mathbb{R}$ , define

$$A(E) = \begin{pmatrix} 0 & e^{iE} \\ e^{-iE} & 0 \end{pmatrix}, \quad B(E) = \begin{pmatrix} 0 & -ie^{iE} \\ ie^{-iE} & 0 \end{pmatrix}. \quad (13)$$

In terms of these new notations, we can rewrite  $H_1(t) = \varepsilon_1 u(\varepsilon_1 \varepsilon_2 t) A(E_1(t)) + \varepsilon_1 u(\varepsilon_1 \varepsilon_2 t) A(E_2(t))$ ,  $t \in [0, \frac{1}{\varepsilon_1 \varepsilon_2}]$ .

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., [16] and [17]). Inspired by this, we apply the unitary change of variables

$$\tilde{\psi}_I(t) = \exp\left(i\varepsilon_1 \frac{u(\varepsilon_1\varepsilon_2 t)}{f_2(t)} B(E_2(t))\right) \psi_I(t). \quad (14)$$

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 7.** *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 8.** • 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  $\tilde{\psi}_I(0) = \psi_I(0)$  and  $\tilde{\psi}_I(\frac{1}{\varepsilon_1 \varepsilon_2}) = \psi_I(\frac{1}{\varepsilon_1 \varepsilon_2})$ .

- Let  $\psi_{\text{RWA}}$  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 22). 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  $\varepsilon_1$  is not fixed) as illustrated in Figure 4.

## 2.1 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 (14). At each step, the obtained effective Hamiltonian will be more complicated but will provide 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.

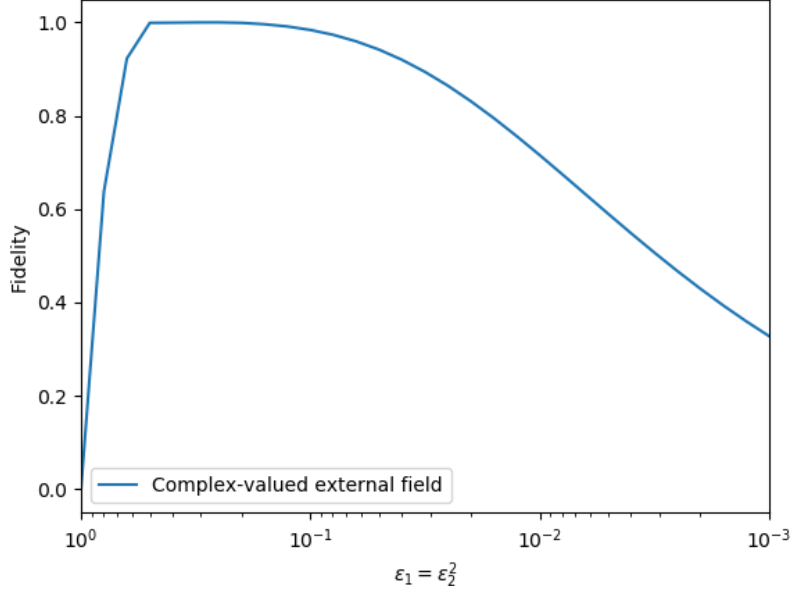


Figure 4: Taking  $v_0 = -0.5$ ,  $v_1 = 0.5$ ,  $E = 0$ , and  $\alpha = 0$ , we observe that the fidelity  $|\langle \psi_{\text{RWA}}(\frac{1}{\varepsilon_1 \varepsilon_2}) | e_2 \rangle|$  does not converge to 1 as  $(\varepsilon_1, \varepsilon_2) \rightarrow 0$  in the regime  $\varepsilon_1 \ll \varepsilon_2$ . The plot corresponds to the choice  $\varepsilon_1 = \varepsilon_2^2$ .

**Theorem 9.** *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  $H_{\text{RWA}}$  of the form*

$$H_{\text{RWA}}(t) = \varepsilon_1 h_1(\varepsilon_1 \varepsilon_2 t) A(E_1(t)) + \varepsilon_1^2 h_2(\varepsilon_1 \varepsilon_2 t) B(E_2(t)) + \varepsilon_1^2 h_3(\varepsilon_1 \varepsilon_2 t) \sigma_z, \quad (15)$$

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  $\psi_{\text{RWA}}$  of the Cauchy problem

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

satisfies  $|\psi_{\text{RWA}}(\frac{1}{\varepsilon_1 \varepsilon_2}) - \psi_I(\frac{1}{\varepsilon_1 \varepsilon_2})| = O(\varepsilon_1^2 \varepsilon_2 + \varepsilon_1^{N_0-1} / \varepsilon_2)$ . 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  $H_{\text{RWA}}$  induces a transition between eigenstates with an error of order  $O(\varepsilon_2 / \varepsilon_1)$ , which will be enough to prove Theorem 3.

