

Adiabatic theorem for bipartite quantum systems in weak coupling limit

David Viennot and Lucile Aubourg

Institut UTINAM (CNRS UMR 6213, Université de Franche-Comté), 41bis Avenue de l'Observatoire, BP1615, 25010 Besançon cedex, France

E-mail: david.viennot@utinam.cnrs.fr

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Abstract

We study the adiabatic approximation of the dynamics of a bipartite quantum system with respect to one of its components, when the coupling between the two components is perturbative. We show that the density matrix of the considered component is described by adiabatic transport formulae exhibiting operator-valued geometric and dynamical phases. The present results can be used to study the quantum control of the dynamics of qubits and of open quantum systems where the two components are the system and its environment. We treat two examples, the control of an atomic qubit interacting with another one and the control of a spin in the middle of a Heisenberg spin chain.

Keywords: geometric phase, adiabatic approximation, bipartite quantum system

(Some figures may appear in colour only in the online journal)

1. Introduction

A bipartite quantum system consists of two quantum subsystems denoted by S and \mathcal{E} and described by the Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_{\mathcal{E}}$. We are interested only in the behaviour of the component S with a loss of the information concerning the component \mathcal{E} . If $\psi \in \mathcal{H}_S \otimes \mathcal{H}_{\mathcal{E}}$ is the state of the bipartite system, the subsystem S is described by the density matrix (the mixed state) $\rho = \text{tr}_{\mathcal{E}} |\psi\rangle\langle\psi|$ (where $\langle\cdot|\langle\cdot|$ denotes the inner product of $\mathcal{H}_S \otimes \mathcal{H}_{\mathcal{E}}$) where the partial trace $\text{tr}_{\mathcal{E}}$ on $\mathcal{H}_{\mathcal{E}}$ suppresses the information concerning \mathcal{E} . ρ takes into account the entanglement of S with \mathcal{E} . An interesting problem in the dynamics of a bipartite quantum system is the control of the component S 'hampered' by \mathcal{E} . Quantum control has potentially many applications in nanoscience and in quantum computing. A problem of quantum control consists in finding out how to act on S (by laser fields, magnetic fields, etc) in order for S to

evolve from its initial state ρ_0 to a predetermined target state ρ_{target} (the goal of the control). The presence of \mathcal{E} can considerably modify the control problem with regard to the control of a pure state in \mathcal{H}_S for S alone. Moreover the control can affect \mathcal{E} directly or indirectly by the coupling between \mathcal{E} and S . The understanding of the dynamics of S in contact with \mathcal{E} is crucial.

Such a situation occurs in quantum information theory where S and \mathcal{E} are two qubits of a quantum computer or two ensembles of qubits. In this case the control consists in performing a logical gate or a quantum algorithm on S in the presence of other qubits (\mathcal{E}) of the quantum computer. In this example, S and \mathcal{E} have similar sizes and the roles of S and \mathcal{E} can be exchanged. However, dynamics of bipartite quantum systems also occur in the control of open quantum systems where S is a small subsystem and \mathcal{E} is a large environment responsible for decoherence effects on S . In this case the loss of information models the observer's lack of knowledge concerning \mathcal{E} due to its large size and its complexity.

An adiabatic approach [1] can be used to describe quantum control, since the variations of the control parameters are often slow. Quantum control schemes based on the adiabatic approximation have been proposed for different closed systems [2–5]. For open quantum systems, adiabatic approaches based on non-hermitian Hamiltonians have been studied [6–8]. For example, the Lindblad equation (a Markovian approximation of the dynamics of S in the environment [9]) is considered as a non-hermitian Schrödinger equation in the Hilbert–Schmidt space (the so-called Liouville space describing the square trace class operators of \mathcal{H}_S , i.e. $\text{tr}_S(A^\dagger A) < \infty$). In these cases the adiabatic approximation is based on adiabatic theorems for non-self-adjoint Hamiltonians [10–12]. However, these works do not focus on the bipartite aspect of quantum dynamics, which has been studied by Sjöqvist *et al* with the viewpoint of nonadiabatic geometric phases [13–15]. Recently operator-valued geometric phases have been proposed as generalizations of the Sjöqvist geometric phases, in the context of cyclic (nonadiabatic) evolutions [16] and of adiabatic evolutions [17, 18]. Nevertheless a rigorous study of the adiabatic regime of a bipartite quantum system exhibiting operator-valued geometric phases has never been realized.

The goal of this paper is to show that, under common assumptions concerning the evolution of the bipartite system, the evolution of the density matrix satisfies adiabatic transport formulae exhibiting operator-valued geometric (and dynamical) phases. Section 2 establishes adiabatic theorems with regard to a discussion concerning the different time scales involved in the dynamics of a bipartite quantum system. In particular we consider two adiabatic regimes. These results are based on the Nenciu adiabatic theorem [19], which considers spectral components and not only one eigenvalue. Adiabatic transport formulae for the density matrix are obtained in section 3. We show that these formulae (for the weak adiabatic regime) exhibit operator-valued geometric phases similar to the ones introduced in the previous works [13–18]. The generator of the operator-valued dynamical phase also exhibited by these formulae can appear as an effective Hamiltonian of S dressed by \mathcal{E} . The adiabatic transport of the density matrix for the second order perturbative expansion satisfies a kind of effective Lindblad equation. We discuss also in this section the specific case of the open quantum systems where \mathcal{E} is a thermal bath. Throughout this paper we consider the case of a weak coupling between S and \mathcal{E} . Indeed to enlighten the individual behaviour of the component S inside the bipartite system through the viewpoint of the adiabatic approximation, it is necessary to explain the relation between the eigenvectors of the bipartite system and the eigenvectors of its component S . This requires a perturbative analysis. Finally section 4 presents two examples: a qubit realized as a two level atom in a laser field in the rotating wave approximation with a perturbative interaction with another atom; and a spin

controlled by a magnetic field in the middle of a ferromagnetic spin chain with Heisenberg coupling between the nearest neighbours.

2. Strong and weak adiabatic theorems

2.1. Preliminary discussion

We consider a bipartite quantum system of Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_E$ governed by the time-dependent Hamiltonian

$$H(t) = H_S(t) \otimes 1_E + 1_S \otimes H_E(t) + \epsilon V(t) \quad (1)$$

where $H_S \in \mathcal{L}(\mathcal{H}_S)$ is the self-adjoint Hamiltonian of the component S , $H_E \in \mathcal{L}(\mathcal{H}_E)$ is the self-adjoint Hamiltonian of the component E , $V \in \mathcal{L}(\mathcal{H}_S \otimes \mathcal{H}_E)$ is the coupling operator between S and E , and $\epsilon \in \mathcal{V}(0)$ is a perturbative parameter ($\mathcal{V}(0)$ denotes the neighbourhood of 0). Let $\{\mu_b\}_b$ and $\{\nu_\beta\}_\beta$ be the pure point spectra of H_S and H_E (for the sake of simplicity we suppose that all these eigenvalues are not globally degenerate, e.g. these eigenvalues are nondegenerate for all $t > 0$ except possibly for a finite number of isolated moments t_*) and $\{\zeta_b\}_b$ and $\{\xi_\beta\}_\beta$ be the associated normalized eigenvectors. The eigenvalues are supposed to be at least C^0 and the eigenvectors at least C^1 with respect to t .

$$H_S(t)\zeta_b(t) = \mu_b(t)\zeta_b(t) \quad \zeta_b \in \mathcal{H}_S, \mu_b \in \mathbb{R} \quad (2)$$

$$H_E(t)\xi_\beta(t) = \nu_\beta(t)\xi_\beta(t) \quad \xi_\beta \in \mathcal{H}_E, \nu_\beta \in \mathbb{R}. \quad (3)$$

Let $\{\lambda_{b\beta}\}_{b,\beta}$ be the perturbed pure point spectrum of H and $\{\phi_{b\beta}\}_{b,\beta}$ be the associated eigenvectors.

$$H(t)\phi_{b\beta}(t) = \lambda_{b\beta}(t)\phi_{b\beta}(t) \quad \phi_{b\beta} \in \mathcal{H}_S \otimes \mathcal{H}_E, \lambda_{b\beta} \in \mathbb{R} \quad (4)$$

$$\lim_{\epsilon \rightarrow 0} \phi_{b\beta}(t) = \zeta_b(t) \otimes \xi_\beta(t) \quad (5)$$

$$\lim_{\epsilon \rightarrow 0} \lambda_{b\beta}(t) = \mu_b(t) + \nu_\beta(t) \quad (6)$$

(with the quantum state limit defined with the norm topology associated with $\langle\langle \cdot | \cdot \rangle\rangle$). The first order approximations (by using the Rayleigh–Schrödinger perturbation method) are

$$\lambda_{b\beta} = \mu_b + \nu_\beta + \epsilon V_{b\beta,b\beta} + \mathcal{O}(\epsilon^2) \quad (7)$$

$$\phi_{b\beta} = \zeta_b \otimes \xi_\beta + \epsilon \sum_{(c\gamma) \neq (b\beta)} \frac{V_{c\gamma,b\beta}}{\mu_b - \mu_c + \nu_\beta - \nu_\gamma} \zeta_c \otimes \xi_\gamma + \mathcal{O}(\epsilon^2) \quad (8)$$

where $V_{c\gamma,b\beta} = \langle\langle \zeta_c \otimes \xi_\gamma | V | \zeta_b \otimes \xi_\beta \rangle\rangle$. We consider the dynamics of the bipartite system starting from $\phi_{a\alpha}$, i.e.

$$i\hbar \frac{d\psi(t)}{dt} = H(t)\psi(t) \quad \psi(0) = \phi_{a\alpha}(0). \quad (9)$$

From the viewpoint of the control of S , there are three time scales:

- T , the total duration of the evolution (the duration of the control);
- τ_S , the quantum proper time characterizing the transition of S from ζ_a to another eigenvector, induced by the control (the Rabi period of the first transition involving ζ_a , e.g. $\tau_S = \sup_{t \in [0, T]} \max_{b \neq a} \frac{\hbar}{|\mu_b - \mu_a|}$);

- θ^ϵ , the time characterizing the perturbation of S by \mathcal{E} .