## 2.2 The rotating wave approximation

**Definition 10.** 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 7) 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 11.** • The functions  $f_1$  and  $f_2$  defined in (11) and (12) are slow.

- $\mathcal{S}$  is isometric to the Banach algebra  $C^\infty([0, 1], \mathbb{R})$ .
- 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

$$\begin{aligned} \Lambda_j &= (j+1)E_1 - jE_2, & \tilde{\phi}_j &= jE_1 - jE_2, \\ \lambda_j &= (j+1)f_1 - jf_2, & \phi_j &= jf_1 - jf_2. \end{aligned} \quad (16)$$

**Definition 12.** 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 13.**  $G$  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 14.** Define the vector space  $\mathcal{E}$  as the set of entire series in  $(\varepsilon_1, \varepsilon_2)$  whose  $(j, k)$ -th coefficient is in the set  $\text{Span}_{\mathcal{S}}G$ , i.e.,

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

### 2.2.1 The elimination procedure

In order to generalize (14), we introduce the operation of elimination of an oscillating term of a coefficient of  $\mathcal{E}$ .

**Definition 15.** 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 16.** 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

$$\begin{aligned}
\text{El}(c, Z(E))(H) &= i \frac{d}{dt} \left[ \exp \left( i(c/f) \text{Pr}(Z)(E) \right) \right] \exp \left( -i(c/f) \text{Pr}(Z)(E) \right) \\
&\quad + \exp \left( i(c/f) \text{Pr}(Z)(E) \right) H \exp \left( -i(c/f) \text{Pr}(Z)(E) \right), \quad (17) \\
\tilde{\text{El}}(c, Z(E))(\psi) &= \exp \left( ic/f \text{Pr}(Z)(E) \right) \psi.
\end{aligned}$$

In fact, the elimination procedure is the generalization of the change of variables in Equation (14). 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  $\eta = \tilde{\text{El}}(c, Z(E)) \psi$ . 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 17.** Take  $H, Z(E), j, k, c$  as in Definition 16. 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

$$\text{El}(c, A(\Lambda_p))(H) = J_1 + J_2 + J_3, \quad (18)$$

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 13,  $J_3$  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

$$\text{El}(c, \cos(\Phi_p)\sigma_z)(H) = J_1 + J_2 + J_3, \quad (19)$$

$$J_1 = -\frac{d}{dt}(c/f) \sin(\Phi_p)\sigma_z,$$

$$J_2 = -c \cos(\Phi_p)\sigma_z,$$

$$J_3 = (\cos(c/f \sin(\Phi_p))I + i \sin(c/f \sin(\Phi_p))\sigma_z)H(\cos(c/f \sin(\Phi_p))I - i \sin(c/f \sin(\Phi_p))\sigma_z).$$

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 13 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 17 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 18.** *Let  $j \in \mathbb{Z}$  be nonzero. Then the functions  $\lambda_j$  and  $\phi_j$ , defined as in (16), are nowhere vanishing in  $[0, \frac{1}{\varepsilon_1 \varepsilon_2}]$ .*

*Proof.* Let us first prove that

$$2f_1(t) < f_2(t), \quad \forall t \in \left[0, \frac{1}{\varepsilon_1 \varepsilon_2}\right], \quad (20)$$

where we recall that  $f_1, f_2$  are defined in (11), (12). 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,  $\Delta'$  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 (20).

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  $\phi_j$  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  $j < 0$ .  $\square$

### 2.2.2 Algorithm description

We can now introduce an algorithm to simplify the Hamiltonian  $H_I$ . The cleaning operation  $\text{cl}_{\bar{p}}(p_0, q_0)$ , with  $p_0 \leq \bar{p}$ , consists in eliminating from  $H_I$  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:

- $\text{cl}_p(0, 0) = H_I$ ;
- 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 17;
- $\text{cl}_p(0, q + 1) = \text{cl}_p(p, q)$ . 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  $\psi_I$  by applying, at every use of Lemma 17, the corresponding transformation  $\tilde{\text{El}}$ .

**Remark 19.** According to Lemma 17, 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 20.** 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  $\varepsilon_1$  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 (17). 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 (18) and (19) (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 17.  $\square$

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

**Lemma 21.** Assume that (20) 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  $\varepsilon_1$  with coefficients in  $\text{Span}_{\mathcal{S}_0} G_0$ ,
2.  $H'_{N_0}$  is a polynomial of degree  $N_0 - 2$  in  $\varepsilon_1$  with coefficients in  $\text{Span}_{\mathcal{S}} G_0$ ,
3.  $H_{r, N_0}$  is an entire series in  $\varepsilon_1$  with coefficients in  $\text{Span}_{\mathcal{S}_0} G$ ,
4.  $H'_{r, N_0}$  is an entire series in  $\varepsilon_1$  with coefficients in  $\text{Span}_{\mathcal{S}} G$ ,
5.  $H''_r$  is an entire series in  $\varepsilon_1, \varepsilon_2$  with coefficients in  $\text{Span}_{\mathcal{S}} G$ .

*Proof.* Points 1 and 3 follow from Lemma 20, while points 2, 4, and 5 follow from Lemma 17.  $\square$

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  $\psi_{\text{RWA}}$  the solution of

$$i \frac{d}{dt} \psi_{\text{RWA}} = H_{\text{RWA}} \psi_{\text{RWA}}, \quad \psi_{\text{RWA}}(0) = \psi_{N_0}(0), \quad (21)$$

where  $\psi_{N_0} = \widetilde{\text{cl}}_{N_0}(N_0, 1)$ . Notice that, even if we are using the same notation  $\psi_{\text{RWA}}$ , we are considering here a RWA of higher-order than the one discussed in Remark 8.



**Lemma 22.** *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 20, 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

$$\sup_{t \in [0, \frac{1}{\varepsilon_1\varepsilon_2}]} |\widetilde{\text{cl}}_{N_0}(N_0, 0)(t) - \psi_{N_0}(t)| = O(\varepsilon_1^2\varepsilon_2), \quad (22)$$

which concludes the proof of the first estimate.

Notice that

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

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 9.

### 2.3 Two scales adiabatic approximation

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

**Lemma 23.** *There exists  $\delta > 0$  such that the solution  $\psi_{\text{RWA}}$  of (21) 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

$$\forall \varepsilon_1, \varepsilon_2 \in (0, \delta)^2, \forall s \in [0, 1], |f_{\varepsilon_1, \varepsilon_2}(s)| \leq M g(\varepsilon_1, \varepsilon_2) \quad (\text{respectively, } |f_{\varepsilon_1, \varepsilon_2}(s)| \geq M g(\varepsilon_1, \varepsilon_2)). \quad (23)$$

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 9. 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  $\psi_{\text{slow}}$  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

$$H_{\text{slow}}(s) = \varepsilon_1 h_1(s) \sigma_x + \varepsilon_1^2 h_2(s) \sigma_y + \left( \alpha - \frac{\Delta'(s)}{2} + \varepsilon_1^2 h_3(s) \right) \sigma_z. \quad (24)$$

We cannot directly apply a ‘standard adiabatic theorem’ to describe the evolution of  $\psi_{\text{slow}}$  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 24.** *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  $\nu$

$$\frac{d^\nu}{ds^\nu} H_{\text{slow}}(s) = \frac{d^\nu}{ds^\nu} \tilde{H}_{\text{slow}}(s) + \frac{d^\nu}{ds^\nu} R(\varepsilon_1, \varepsilon_2, s), \quad (25)$$

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  $C^\infty$  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 (25) 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  $-1$ ,  $d^2P$  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  $C' = \sup_{L \in \mathcal{K}} |d^2P_L|$ . 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 25.** *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  $\varepsilon_1$  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

$$\tilde{P}_{\varepsilon_1} = \begin{pmatrix} \sin^2(\tilde{\theta}/2) & -e^{-i\tilde{\phi}} \sin(\tilde{\theta}/2) \cos(\tilde{\theta}/2) \\ -e^{i\tilde{\phi}} \sin(\tilde{\theta}/2) \cos(\tilde{\theta}/2) & \cos^2(\tilde{\theta}/2) \end{pmatrix}. \quad (26)$$