We remark that the non-self-adjoint models [10–12] also exhibit three time scales (the duration of the evolution, the time characterizing the quantum transitions, and the time characterizing the dissipation—the inverse of the resonance width). There are then three adiabatic regimes:

- $\tau_S \ll \theta^\epsilon$ and $\tau_S \ll T$ (very strong adiabatic regime);
- $\tau_S \sim \theta^\epsilon$ and $\theta^\epsilon \ll T$ (strong adiabatic regime);
- $\tau_S \sim \theta^\epsilon$ and $\theta^\epsilon \sim T$, the evolution of \mathcal{E} being assumed to be very strongly adiabatic (weak adiabatic regime).

More precisely, consider the nonadiabatic couplings (for $(b\beta) \neq (a\alpha)$):

$$\left\langle\left\langle \phi_{a\alpha} \left| \dot{\phi}_{b\beta} \right. \right\rangle\right\rangle = \frac{\hbar}{T(\lambda_{b\beta} - \lambda_{a\alpha})} \left\langle\left\langle \phi_{a\alpha} \left| \hbar^{-1} H' \right. \right| \phi_{b\beta} \right\rangle\right\rangle \quad (10)$$

where a dot denotes the derivative with respect to t and a prime denotes the derivative with respect to the reduced time $s = t/T$. If $\forall b \neq a$, $\inf_{t \in [0, T]} |\mu_b - \mu_a| = \mathcal{O}(1)$ ($\Leftrightarrow \tau_S \ll \theta^\epsilon$, $\mathcal{O}(1)$ means a gap condition very large with respect to ϵ —a value of zero order in ϵ) then

$$\begin{aligned} \frac{\hbar}{T(\lambda_{b\beta} - \lambda_{a\alpha})} &= \frac{\hbar}{T(\mu_b - \mu_a) \left(1 + \frac{\nu_\beta - \nu_\alpha}{\mu_b - \mu_a} \right)} \\ &\quad - \frac{\hbar \epsilon (V_{b\beta, b\beta} - V_{a\alpha, a\alpha})}{T(\mu_b - \mu_a)^2 \left(1 + \frac{\nu_\beta - \nu_\alpha}{\mu_b - \mu_a} \right)^2} + \mathcal{O}(\epsilon^2). \end{aligned} \quad (11)$$

By assuming that $\Delta = \inf_{t \in [0, T]} \min_{\beta \neq \alpha} \max_{b \neq a} \left| 1 + \frac{\nu_\beta - \nu_\alpha}{\mu_b - \mu_a} \right| = \mathcal{O}(1)$ (no resonance between a transition of S from ζ_a and a transition of \mathcal{E} from ξ_a) we have

$$\left| \frac{\hbar}{T(\lambda_{b\beta} - \lambda_{a\alpha})} \right| \leq \frac{\tau_S}{T\Delta} + \frac{\tau_S^2}{T\theta^\epsilon \Delta^2} + \mathcal{O}(\epsilon^2) \quad (12)$$

with $\tau_S = \sup_{t \in [0, 1]} \max_{b \neq a} \frac{\hbar}{|\mu_b - \mu_a|}$ and $\theta^\epsilon = \inf_{t \in [0, T]} \min_{(b\beta) \neq (a\alpha)} \frac{\hbar}{\epsilon |V_{b\beta, b\beta} - V_{a\alpha, a\alpha}|}$. If T is chosen like $\tau_S \ll T$, then $\forall (b\beta) \neq (a\alpha)$, $|\langle\langle \phi_{a\alpha} | \dot{\phi}_{b\beta} \rangle\rangle| \ll 1$. All nonadiabatic couplings being negligible, we can think that the system remains projected only onto $\phi_{a\alpha}(t)$ during the whole dynamics. This is the very strong adiabatic regime which corresponds to an adiabatic evolution of the whole bipartite system. Now if $\inf_{t \in [0, T]} \min_{b \neq a} |\mu_b - \mu_a| = \mathcal{O}(\epsilon)$ ($\Leftrightarrow \tau_S \sim \theta^\epsilon$) we have the following.

- If $\alpha \neq \beta$ and $\inf_{t \in [0, T]} |\nu_\beta - \nu_\alpha| = \mathcal{O}(1)$:

$$\begin{aligned} \frac{\hbar}{T(\lambda_{b\beta} - \lambda_{a\alpha})} &= \frac{\hbar}{T(\nu_\beta - \nu_\alpha)} \\ &\quad - \frac{\hbar \epsilon (\tilde{\mu}_b - \tilde{\mu}_a + V_{b\beta, b\beta} - V_{a\alpha, a\alpha})}{T(\nu_\beta - \nu_\alpha)^2} + \mathcal{O}(\epsilon^2) \end{aligned} \quad (13)$$

where $\tilde{\mu}_b = \frac{\mu_b}{\epsilon}$ ($\inf_{t \in [0, T]} \min_{b \neq a} |\tilde{\mu}_b - \tilde{\mu}_a| = \mathcal{O}(1)$).

- If $\alpha = \beta$ or $\exists t_*$ such that $\nu_\beta(t_*) = \nu_\alpha(t_*)$: since $\lambda_{b\beta} = \epsilon(\tilde{\mu}_b + V_{b\beta,b\beta}) + \nu_\beta$ we have

$$\frac{\hbar}{T(\lambda_{b\beta} - \lambda_{a\alpha})} = \frac{\hbar}{T\epsilon(\tilde{\mu}_b - \tilde{\mu}_a + V_{b\beta,b\beta} - V_{a\alpha,a\alpha})} \quad (14)$$

for all t if $\alpha = \beta$ or only at $t = t_*$.

We have the following.

- If $\alpha \neq \beta$ and $\inf_{t \in [0, T]} |\nu_\beta - \nu_\alpha| = \mathcal{O}(1)$:

$$\left| \frac{\hbar}{T(\lambda_{b\beta} - \lambda_{a\alpha})} \right| \leq \frac{\tau_\mathcal{E}}{T} + \frac{\tau_\mathcal{E}^2}{T\theta^\epsilon} + \mathcal{O}(\epsilon^2). \quad (15)$$

- If $\alpha = \beta$ or $\exists t_*$ such that $\nu_\beta(t_*) = \nu_\alpha(t_*)$:

$$\left| \frac{\hbar}{T(\lambda_{b\beta} - \lambda_{a\alpha})} \right| \leq \frac{\tau_S^\epsilon}{T} \quad (16)$$

for all t if $\alpha = \beta$ or only at $t = t_*$.

Here $\tau_\mathcal{E} = \sup_{t \in [0, T]} \max_{\beta \neq \alpha} \frac{\hbar}{|\nu_\beta - \nu_\alpha|}$, $\theta^\epsilon = \inf_{t \in [0, T]} \min_{(b\beta) \neq (a\alpha)} \frac{\hbar}{\epsilon(\tilde{\mu}_b - \tilde{\mu}_a + V_{b\beta,b\beta} - V_{a\alpha,a\alpha})}$ and $\tau_S^\epsilon = \sup_{t \in [0, T]} \max_{\beta \neq \alpha} \frac{\hbar}{\epsilon(\tilde{\mu}_b - \tilde{\mu}_a + V_{b\beta,b\beta} - V_{a\alpha,a\alpha})}$ (τ_S^ϵ is the time characterizing the transition of S from ζ_a to another eigenvector induced by the action of \mathcal{E} on S). If T and ϵ are chosen such that $\theta^\epsilon \sim \tau_S^\epsilon \ll T$, then $\forall (b\beta) \neq (a\alpha)$, $|\langle\langle \phi_{a\alpha} | \dot{\phi}_{b\beta} \rangle\rangle| \ll 1$. In this strong adiabatic regime, as in the very strong adiabatic regime, the system remains projected only onto $\phi_{a\alpha}(t)$ during the whole dynamics. In contrast, if T and ϵ are chosen such that $\theta^\epsilon \sim \tau_S^\epsilon \sim T$, then $\forall \beta \neq \alpha$, $|\langle\langle \phi_{a\alpha} | \dot{\phi}_{b\beta} \rangle\rangle| \ll 1$ if we assume that $\tau_\mathcal{E} \ll T$, but $|\langle\langle \phi_{a\alpha} | \dot{\phi}_{b\alpha} \rangle\rangle| \ll 1$. In this weak adiabatic regime, the system remains projected onto the space spanned by the eigenvectors related to ξ_a , but transitions between the eigenstate related to ζ_a and an eigenstate related to another ζ_b are possible due to nonadiabatic transitions induced by \mathcal{E} on S (and not directly by the control).