**Lemma 26.** *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.  $\int_0^1 \left| \left( \frac{d}{ds} P_{\varepsilon_1, \varepsilon_2} \right)(s) \right|^2 ds = O(1/\varepsilon_1)$ ;
3.  $\int_0^1 \left| \left( \frac{d^2}{ds^2} P_{\varepsilon_1, \varepsilon_2} \right)(s) \right| ds = O(1/\varepsilon_1)$ ;
4.  $\int_0^1 \left| \frac{1}{\omega_{\varepsilon_1, \varepsilon_2}(s)^2} \frac{d}{ds} P_{\varepsilon_1, \varepsilon_2}(s) \right| \left| \frac{d}{ds} H_{\text{slow}}(s) \right| ds = O(1/\varepsilon_1^2)$ .

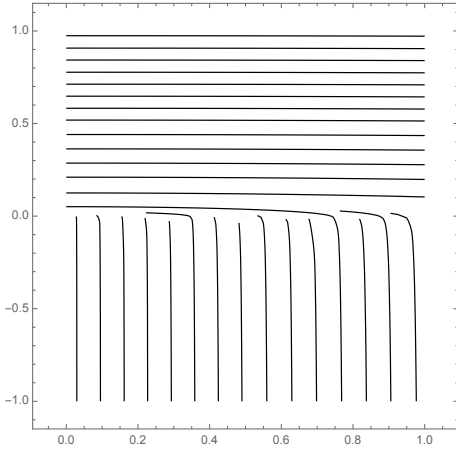


Figure 5: Eigendirection corresponding to the negative eigenvalue of  $\tilde{H}_{\text{slow}}$  as a function of  $(u, \Delta') \in \mathbb{R}^2$ , for  $\varepsilon_1 = 0.01$  and  $\alpha = 0$ .

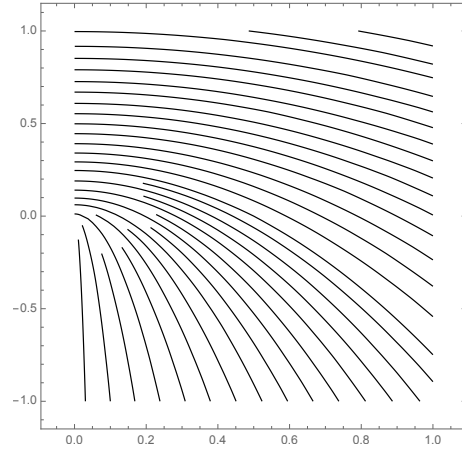


Figure 6: Eigendirection corresponding to the negative eigenvalue of  $\tilde{H}_{\text{slow}}$  as a function of  $(u, \Delta') \in \mathbb{R}^2$ , for  $\varepsilon_1 = 1$  and  $\alpha = 0$ .

*Proof.* Point 1 is a simple consequence of points 1, 2 and 3 in Theorem 9.

Concerning the other three points, thanks to Lemma 24 we are left to prove the corresponding estimates for  $\tilde{P}_{\varepsilon_1, \varepsilon_2}$  and  $\tilde{H}_{\text{slow}}$ . 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

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

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

Using formula (26), 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  $1/\varepsilon_1^2$ .  $\square$

To conclude the proof of Lemma 23, we deduce from [23, 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 23 together with Theorem 9 conclude the proof of Theorem 3 for a given  $\alpha$ . To get uniformity on the range of  $\alpha$ , notice that the algorithm does not depend on  $\alpha$  elsewhere than in the expression of  $E_1$  and  $E_2$  (see (11) and (12)). For the adiabatic part, if we restrict  $\alpha$  to a compact interval  $I \subset (v_0, v_1)$ , the estimates of Lemma 26 can be taken uniform with respect to  $\alpha$ .

**Remark 27.** *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 22), whereas the error is of order  $\varepsilon_1$  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  $\varepsilon_2 \ll \varepsilon_1$ .*

### 3 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  $\alpha$ , while  $\varepsilon_1$  and  $\varepsilon_2$  (and hence  $\mathcal{T}$ ) are fixed.

Figure 9 shows the fidelity as a function of the reduced time for three values of  $\alpha$ , while  $\varepsilon_1$  and  $\varepsilon_2$  (and hence  $\mathcal{T}$ ) are fixed. We clearly see that the RWA produces large oscillations (of magnitude of order  $\varepsilon_1$ ), which become much smaller at the endpoints, as described in Remark 27, point 3.

Finally, Figure 10 illustrates the conflict between the AA and RWA. At  $\mathcal{T} = 0.05$  fixed, for smaller  $\varepsilon_1$  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  $\varepsilon_1$  decreases, the ratio  $\varepsilon_2/\varepsilon_1$  increases and the AA becomes less accurate.

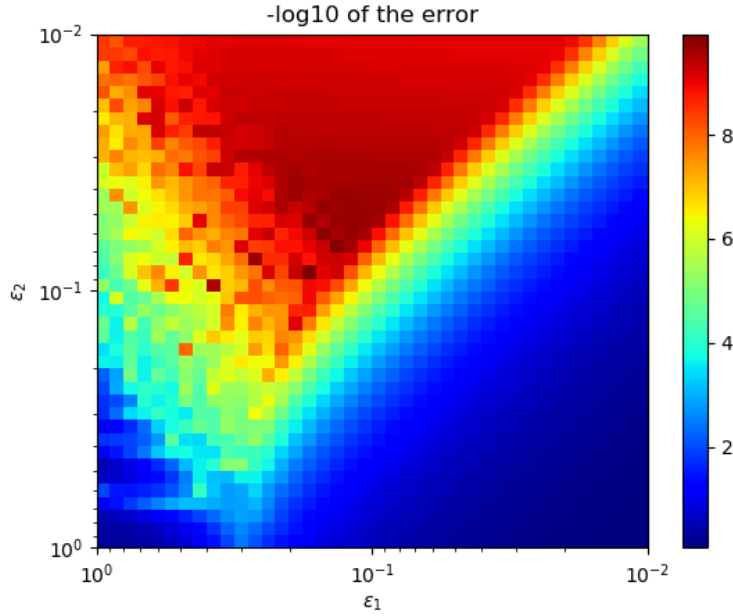


Figure 7: Log of the distance from  $\psi_{\varepsilon_1, \varepsilon_2}^0(\frac{1}{\varepsilon_1 \varepsilon_2})$  to the orbit of  $(1, 0)$ .

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## References

- [1] A. A. Agrachev and Y. L. Sachkov. *Control theory from the geometric viewpoint*, volume 87 of *Encyclopaedia of Mathematical Sciences*. Springer-Verlag, Berlin, 2004. Control Theory and Optimization, II.

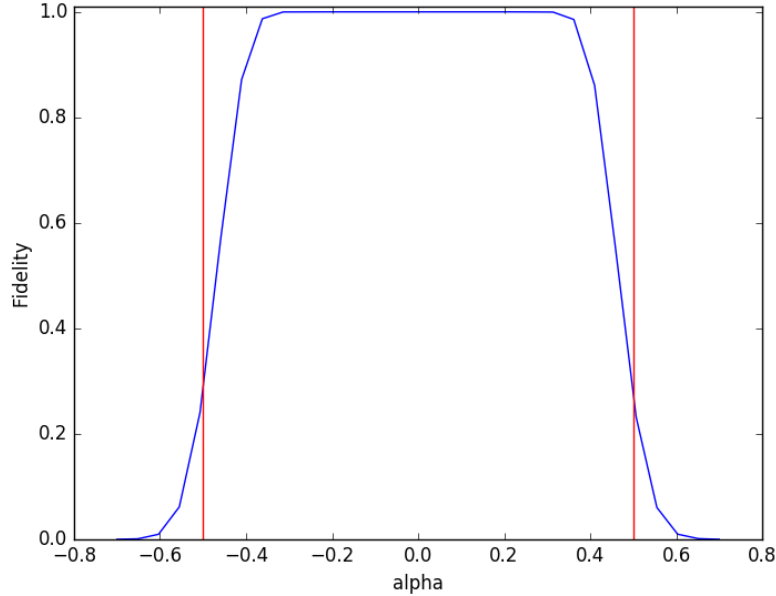


Figure 8: Population transfer as a function of  $\alpha$  for  $E = 1$ ,  $\varepsilon_1 = 0.5$  and  $\varepsilon_2 = 0.1$ .