In the strong and the very strong adiabatic regimes S and \mathcal{E} evolve adiabatically with regard to the control (and S evolves adiabatically with regard to \mathcal{E} in the very strong adiabatic regime). In the weak adiabatic regime, only \mathcal{E} evolves adiabatically with regard to the control, then the evolution of S can be richer and it is in this case that the adiabatic transport of the density matrix can potentially exhibit operator-valued phases. We note that this weak adiabatic regime is more interesting from the viewpoint of the quantum control. Indeed, in general, quantum control problems are characterized by the condition $H(T) = H(0)$ since we start and end with the control system off. This induces $\phi_{a\alpha}(T) = \phi_{a\alpha}(0)$ and in the strong and the very strong adiabatic regimes we have $\rho(T) = \rho(0)$. In contrast due to the possible transitions in the weak adiabatic regime, which are characterized by an operator-valued phase $U \in \mathcal{U}(\mathcal{H}_S)$, we can have $\rho(T) = U\rho(0)U^\dagger$ ($\mathcal{U}(\mathcal{H}_S)$ denotes the set of unitary operators of \mathcal{H}_S). The answer to the control problem consists then in finding the time dependent modulation of the control system such that U transforms $\rho(0)$ to ρ_{target} (or at least such that $\|U\rho(0)U^\dagger - \rho_{\text{target}}\|$ is minimal). The assumption stating that the evolution of \mathcal{E} must be adiabatic is natural in this context, since it corresponds to requiring that transitions in \mathcal{E} do not hamper the adiabatic control by generating kinematic decoherence (see section 3.7 and [20]).

The discussion presented here is heuristic; the following section presents rigorous results.

2.2. Adiabatic theorems

Theorem 1 (Strong adiabatic theorem for bipartite quantum systems). *Let $[0, 1] \ni s \mapsto H(s) = H_S(s) \otimes 1_{\mathcal{E}} + 1_S \otimes H_{\mathcal{E}}(s) + \epsilon V(s)$ be a family of self-adjoint Hamiltonians of a bipartite quantum system such that $\forall T > 0$, $i\hbar\psi'(s) = TH(s)\psi(s)$ has continuous solutions in the norm topology, and such that V is $(H_S \otimes 1_{\mathcal{E}} + 1_S \otimes H_{\mathcal{E}})$ bounded. Let $\{\mu_b\}_b$ and $\{\nu_\beta\}_\beta$ be the pure point spectra of H_S and $H_{\mathcal{E}}$ and $\{\zeta_b\}_b$ and $\{\xi_\beta\}_\beta$ be the associated normalized eigenvectors. Let $\{\phi_{b\beta}\}_{b\beta}$ be the normalized eigenvectors of H continuously linked to $\{\zeta_b \otimes \xi_\beta\}_{b\beta}$ when $\epsilon \rightarrow 0$ (in the norm topology). We consider the case where $\psi(0) = \phi_{\alpha\alpha}(0)$. For the sake of simplicity we suppose that each eigenvalue is nondegenerate and that H_S and $H_{\mathcal{E}}$ do not have continuous spectra. We assume the following conditions.*

- (i) $\forall b, \beta, s \mapsto \mu_b(s)$ and $s \mapsto \nu_\beta(s)$ are C^1 ; $s \mapsto \zeta_b(s)$ and $s \mapsto \xi_\beta(s)$ are C^2 in the norm topology.
- (ii) No resonance between transitions of S and \mathcal{E} involving $\zeta_\alpha \otimes \xi_\alpha$ occurs, i.e. $\forall s \in [0, 1]$, $\forall (b\beta) \neq (\alpha\alpha)$, $\mu_b(s) + \nu_\beta(s) + \epsilon V_{b\beta}(s) \neq \mu_\alpha(s) + \nu_\alpha(s) + \epsilon V_{\alpha\alpha}(s)$.
- (iii) The perturbed energies of S satisfy a gap condition of order ϵ with μ_α :

$$\inf_{s \in [0,1]} \min_{(b\beta) \neq (\alpha\alpha)} \left| \mu_b(s) + \epsilon V_{b\beta}(s) - \mu_\alpha(s) - \epsilon V_{\alpha\alpha}(s) \right| = \mathcal{O}(\epsilon). \quad (17)$$

Then we have

$$\forall s \in [0, 1], \quad P_{\alpha\alpha}(s)\psi(s) = \psi(s) + \mathcal{O}\left(\frac{1}{T\epsilon}\right) \quad (18)$$

with $P_{\alpha\alpha}(s) = |\phi_{\alpha\alpha}(s)\rangle\langle\phi_{\alpha\alpha}(s)|$ the orthogonal projection onto $\phi_{\alpha\alpha}$.

We remark that we can also write $P_{\alpha\alpha}(s)\psi(s) = \psi(s) + \mathcal{O}\left(\frac{\theta^\epsilon}{T}\right)$.

Proof. $\forall s \in [0, 1]$, $(\phi_{d\delta}(s))_{d,\delta}$ being a complete basis of the domain of $H(s)$, we can write

$$\psi(s) = \sum_{d\delta} c_{d\delta}(s) e^{-i\hbar^{-1}T \int_0^s \lambda_{d\delta}(\sigma) d\sigma} \phi_{d\delta}(s) \quad (19)$$

for some $c_{d\delta}(s) \in \mathbb{C}$. By injecting this expression into the Schrödinger equation $i\hbar\psi' = TH\psi$ and projecting the result onto $\phi_{b\beta}(s)$, we find

$$c'_{b\beta}(s) = - \sum_{d\delta} c_{d\delta}(s) e^{i\hbar^{-1}T \int_0^s (\lambda_{b\beta}(\sigma) - \lambda_{d\delta}(\sigma)) d\sigma} \left\langle \phi_{b\beta}(s) \left| \phi'_{d\delta}(s) \right. \right\rangle. \quad (20)$$

By an integration of this expression with respect to s , we find

$$\begin{aligned} c_{b\beta}(s) &= c_{b\beta}(0) \\ &- \sum_{d\delta} \int_0^s c_{d\delta}(\sigma) e^{i\hbar^{-1}T \int_0^\sigma (\lambda_{b\beta}(\zeta) - \lambda_{d\delta}(\zeta)) d\zeta} \left\langle \phi_{b\beta}(\sigma) \left| \phi'_{d\delta}(\sigma) \right. \right\rangle d\sigma. \end{aligned} \quad (21)$$

With an integration by parts we have

$$\begin{aligned}
 c_{b\beta}(s) &= c_{b\beta}(0) - \int_0^s c_{b\beta}(\sigma) \left\langle \left\langle \phi_{b\beta}(\sigma) \left| \phi'_{b\beta}(\sigma) \right. \right\rangle \right\rangle d\sigma \\
 &\quad - \sum_{(d\delta) \neq (b\beta)} \left[\left[\frac{c_{d\delta}(\sigma) \left\langle \left\langle \phi_{b\beta}(\sigma) \left| \phi'_{d\delta}(\sigma) \right. \right\rangle \right\rangle}{i\hbar^{-1}T(\lambda_{b\beta}(\sigma) - \lambda_{d\delta}(\sigma))} e^{i\hbar^{-1}T \int_0^\sigma (\lambda_{b\beta}(\xi) - \lambda_{d\delta}(\xi)) d\xi} \right]_0^s \right. \\
 &\quad \left. + \int_0^s \frac{e^{i\hbar^{-1}T \int_0^\sigma (\lambda_{b\beta}(\xi) - \lambda_{d\delta}(\xi)) d\xi}}{i\hbar^{-1}T} \left(\frac{c_{d\delta}(\sigma) \left\langle \left\langle \phi_{b\beta}(\sigma) \left| \phi'_{d\delta}(\sigma) \right. \right\rangle \right\rangle}{(\lambda_{b\beta}(\sigma) - \lambda_{d\delta}(\sigma))} \right)' d\sigma \right]. \tag{22}
 \end{aligned}$$

By a first order perturbation we have $\forall (d\delta) \neq (a\alpha)$

$$\lambda_{a\alpha} - \lambda_{d\delta} = \mu_a - \mu_d + \nu_\alpha - \nu_\delta + \epsilon (V_{a\alpha, a\alpha} - V_{d\delta, d\delta}) + \mathcal{O}(\epsilon^2). \tag{23}$$

Because of the gap and the no resonance conditions, at least $|\lambda_{a\alpha} - \lambda_{d\delta}| = \mathcal{O}(\epsilon)$ even if $\alpha = \delta$ or $\exists s_*$ such that $\nu_\delta(s_*) = \nu_\alpha(s_*)$. All the other quantities appearing in equation (22) are bounded. Indeed, the eigenvectors being \mathcal{C}^2 , $\phi'_{d\delta}$ and $\phi''_{d\delta}$ are defined and bounded on $[0, 1]$ ($\sup_{s \in [0,1]} \|\phi'_{d\delta}\| < +\infty$ and $\sup_{s \in [0,1]} \|\phi''_{d\delta}\| < +\infty$); the eigenvalues being \mathcal{C}^1 , $\lambda'_{d\delta}$ is defined and is bounded on $[0, 1]$ ($\sup_{s \in [0,1]} |\lambda'_{d\delta}| < +\infty$); moreover $c_{d\delta} < 1$ and is \mathcal{C}^1 (because $c_{d\delta} = e^{i\hbar^{-1}T \int_0^s \lambda_{d\delta} d\sigma} \langle \langle \phi_{d\delta} | \psi \rangle \rangle$ with ψ which is \mathcal{C}^1 as a solution of the Schrödinger equation). It follows that

$$\left| \frac{c_{d\delta} \left\langle \left\langle \phi_{b\beta} \left| \phi'_{d\delta} \right. \right\rangle \right\rangle}{i\hbar^{-1}T} \right| \leq \frac{\sup_{s \in [0,1]} \|\phi'_{d\delta}\|}{\hbar^{-1}T} = \mathcal{O}\left(\frac{1}{T}\right) \tag{24}$$

implying that the third term of equation (22) is $\mathcal{O}\left(\frac{1}{T\epsilon}\right)$.

$$\begin{aligned}
 \left(\frac{c_{d\delta} \left\langle \left\langle \phi_{b\beta} \left| \phi'_{d\delta} \right. \right\rangle \right\rangle}{i\hbar^{-1}T(\lambda_{b\beta} - \lambda_{d\delta})} \right)' &= \frac{c'_{d\delta} \left\langle \left\langle \phi_{b\beta} \left| \phi'_{d\delta} \right. \right\rangle \right\rangle}{i\hbar^{-1}T(\lambda_{b\beta} - \lambda_{d\delta})} \\
 &\quad + \frac{c_{d\delta} \left\langle \left\langle \phi'_{b\beta} \left| \phi'_{d\delta} \right. \right\rangle \right\rangle}{i\hbar^{-1}T(\lambda_{b\beta} - \lambda_{d\delta})} \\
 &\quad + \frac{c_{d\delta} \left\langle \left\langle \phi_{b\beta} \left| \phi''_{d\delta} \right. \right\rangle \right\rangle}{i\hbar^{-1}T(\lambda_{b\beta} - \lambda_{d\delta})} \\
 &\quad - \frac{(\lambda'_{b\beta} - \lambda'_{d\delta}) c_{d\delta} \left\langle \left\langle \phi_{b\beta} \left| \phi'_{d\delta} \right. \right\rangle \right\rangle}{i\hbar^{-1}T(\lambda_{b\beta} - \lambda_{d\delta})^2} \tag{25}
 \end{aligned}$$

then

$$\left| \frac{c'_{d\delta} \left\langle \left\langle \phi_{b\beta} \left| \phi'_{d\delta} \right. \right\rangle \right\rangle}{i\hbar^{-1}T} \right| \leq \frac{\sup_{s \in [0,1]} |c'_{d\delta}| \sup_{s \in [0,1]} \|\phi'_{d\delta}\|}{\hbar^{-1}T} = \mathcal{O}\left(\frac{1}{T}\right) \tag{26}$$

$$\left| \frac{c_{d\delta} \langle\langle \phi'_{b\beta} | \phi'_{d\delta} \rangle\rangle}{i\hbar^{-1}T} \right| \leq \frac{\sup_{s \in [0,1]} \|\phi'_{b\beta}\| \sup_{s \in [0,1]} \|\phi'_{d\delta}\|}{\hbar^{-1}T} = \mathcal{O}\left(\frac{1}{T}\right) \quad (27)$$

$$\left| \frac{c_{d\delta} \langle\langle \phi_{b\beta} | \phi''_{d\delta} \rangle\rangle}{i\hbar^{-1}T} \right| \leq \frac{\sup_{s \in [0,1]} \|\phi''_{d\delta}\|}{\hbar^{-1}T} = \mathcal{O}\left(\frac{1}{T}\right) \quad (28)$$

$$\begin{aligned} \left| \frac{(\lambda'_{b\beta} - \lambda'_{d\delta}) c_{d\delta} \langle\langle \phi_{b\beta} | \phi'_{d\delta} \rangle\rangle}{i\hbar^{-1}T} \right| &\leq \frac{\sup_{s \in [0,1]} |\lambda'_{b\beta} - \lambda'_{d\delta}| \sup_{s \in [0,1]} \|\phi'_{d\delta}\|}{\hbar^{-1}T} \\ &= \mathcal{O}\left(\frac{1}{T}\right). \end{aligned} \quad (29)$$

This implies that the fourth term of equation (22) is $\mathcal{O}\left(\frac{1}{T\epsilon}\right)$. Finally for $(b\beta) = (a\alpha)$ we have

$$c_{a\alpha}(s) = 1 - \int_0^s c_{a\alpha}(\sigma) \langle\langle \phi_{a\alpha}(\sigma) | \phi'_{a\alpha}(\sigma) \rangle\rangle d\sigma + \mathcal{O}\left(\frac{1}{T\epsilon}\right) \quad (30)$$

and for $\forall (b\beta) \neq (a\alpha)$ we have

$$c_{b\beta}(s) = - \sum_{(d\delta) \neq (a\alpha)} \int_0^s c_{d\delta}(\sigma) e^{i\hbar^{-1}T \int_0^\sigma (\lambda_{b\beta}(\xi) - \lambda_{d\delta}(\xi)) d\xi} \langle\langle \phi_{b\beta}(\sigma) | \phi'_{d\delta}(\sigma) \rangle\rangle d\sigma + \mathcal{O}\left(\frac{1}{T\epsilon}\right) \quad (31)$$

(note that $c_{a\alpha}(0) = 1$ and $c_{b\beta}(0) = 0$). This last expression being the integral equation of the Dyson series for the null initial condition, we have $c_{b\beta}(s) = \mathcal{O}\left(\frac{1}{T\epsilon}\right)$. Finally we conclude that

$$\psi(s) = c_{a\alpha}(s) e^{-i\hbar^{-1}T \int_0^s \lambda_{a\alpha}(\sigma) d\sigma} \phi_{a\alpha}(s) + \mathcal{O}\left(\frac{1}{T\epsilon}\right) \quad (32)$$

with $c_{a\alpha}(s) = e^{-\int_0^s \langle\langle \phi_{a\alpha}(\sigma) | \phi'_{a\alpha}(\sigma) \rangle\rangle d\sigma}$ because equation (30) is the integral equation of an exponential map with the initial condition equal to 1. \square

As the very strong adiabatic regime is obtained with a usual adiabatic theorem applied on the bipartite quantum system, it can be considered as a particular case of the previous theorem where the gap condition is stronger and where the remainder of the adiabatic approximation is smaller ($\mathcal{O}\left(\frac{1}{T}\right)$ in place of $\mathcal{O}\left(\frac{1}{T\epsilon}\right)$).

We can remark that assumption (iii) is equivalent to $\tau_S \sim \theta^\epsilon$ as expressed in section 2.1. The condition $T \gg \theta^\epsilon$ is equivalent to requiring that the remainder $\mathcal{O}\left(\frac{1}{T\epsilon}\right)$ must be small.

Theorem 1 can be viewed as a corollary of the usual adiabatic theorem since their assumptions are very similar. Nevertheless, theorem 1 corresponds to an adiabatic theorem with a gap condition which is asymptotically small (i.e. $\mathcal{O}(\epsilon)$). The remainder of the adiabatic approximation ($\mathcal{O}\left(\frac{1}{T\epsilon}\right)$) is then larger than that of the usual adiabatic approximation ($\mathcal{O}\left(\frac{1}{T}\right)$). As stated above, the very strong adiabatic regime is a particular case of theorem 1 where the gap is not chosen asymptotically small and corresponds exactly to the usual adiabatic theorem.

Theorem 2 (Weak adiabatic theorem for bipartite quantum systems). *Let $[0, 1] \ni s \mapsto H(s) = H_S(s) \otimes 1_\mathcal{E} + 1_S \otimes H_\mathcal{E}(s) + \epsilon V(s)$ be a family of self-adjoint*

Hamiltonians of a bipartite quantum system such that $\forall T > 0$, $i\hbar\psi'(s) = TH(s)\psi(s)$ has continuous solutions in the norm topology, and such that V is $(H_S \otimes 1_{\mathcal{E}} + 1_S \otimes H_{\mathcal{E}})$ bounded. Let $\{\mu_b\}_b$ and $\{\nu_\beta\}_\beta$ be the pure point spectra of H_S and $H_{\mathcal{E}}$ and $\{\zeta_b\}_b$ and $\{\xi_\beta\}_\beta$ be the associated normalized eigenvectors. Let $\{\phi_{b\beta}\}_{b\beta}$ be the normalized eigenvectors of H continuously linked to $\{\zeta_b \otimes \xi_\beta\}_{b\beta}$ when $\epsilon \rightarrow 0$ (in the norm topology). We consider the case where $\psi(0) = \phi_{\alpha\alpha}(0)$. For the sake of simplicity we suppose that each eigenvalue is nondegenerate and that H_S and $H_{\mathcal{E}}$ do not have continuous spectra. We assume the following conditions.