- [2] S. Ashhab, J. R. Johansson, A. M. Zagoskin, and F. Nori. Two-level systems driven by large-amplitude fields. *Phys. Rev. A*, 75:063414, Jun 2007.
- [3] N. Augier, U. Boscain, and M. Sigalotti. Adiabatic ensemble control of a continuum of quantum systems. *SIAM J. Control Optim.*, 56(6):4045–4068, 2018.
- [4] N. Augier, U. Boscain, and M. Sigalotti. On the compatibility between the adiabatic and the rotating wave approximations in quantum control. In *Proceedings of the 58th IEEE Conference on Decision and Control*, 2019.
- [5] N. Augier, U. Boscain, and M. Sigalotti. Semi-conical eigenvalue intersections and the ensemble controllability problem for quantum systems. *Math. Control Relat. Fields*, to appear.
- [6] K. Beauchard, J.-M. Coron, and P. Rouchon. Controllability issues for continuous-spectrum systems and ensemble controllability of Bloch equations. *Comm. Math. Phys.*, 296(2):525–557, 2010.
- [7] X. Cao, J. Q. You, H. Zheng, A. G. Kofman, and F. Nori. Dynamics and quantum zeno effect for a qubit in either a low- or high-frequency bath beyond the rotating-wave approximation. *Phys. Rev. A*, 82:022119, Aug 2010.
- [8] M. Garwood and L. DelaBarre. The return of the frequency sweep: Designing adiabatic pulses for contemporary NMR. *Journal of magnetic resonance (San Diego, Calif.: 1997)*, 153:155–77, 01 2002.

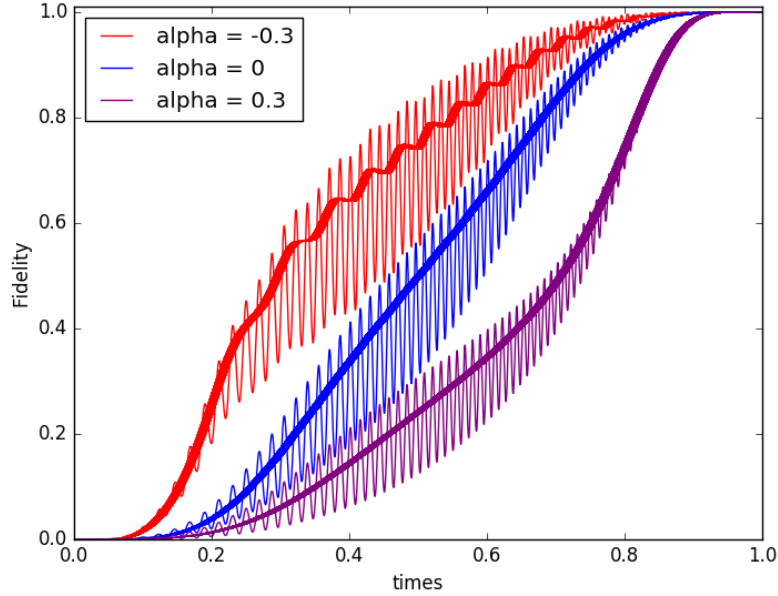


Figure 9:  $\varepsilon_1 = 0.5$ ,  $\varepsilon_2 = 0.1$  and  $\alpha = 0$ . In thick line are the trajectories corresponding to the equivalent 1st order RWA system.

- [9] H. Jo, H.-g. Lee, S. Gurin, and J. Ahn. Robust two-level system control by a detuned and chirped laser pulse. *Physical Review A*, 96(3), Sep 2017.
- [10] Z. Leghtas, A. Sarlette, and P. Rouchon. Adiabatic passage and ensemble control of quantum systems. *Journal of Physics B*, 44(15), 2011.
- [11] J.-S. Li and N. Khaneja. Control of inhomogeneous quantum ensembles. *Phys. Rev. A*, 73:030302, 2006.
- [12] J.-S. Li and N. Khaneja. Ensemble control of Bloch equations. *IEEE Trans. Automat. Control*, 54(3):528–536, 2009.
- [13] U. A. Maciel Neto, P. S. Pereira da Silva, K. Beauchard, and P. Rouchon.  $H^1$ -control of an ensemble of half-spin systems replacing Rabi pulses by adiabatic following. In *Proceedings of the 58th IEEE Conference on Decision and Control*, 2019.
- [14] V. Malinovsky and J. Krause. General theory of population transfer by adiabatic rapid passage with intense, chirped laser pulses. *Eur. Phys. J. D*, 1450:147–155, 05 2001.
- [15] M. H. Mittleman. *Introduction to the theory of laser-atom interactions*. Springer Science & Business Media, 2013.
- [16] P. Rouchon. Quantum systems and control 1. *Revue Africaine de la Recherche en Informatique et Mathématiques Appliquées*, Volume 9, Conference in Honor of Claude Lobry, 2008.