- (i) $\forall b, \beta, s \mapsto \mu_b(s)$ and $s \mapsto \nu_\beta(s)$ are C^1 ; $s \mapsto \zeta_b(s)$ and $s \mapsto \xi_\beta(s)$ are C^2 in the norm topology.
- (ii) No quasi-resonance between transitions of S and \mathcal{E} involving ξ_α occurs, i.e. $\forall s \in [0, 1], \forall c, \forall (b\beta) \neq (c\alpha), |\mu_b(s) + \nu_\beta(s) - \mu_c(s) - \nu_\alpha(s)| = \mathcal{O}(1)$.
- (iii) The energies of \mathcal{E} satisfy a gap condition of order 0 with ν_α :

$$\inf_{s \in [0, 1]} \min_{\beta \neq \alpha} |\nu_\beta(s) - \nu_\alpha(s)| = \mathcal{O}(1). \quad (33)$$

- (iv) $[0, 1] \times \mathbb{C} \ni (s, z) \mapsto R(s, z) = (H(s) - z)^{-1}$ is strongly C^1 with respect to s and for every $\delta > 0$, $\exists K_\delta \in \mathbb{R}^+$, such that $\|R(s, z)\| \leq \frac{K_\delta}{\text{dist}(z, \{\lambda_{b\beta}(s)\}_{b\beta})} \forall z$ satisfying $\text{dist}(z, \{\lambda_{b\beta}(s)\}_{b\beta}) > \delta$.

Then we have

$$\forall s \in [0, 1], \quad P_\alpha(s)\psi(s) = \psi(s) + \mathcal{O}\left(\frac{1}{T}\right) \quad (34)$$

with $P_\alpha(s) = \sum_b |\phi_{b\alpha}(s)\rangle\langle\phi_{b\alpha}(s)|$.

Proof. Let $\sigma_\alpha(s) = \{\lambda_{c\alpha}(s)\}_c$ and $\sigma_\perp(s) = \{\lambda_{b\beta}(s)\}_{b,\beta \neq \alpha}$ be a decomposition of the spectrum of $H(s)$ into the part linked to ν_α and its complement. By a first order perturbation we have

$$\lambda_{c\alpha} - \lambda_{b\beta} = \mu_c - \mu_b + \nu_\alpha - \nu_\beta + \epsilon(V_{c\alpha, c\alpha} - V_{b\beta, b\beta}) + \mathcal{O}(\epsilon^2). \quad (35)$$

With the gap and the no quasi-resonance conditions we have then

$$\inf_{s \in [0, 1]} \text{dist}(\sigma_\alpha(s), \sigma_\perp(s)) = \inf_{s \in [0, 1]} \min_{c, b} \min_{\beta \neq \alpha} |\lambda_{c\alpha} - \lambda_{b\beta}| = \mathcal{O}(1). \quad (36)$$

We are in the conditions of the Nenciu adiabatic theorem [19] (condition (iv) is a requirement of this theorem) which ensures that during the whole evolution, the system remains projected onto the spectral subspace associated with the isolated part of the spectrum $\sigma_\alpha = \{\lambda_{c\alpha}\}_c$. The application of the Nenciu theorem proves the present one which is just a special version. \square

We note that the no quasi-resonance condition (ii) can be relaxed as a no resonance condition $\mu_b(s) + \nu_\beta(s) \neq \mu_c(s) + \nu_\alpha(s)$ (permitting $|\mu_b(s) + \nu_\beta(s) - \mu_c(s) - \nu_\alpha(s)| = \mathcal{O}(\epsilon)$) and moreover it could be suppressed if $V_{c\alpha, c\alpha}(s_*) \neq V_{b\beta, b\beta}(s_*)$ for s_* such that $\mu_b(s_*) + \nu_\beta(s_*) = \mu_c(s_*) + \nu_\alpha(s_*)$. But with these weaker conditions, the remainder of the adiabatic approximation is larger: $\mathcal{O}\left(\frac{1}{T\epsilon}\right)$. Nevertheless the main interest of this theorem is the

weak adiabatic regime $\frac{1}{T\epsilon} \notin \mathcal{V}(0)$ (where we cannot apply the strong adiabatic theorem), where the following optional condition is satisfied.

(v) The energies of \mathcal{S} satisfy a gap condition of order ϵ with μ_a :

$$\inf_{s \in [0, 1]} \min_{b \neq a} |\mu_b(s) - \mu_a(s)| = \mathcal{O}(\epsilon). \quad (37)$$

Condition (v) is compatible with theorem 2 but it is not necessary. Nevertheless it corresponds to the interesting physical situations.

Assumption (iii) implies that \mathcal{E} evolves adiabatically with regard to the control. This is a natural assumption because it corresponds to requiring that transitions in \mathcal{E} do not hamper the control of \mathcal{S} , as explained at the end of section 2.1. But if in practice it is necessary to relax this assumption for a single instant (or for a small number of instants) it is possible to generalize the application of theorem 2; we discuss this point in section 3.7.

We can remark that assumption (iii) is equivalent to $T \gg \tau_{\mathcal{E}}$ as expressed in section 2.1, whereas condition (v) is equivalent to $\tau_{\mathcal{S}} \sim \theta^{\epsilon}$.

3. Adiabatic transport of the density matrix

We are now able to find adiabatic transport formulae for the density matrix of \mathcal{S} : $\rho(s) = \text{tr}_{\mathcal{E}} |\psi(s)\rangle\langle\psi(s)|$.

3.1. Strong adiabatic regime

Proposition 1. *In the conditions of the strong adiabatic theorem (theorem 1) we have*

$$\forall s \in [0, 1] \quad \rho(s) = \rho_{aa}(s) + \mathcal{O}\left(\frac{1}{T\epsilon}\right) \quad (38)$$

where $\rho_{aa}(s) = \text{tr}_{\mathcal{E}} |\phi_{aa}(s)\rangle\langle\phi_{aa}(s)|$ is the ‘density eigenmatrix’.

Proof. By applying theorem 1 we have

$$|\psi(s)\rangle = e^{-i\hbar^{-1}T \int_0^s \lambda_{aa}(\sigma) d\sigma} \int_0^s \langle\phi_{aa}(\sigma)| \phi'_{aa}(\sigma)\rangle d\sigma |\phi_{aa}(s)\rangle + \mathcal{O}\left(\frac{1}{T\epsilon}\right) \quad (39)$$

Since $\langle\phi_{aa}(s)|\phi_{aa}(s)\rangle = 1 \Rightarrow \langle\phi_{aa}(s)|\phi'_{aa}(s)\rangle \in i\mathbb{R}$, we have $|\psi(s)\rangle\langle\psi(s)| = |\phi_{aa}(s)\rangle\langle\phi_{aa}(s)|$. \square

We can approach ρ_{aa} by a perturbative method (using the Wigner–Brillouin approach):

$$\begin{aligned} \rho(s) &= |\zeta_a(s)\rangle\langle\zeta_a(s)| + \epsilon \sum_{b \neq a} \frac{V_{b\alpha, a\alpha}(s)}{\mu_a(s) - \mu_b(s) + \epsilon V_{aa, aa}} |\zeta_b(s)\rangle\langle\zeta_a(s)| \\ &+ \epsilon \sum_{b \neq a} \frac{V_{\alpha, b\alpha}(s)}{\mu_b(s) - \mu_a(s) + \epsilon V_{aa, aa}} |\zeta_a(s)\rangle\langle\zeta_b(s)| \\ &+ \mathcal{O}\left(\max\left(\frac{1}{T\epsilon}, \epsilon^2\right)\right). \end{aligned} \quad (40)$$

3.2. Zero order weak adiabatic regime

We denote by $\overleftarrow{\mathbb{T}e}$ and $\overrightarrow{\mathbb{T}e}$ the time ordered and the time anti-ordered exponentials, i.e. for $s \mapsto A(s)$ a bounded anti-self-adjoint operator, $\overleftarrow{\mathbb{T}e}^{-\int_0^s A(\sigma) d\sigma}$ is the unitary operator solution of

$$\left(\mathbb{T}e^{-\int_0^s A(\sigma) d\sigma} \right)' = -A(s) \mathbb{T}e^{-\int_0^s A(\sigma) d\sigma} \quad \mathbb{T}e^{-\int_0^0 A(\sigma) d\sigma} = 1 \quad (41)$$

and $\mathbb{T}e^{-\int_0^s A(\sigma) d\sigma}$ is the unitary operator solution of

$$\left(\mathbb{T}e^{-\int_0^s A(\sigma) d\sigma} \right)' = -\mathbb{T}e^{-\int_0^s A(\sigma) d\sigma} A(s) \quad \mathbb{T}e^{-\int_0^0 A(\sigma) d\sigma} = 1. \quad (42)$$