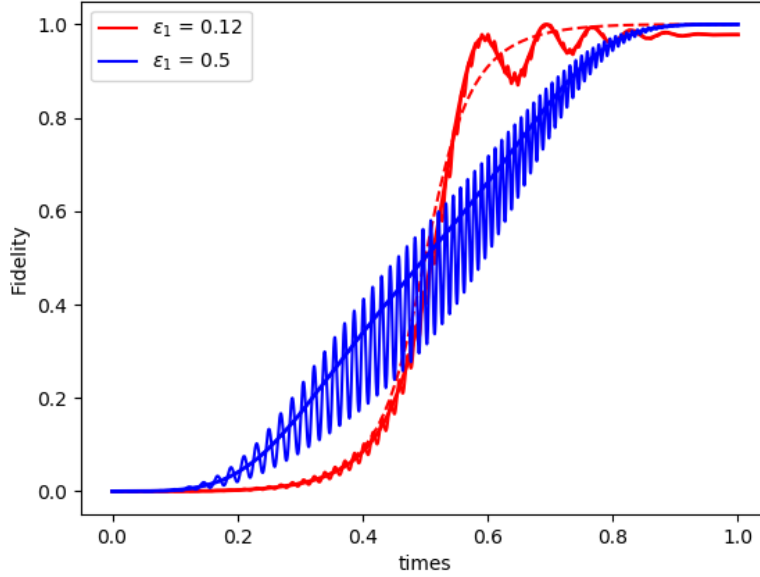


Figure 10:  $\varepsilon_1\varepsilon_2 = 0.05$ ,  $\alpha = 0$ . In thick line are the trajectories corresponding to the equivalent 1st order RWA system and in dotted line the theoretical AA trajectories.

- [17] J. Sanders, F. Verhulst, and J. Murdock. *Averaging methods in nonlinear dynamical systems*. Number 59 in Applied Mathematical Sciences. Springer, 2007.
- [18] J. Scheuer, X. Kong, R. S. Said, J. Chen, A. Kurz, L. Marseglia, J. Du, P. R. Hemmer, S. Montangero, T. Calarco, B. Naydenov, and F. Jelezko. Precise qubit control beyond the rotating wave approximation. *New Journal of Physics*, 16(9):093022, sep 2014.
- [19] P. Shapiro, Moshe; Brumer. *Quantum Control of Molecular Processes*. John Wiley & Sons, Ltd, 2012.
- [20] B. Shore. Coherent manipulations of atoms using laser light. *Acta Physica Slovaca*, 58, 07 2008.
- [21] B. W. Shore. *Manipulating Quantum Structures Using Laser Pulses*. Cambridge University Press, 2011.
- [22] C.-M. Simon, T. Belhadj, B. Chatel, T. Amand, P. Renucci, A. Lemaitre, O. Krebs, P. A. Dalgarno, R. J. Warburton, X. Marie, and B. Urbaszek. Robust quantum dot exciton generation via adiabatic passage with frequency-swept optical pulses. *Phys. Rev. Lett.*, 106:166801, Apr 2011.
- [23] S. Teufel. *Adiabatic perturbation theory in quantum dynamics*, volume 1821 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin, 2003.
- [24] B. T. Torosov, S. Guérin, and N. V. Vitanov. High-fidelity adiabatic passage by composite sequences of chirped pulses. *Phys. Rev. Lett.*, 106:233001, Jun 2011.

- [25] N. V. Vitanov, M. Fleischhauer, B. W. Shore, and K. Bergmann. Coherent manipulation of atoms and molecules by sequential laser pulses. *Advances in Atomic Molecular and Optical Physics*, 46:55–190, Jan. 2001.
- [26] Y. Wu, I. M. Piper, M. Ediger, P. Brereton, E. R. Schmidgall, P. R. Eastham, M. Hugues, M. Hopkinson, and R. T. Phillips. Population inversion in a single InGaAs quantum dot using the method of adiabatic rapid passage. *Phys. Rev. Lett.*, 106:067401, Feb 2011.