Moreover we denote by \mathfrak{Ad} the adjoint action of a transformation U on a density matrix ρ :

$$\mathfrak{Ad}[U]\rho = U\rho U^\dagger. \quad (43)$$

Proposition 2. *In the conditions of the weak adiabatic theorem (theorem 2) we have $\forall s \in [0, 1]$*

$$\begin{aligned} \rho(s) = \mathfrak{Ad} \left[\mathbb{T}e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(0)}(\sigma) d\sigma} \mathbb{T}e^{-\int_0^s A^{(0)}(\sigma) d\sigma} \right] \rho_{\alpha\alpha}(s) \\ + \mathcal{O} \left(\max \left(\frac{1}{T}, \epsilon \right) \right) \end{aligned} \quad (44)$$

with the zero order dynamical phase generator defined as being

$$E_\alpha^{(0)}(s) = \sum_b \lambda_{b\alpha}(s) |\zeta_b(s)\rangle \langle \zeta_b(s)| \in \mathcal{L}(\mathcal{H}_S) \quad (45)$$

and the zero order geometric phase generator defined as being

$$A^{(0)}(s) = \sum_{b,c} \langle \zeta_b(s) | \zeta'_c(s) \rangle |\zeta_b(s)\rangle \langle \zeta_c(s)| \in \mathcal{L}(\mathcal{H}_S). \quad (46)$$

Proof. By applying theorem 2 and an adiabatic transport formula for several eigenvalues [21, 22] we have

$$\psi(s) = \sum_b \left[\mathbb{T}e^{-i\hbar^{-1}T \int_0^s \Lambda_\alpha d\sigma - \int_0^s K_\alpha d\sigma} \right]_{ba} \phi_{b\alpha} + \mathcal{O} \left(\frac{1}{T} \right) \quad (47)$$

with $\Lambda_\alpha, K_\alpha \in \mathfrak{M}_{n \times n}(\mathbb{C})$ being the square matrices of order n (n is the dimension of \mathcal{H}_S) such that $[\Lambda_\alpha]_{ab} = \lambda_{a\alpha} \delta_{ab}$ and $[K_\alpha]_{ab} = \langle \phi_{a\alpha} | \phi'_{b\alpha} \rangle$ ($[\cdot]_{ab}$ denotes the matrix element at the a th line and the b th column). Since $|\zeta_b\rangle \langle \zeta_c| \phi_{\alpha\alpha} = \phi_{b\alpha} \delta_{ca} + \mathcal{O}(\epsilon)$ we have

$$\psi(s) = \sum_{b,c} \left[\mathbb{T}e^{-i\hbar^{-1}T \int_0^s \Lambda_\alpha d\sigma - \int_0^s K_\alpha d\sigma} \right]_{bc} |\zeta_b\rangle \langle \zeta_c| \phi_{\alpha\alpha} + \mathcal{O} \left(\max \left(\frac{1}{T}, \epsilon \right) \right). \quad (48)$$

By applying corollary 1 (appendix) we have

$$\begin{aligned} \sum_{b,c} \left[\mathbb{T}e^{-i\hbar^{-1}T \int_0^s \Lambda_\alpha d\sigma - \int_0^s K_\alpha d\sigma} \right]_{bc} |\zeta_b\rangle \langle \zeta_c| \\ = \sum_{bd} \left[\mathbb{T}e^{-\int_0^s X d\sigma} \right]_{bd} |\zeta_b\rangle \langle \zeta_d| \sum_{f,c} \left[\mathbb{T}e^{-\int_0^s K_\alpha d\sigma} \right]_{fc} |\zeta_f\rangle \langle \zeta_c| \end{aligned} \quad (49)$$

with $X = i\hbar^{-1}T\Lambda_\alpha + K_\alpha - \mathbb{T}e^{-\int_0^s X d\sigma} K_\alpha \left(\mathbb{T}e^{-\int_0^s X d\sigma} \right)^{-1}$.

• Let $Y \in \mathfrak{M}_{n \times n}(\mathbb{C})$ be such that $\mathbb{T}e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(0)} d\sigma} = \sum_{b,d} \left[\mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} |\zeta_b\rangle \langle \zeta_d|$.

$$\left(\mathbb{T}e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(0)} d\sigma} \right)' = -i\hbar^{-1}TE_\alpha^{(0)} \mathbb{T}e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(0)} d\sigma} \quad (50)$$

implies that

$$\begin{aligned} & -i\hbar^{-1}TE_\alpha^{(0)} \sum_{b,d} \left[\mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} |\zeta_b\rangle \langle \zeta_d| \\ &= \sum_{b,d} \left[-Y \mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} |\zeta_b\rangle \langle \zeta_d| \\ &+ \sum_{b,d} \left[\mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} |\zeta'_b\rangle \langle \zeta_d| \\ &+ \sum_{b,d} \left[\mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} |\zeta_b\rangle \langle \zeta'_d| \end{aligned} \quad (51)$$

but

$$\begin{aligned} & -i\hbar^{-1}TE_\alpha^{(0)} \sum_{b,d} \left[\mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} |\zeta_b\rangle \langle \zeta_d| \\ &= -i\hbar^{-1}T \sum_{b,d} \lambda_{b\alpha} \left[\mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} |\zeta_b\rangle \langle \zeta_d| \end{aligned} \quad (52)$$

$$= \sum_{b,d} \left[-i\hbar^{-1}T \Lambda_\alpha \mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} |\zeta_b\rangle \langle \zeta_d| \quad (53)$$

and

$$|\zeta'_b\rangle \langle \zeta_d| = \sum_f \langle \zeta_f | \zeta'_b \rangle |\zeta_f\rangle \langle \zeta_d| \quad (54)$$

$$|\zeta_b\rangle \langle \zeta'_d| = \sum_f \langle \zeta'_d | \zeta_f \rangle |\zeta_b\rangle \langle \zeta_f|. \quad (55)$$

Equation (51) becomes

$$\begin{aligned} -i\hbar^{-1}T \Lambda_\alpha \mathbb{T}e^{-\int_0^s Y d\sigma} &= -Y \mathbb{T}e^{-\int_0^s Y d\sigma} + \mathring{K} \mathbb{T}e^{-\int_0^s Y d\sigma} \\ &\quad - \mathbb{T}e^{-\int_0^s Y d\sigma} \mathring{K} \end{aligned} \quad (56)$$

because $\langle \zeta_d | \zeta_f \rangle = \delta_{df} \Rightarrow \langle \zeta'_d | \zeta_f \rangle = -\langle \zeta_d | \zeta'_f \rangle$ with $\mathring{K} \in \mathfrak{M}_{n \times n}(\mathbb{C})$ defined as $[\mathring{K}]_{df} = \langle \zeta_d | \zeta'_f \rangle$. But

$$[K_\alpha]_{bc} = \langle \langle \phi_{b\alpha} | \phi'_{c\alpha} \rangle \rangle \quad (57)$$

$$= \langle \zeta_b | \zeta'_c \rangle + \langle \xi_\alpha | \xi'_\alpha \rangle + \mathcal{O}(\epsilon) \quad (58)$$

$$\Rightarrow K_\alpha = \overset{\circ}{K} + \langle \xi_\alpha | \xi'_\alpha \rangle + \mathcal{O}(\epsilon) \tag{59}$$

and then $X = i\hbar^{-1}T\Lambda_\alpha + \overset{\circ}{K} - \overleftarrow{\mathbb{T}}e^{-\int_0^s X d\sigma} \overset{\circ}{K} \left(\overleftarrow{\mathbb{T}}e^{-\int_0^s X d\sigma} \right)^{-1} + \mathcal{O}(\epsilon)$ ($\langle \xi_\alpha | \xi'_\alpha \rangle \in i\mathbb{R}$). A comparison with equation (56) shows that $Y = X + \mathcal{O}(\epsilon)$ and then

$$\sum_{bd} \left[\overleftarrow{\mathbb{T}}e^{-\int_0^s X d\sigma} \right]_{bd} |\zeta_b\rangle \langle \zeta_d| = \overleftarrow{\mathbb{T}}e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(0)} d\sigma} + \mathcal{O}(\epsilon). \tag{60}$$

• Let $Z \in \mathfrak{M}_{n \times n}(\mathbb{C})$ be such that $\overleftarrow{\mathbb{T}}e^{-\int_0^s A^{(0)} d\sigma} = \sum_{f,c} \left[\overleftarrow{\mathbb{T}}e^{-\int_0^s Z d\sigma} \right]_{f,c} |\zeta_f\rangle \langle \zeta_c|$.

$$\left(\overrightarrow{\mathbb{T}}e^{-\int_0^s A^{(0)} d\sigma} \right)' = -\overrightarrow{\mathbb{T}}e^{-\int_0^s A^{(0)} d\sigma} A^{(0)} \tag{61}$$

implies that

$$\begin{aligned} & -\sum_{f,c} \left[\overleftarrow{\mathbb{T}}e^{-\int_0^s Z d\sigma} \right]_{f,c} |\zeta_f\rangle \langle \zeta_c| A^{(0)} \\ &= \sum_{f,c} \left[-Z \overleftarrow{\mathbb{T}}e^{-\int_0^s Z d\sigma} \right]_{f,c} |\zeta_f\rangle \langle \zeta_c| \\ &+ \sum_{f,c} \left[\overleftarrow{\mathbb{T}}e^{-\int_0^s Z d\sigma} \right]_{f,c} |\zeta'_f\rangle \langle \zeta_c| \\ &+ \sum_{f,c} \left[\overleftarrow{\mathbb{T}}e^{-\int_0^s Z d\sigma} \right]_{f,c} |\zeta_f\rangle \langle \zeta'_c| \end{aligned} \tag{62}$$

which becomes (since $A^{(0)} = \sum_{cg} [\overset{\circ}{K}]_{cg} |\zeta_c\rangle \langle \zeta_g|$)

$$-\overleftarrow{\mathbb{T}}e^{-\int_0^s Z d\sigma} \overset{\circ}{K} = -Z \overleftarrow{\mathbb{T}}e^{-\int_0^s Z d\sigma} + \overset{\circ}{K} \overleftarrow{\mathbb{T}}e^{-\int_0^s Z d\sigma} - \overleftarrow{\mathbb{T}}e^{-\int_0^s Z d\sigma} \overset{\circ}{K} \tag{63}$$

$Z = \overset{\circ}{K} = K_\alpha - \langle \xi_\alpha | \xi'_\alpha \rangle + \mathcal{O}(\epsilon)$ and then

$$\sum_{f,c} \left[\overleftarrow{\mathbb{T}}e^{-\int_0^s K_\alpha d\sigma} \right]_{f,c} |\zeta_f\rangle \langle \zeta_c| = e^{-\int_0^s \langle \xi_\alpha | \xi'_\alpha \rangle d\sigma} \overrightarrow{\mathbb{T}}e^{-\int_0^s A^{(0)} d\sigma} + \mathcal{O}(\epsilon). \tag{64}$$

Finally we have

$$\begin{aligned} \psi(s) &= e^{-\int_0^s \langle \xi_\alpha | \xi'_\alpha \rangle d\sigma} \overleftarrow{\mathbb{T}}e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(0)} d\sigma} \overrightarrow{\mathbb{T}}e^{-\int_0^s A^{(0)} d\sigma} \phi_{\alpha\alpha}(s) \\ &+ \mathcal{O}\left(\max\left(\frac{1}{T}, \epsilon\right)\right) \end{aligned} \tag{65}$$

and

$$\rho(s) = \text{tr}_{\mathcal{E}} |\psi(s)\rangle \langle \psi(s)| \tag{66}$$

$$= \mathfrak{A} \mathfrak{D} \left[\overleftarrow{\mathbb{T}}e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(0)} d\sigma} \overrightarrow{\mathbb{T}}e^{-\int_0^s A^{(0)} d\sigma} \right] \rho_{\alpha\alpha} + \mathcal{O}\left(\max\left(\frac{1}{T}, \epsilon\right)\right) \tag{67}$$

since $e^{-\int_0^s \langle \xi_\alpha | \xi'_\alpha \rangle d\sigma} \in U(1)$ ($U(1)$ is the set of unit modulus complex numbers) and $\overleftarrow{\mathbb{T}}e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(0)} d\sigma}, \overrightarrow{\mathbb{T}}e^{-\int_0^s A^{(0)} d\sigma} \in \mathcal{U}(\mathcal{H}_S)$. □

In this zero order approximation, the only memory of \mathcal{E} is the elements $T\lambda_{ba}$ in the expression of the operator-valued dynamical phase. We note that we cannot approach λ_{ba} at the zero order perturbative approximation in the dynamical phase because $T\epsilon$ is not negligible in the weak adiabatic regime. In the next section we consider higher accuracy approximations.

3.3. First order weak adiabatic regime

Proposition 3. *In the conditions of the weak adiabatic theorem (theorem 2) we have $\forall s \in [0, 1]$*

$$\rho(s) = \mathfrak{A} \mathfrak{D} \left[\mathbb{T} \overleftarrow{e^{-i\hbar^{-1}T \int_0^s E_a^{(1)}(\sigma) d\sigma}} \mathbb{T} \overrightarrow{e^{-i\hbar^{-1}T \int_0^s A_a^{(1)}(\sigma) d\sigma}} \right] \rho_{aa}(s) + \mathcal{O} \left(\max \left(\frac{1}{T}, \epsilon^2 \right) \right) \quad (68)$$

with the first order dynamical phase generator defined as being

$$E_a^{(1)}(s) = \sum_{b,c} \left(\lambda_{ba}(s) \delta_{bc} - \frac{i\hbar}{T} \eta_{abc}^{(1)}(s) \right) \left| \zeta_{ba}^{(1)}(s) \right\rangle \left\langle \zeta_{ca}^{(1)}(s) \right| \in \mathcal{L}(\mathcal{H}_S) \quad (69)$$

and the first order geometric phase generator defined as being

$$A_a^{(1)}(s) = \sum_{b,c} \left\langle \zeta_{ba}^{(1)}(s) \left| \zeta_{ca}^{(1)'}(s) \right. \right\rangle \left| \zeta_{ba}^{(1)}(s) \right\rangle \left\langle \zeta_{ca}^{(1)}(s) \right| \in \mathcal{L}(\mathcal{H}_S) \quad (70)$$

with

$$\zeta_{ba}^{(1)}(s) = \zeta_b(s) + \epsilon \sum_{d \neq b} \frac{V_{da,ba}(s)}{\mu_b(s) - \mu_d(s) + \epsilon V_{ba,ba}(s)} \zeta_d(s) \quad (71)$$

$$\begin{aligned} \eta_{abc}^{(1)}(s) &= \left\langle \xi_a(s) \left| \xi_a'(s) \right. \right\rangle \delta_{bc} \\ &+ \epsilon \sum_{\gamma \neq \alpha} \frac{V_{b\gamma,ca}(s) \left\langle \xi_a(s) \left| \xi_\gamma'(s) \right. \right\rangle (1 - \delta_{bc})}{\mu_c(s) - \mu_b(s) + \nu_\alpha(s) - \nu_\gamma(s) + \epsilon V_{ca,ca}(s)} \\ &+ \epsilon \sum_{\gamma \neq \alpha} \frac{V_{b\alpha,c\gamma}(s) \left\langle \xi_\gamma(s) \left| \xi_\alpha'(s) \right. \right\rangle (1 - \delta_{bc})}{\mu_b(s) - \mu_c(s) + \nu_\alpha(s) - \nu_\gamma(s) + \epsilon V_{ba,ba}(s)}. \end{aligned} \quad (72)$$

Proof. As for the zero order formula we start with

$$\psi(s) = \sum_b \left[\mathbb{T} \overleftarrow{e^{-i\hbar^{-1}T \int_0^s \Lambda_\alpha d\sigma}} \mathbb{T} \overrightarrow{e^{-i\hbar^{-1}T \int_0^s K_\alpha d\sigma}} \right]_{ba} \phi_{ba} + \mathcal{O} \left(\frac{1}{T} \right) \quad (73)$$

$$= \sum_{b,c} U_{abc} \left| \phi_{ba} \right\rangle \left\langle \left\langle \phi_{ca} \right| \phi_{aa} \right\rangle + \mathcal{O} \left(\frac{1}{T} \right). \quad (74)$$

Let $\zeta_{ba}^{(1)} = \zeta_b + \epsilon \sum_{d \neq b} \mathcal{V}_{da,ba} \zeta_d$ (with $\mathcal{V}_{d\gamma,ba} = \frac{V_{d\gamma,ba}}{\mu_b - \mu_d + \nu_\alpha - \nu_\gamma + \epsilon V_{ba,ba}}$). By using a first order perturbative expansion based on the Wigner–Brillouin method we have

$$\phi_{ba} = \zeta_b \otimes \xi_\alpha + \epsilon \sum_{(d,\gamma) \neq (b,\alpha)} \mathcal{V}_{d\gamma,ba} \zeta_d \otimes \xi_\gamma + \mathcal{O}(\epsilon^2) \quad (75)$$

$$= \zeta_{ba}^{(1)} \otimes \xi_\alpha + \epsilon \sum_{\gamma \neq \alpha} \sum_{d \neq b} \mathcal{V}_{d\gamma,ba} \zeta_d \otimes \xi_\gamma + \mathcal{O}(\epsilon^2). \quad (76)$$

We have then

$$\begin{aligned} |\phi_{ba}\rangle\rangle\langle\langle\phi_{ca}| &= |\zeta_{ba}^{(1)}\rangle\langle\zeta_{ca}^{(1)}| \otimes |\xi_\alpha\rangle\langle\xi_\alpha| \\ &+ \epsilon \sum_{\gamma \neq \alpha} \sum_{d \neq b} \mathcal{V}_{d\gamma,ba} |\zeta_d\rangle\langle\zeta_c| \otimes |\xi_\gamma\rangle\langle\xi_\alpha| \\ &+ \epsilon \sum_{\gamma \neq \alpha} \sum_{d \neq c} \overline{\mathcal{V}_{d\gamma,ca}} |\zeta_b\rangle\langle\zeta_d| \otimes |\xi_\alpha\rangle\langle\xi_\gamma| + \mathcal{O}(\epsilon^2) \end{aligned} \quad (77)$$

$$\begin{aligned} |\phi_{ba}\rangle\rangle\langle\langle\phi_{ca}| \phi_{aa} &= |\zeta_{ba}^{(1)}\rangle\langle\zeta_{ca}^{(1)}| \phi_{aa} \\ &- \epsilon \sum_{\gamma \neq \alpha} \mathcal{V}_{c\gamma,aa} \zeta_b \otimes \xi_\gamma (1 - \delta_{ac}) \\ &+ \epsilon \sum_{\gamma \neq \alpha} \sum_{d \neq b} \mathcal{V}_{d\gamma,ba} \zeta_d \otimes \xi_\gamma \delta_{ac} + \mathcal{O}(\epsilon^2) \end{aligned} \quad (78)$$

$$\begin{aligned} &= |\zeta_{ba}^{(1)}\rangle\langle\zeta_{ca}^{(1)}| \phi_{aa} \\ &- \epsilon \sum_{\gamma \neq \alpha} \sum_{d \neq c} \mathcal{V}_{c\gamma,da} |\zeta_b\rangle\langle\zeta_d| \phi_{a\gamma} \\ &+ \epsilon \sum_{\gamma \neq \alpha} \sum_{d \neq b} \mathcal{V}_{d\gamma,ba} |\zeta_d\rangle\langle\zeta_c| \phi_{a\gamma} + \mathcal{O}(\epsilon^2). \end{aligned} \quad (79)$$

By using this expression with equation (73) we find that

$$\begin{aligned} \psi(s) &= \sum_{bc} U_{abc} |\zeta_{ba}^{(1)}\rangle\langle\zeta_{ba}^{(1)}| \phi_{aa} \\ &- \epsilon \sum_{b,c} \sum_{d \neq c} \sum_{\gamma \neq \alpha} U_{abc} \mathcal{V}_{c\gamma,da} |\zeta_b\rangle\langle\zeta_d| \phi_{a\gamma} \\ &+ \epsilon \sum_{b,c} \sum_{d \neq b} \sum_{\gamma \neq \alpha} U_{abc} \mathcal{V}_{d\gamma,ba} |\zeta_d\rangle\langle\zeta_c| \phi_{a\gamma} + \mathcal{O}\left(\max\left(\frac{1}{T}, \epsilon^2\right)\right) \end{aligned} \quad (80)$$

$$= \mathcal{U}_\alpha \phi_{aa} + \epsilon \sum_{\gamma \neq \alpha} [\mathcal{W}_{\gamma\alpha}, \mathcal{U}_\alpha] \phi_{a\gamma} + \mathcal{O}\left(\max\left(\frac{1}{T}, \epsilon^2\right)\right) \quad (81)$$

with the operators of \mathcal{H}_S : $\mathcal{U}_\alpha = \sum_{b,c} U_{abc} |\zeta_{ba}^{(1)}\rangle\langle\zeta_{ca}^{(1)}|$ and $\mathcal{W}_{\gamma\alpha} = \sum_d \sum_{b \neq d} \mathcal{V}_{d\gamma,ba} |\zeta_{d\gamma}^{(1)}\rangle\langle\zeta_{ba}^{(1)}|$. We have then

$$\begin{aligned}
|\psi\rangle\langle\psi| &= \mathcal{U}_\alpha |\phi_{\alpha\alpha}\rangle\langle\phi_{\alpha\alpha}| \mathcal{U}_\alpha^\dagger \\
&+ \epsilon \sum_{\gamma \neq \alpha} [\mathcal{W}_{\gamma\alpha}, \mathcal{U}_\alpha] |\zeta_\alpha\rangle\langle\zeta_\alpha| \otimes |\xi_\gamma\rangle\langle\xi_\alpha| \mathcal{U}_\alpha^\dagger \\
&+ \epsilon \sum_{\gamma \neq \alpha} \mathcal{U}_\alpha |\zeta_\alpha\rangle\langle\zeta_\alpha| \otimes |\xi_\alpha\rangle\langle\xi_\gamma| [\mathcal{U}_\alpha^\dagger, \mathcal{W}_{\gamma\alpha}^\dagger] \\
&+ \mathcal{O}\left(\max\left(\frac{1}{T}, \epsilon^2\right)\right)
\end{aligned} \tag{82}$$

$$\Rightarrow \rho(s) = \text{tr}_\mathcal{E} |\psi\rangle\langle\psi| = \mathcal{U}_\alpha \rho_{\alpha\alpha} \mathcal{U}_\alpha^\dagger + \mathcal{O}\left(\max\left(\frac{1}{T}, \epsilon^2\right)\right) \tag{83}$$

$$\mathcal{U}_\alpha = \sum_{b,c} \left[\mathbb{E} \left[\leftarrow \mathbb{E}^{-i\hbar^{-1}T \int_0^s \Lambda_\alpha d\sigma - \int_0^s K_\alpha d\sigma} \right]_{bc} \right] |\zeta_{b\alpha}^{(1)}\rangle\langle\zeta_{c\alpha}^{(1)}|. \tag{84}$$

But

$$[K_\alpha]_{bc} = \langle\langle \phi_{b\alpha} | \phi'_{c\alpha} \rangle\rangle \tag{85}$$

$$\begin{aligned}
&= \langle\zeta_{b\alpha}^{(1)} | \zeta_{c\alpha}^{(1)'}\rangle + \langle\xi_\alpha | \xi_\alpha'\rangle \\
&+ \epsilon \sum_{\gamma \neq \alpha} \mathcal{V}_{b\gamma, c\alpha} \langle\xi_\alpha | \xi_\gamma'\rangle (1 - \delta_{bc}) \\
&+ \epsilon \sum_{\gamma \neq \alpha} \overline{\mathcal{V}_{c\gamma, b\alpha}} \langle\xi_\gamma | \xi_\alpha'\rangle (1 - \delta_{bc}) + \mathcal{O}(\epsilon^2)
\end{aligned} \tag{86}$$

$$= [\mathring{K}_\alpha]_{bc} + \eta_{abc}^{(1)} + \mathcal{O}(\epsilon^2) \tag{87}$$

with $[\mathring{K}_\alpha]_{bc} = \langle\zeta_{b\alpha}^{(1)} | \zeta_{c\alpha}^{(1)'}\rangle$ ($\mathring{K}_\alpha \in \mathfrak{M}_{n \times n}(\mathbb{C})$). By using corollary 1 (appendix) we find

$$\begin{aligned}
&\mathcal{U}_\alpha \\
&= \sum_{b,d} \left[\mathbb{E} \left[\leftarrow \mathbb{E}^{-\int_0^s X d\sigma} \right]_{bd} \right] |\zeta_{b\alpha}^{(1)}\rangle\langle\zeta_{d\alpha}^{(1)}| \sum_{f,c} \left[\mathbb{E} \left[\leftarrow \mathbb{E}^{-\int_0^s \mathring{K}_\alpha d\sigma} \right]_{fc} \right] |\zeta_{f\alpha}^{(1)}\rangle\langle\zeta_{c\alpha}^{(1)}| + \mathcal{O}(\epsilon^2)
\end{aligned} \tag{88}$$

with $X = i\hbar^{-1}T\Lambda_\alpha + \eta_\alpha^{(1)} + \mathring{K}_\alpha - \mathbb{E} \left[\leftarrow \mathbb{E}^{-\int_0^s X d\sigma} \mathring{K}_\alpha \left(\mathbb{E} \left[\leftarrow \mathbb{E}^{-\int_0^s X d\sigma} \right] \right)^{-1} \right]$.

- Let $Y \in \mathfrak{M}_{n \times n}(\mathbb{C})$ be such that $\mathbb{E} \left[\leftarrow \mathbb{E}^{-i\hbar^{-1}T \int_0^s E_\alpha^{(1)} d\sigma} \right] = \sum_{b,d} \left[\mathbb{E} \left[\leftarrow \mathbb{E}^{-\int_0^s Y d\sigma} \right]_{bd} \right] |\zeta_{b\alpha}^{(1)}\rangle\langle\zeta_{d\alpha}^{(1)}|$

$$\left(\mathbb{E} \left[\leftarrow \mathbb{E}^{-i\hbar^{-1}T \int_0^s E_\alpha^{(1)} d\sigma} \right] \right)' = -i\hbar^{-1}T E_\alpha^{(1)} \mathbb{E} \left[\leftarrow \mathbb{E}^{-i\hbar^{-1}T \int_0^s E_\alpha^{(1)} d\sigma} \right] \tag{89}$$

implies that

$$\begin{aligned}
 & \sum_{b,d} \left[\left(-i\hbar^{-1}T\Lambda_\alpha - \eta_\alpha^{(1)} \right) \mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} \left| \zeta_{b\alpha}^{(1)} \right\rangle \left\langle \zeta_{d\alpha}^{(1)} \right| \\
 &= \sum_{b,d} \left[-Y \mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} \left| \zeta_{b\alpha}^{(1)} \right\rangle \left\langle \zeta_{d\alpha}^{(1)} \right| \\
 &+ \sum_{b,d,f} \left[\mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} \left\langle \zeta_{f\alpha}^{(1)} \left| \zeta_{b\alpha}^{(1)'} \right\rangle \left| \zeta_{f\alpha}^{(1)} \right\rangle \left\langle \zeta_{d\alpha}^{(1)} \right| \\
 &+ \sum_{b,d,f} \left[\mathbb{T}e^{-\int_0^s Y d\sigma} \right]_{bd} \left\langle \zeta_{d\alpha}^{(1)'} \left| \zeta_{f\alpha}^{(1)} \right\rangle \left| \zeta_{b\alpha}^{(1)} \right\rangle \left\langle \zeta_{f\alpha}^{(1)} \right| \tag{90}
 \end{aligned}$$

$$\begin{aligned}
 & \Rightarrow \left(-i\hbar^{-1}T\Lambda_\alpha - \eta_\alpha^{(1)} \right) \mathbb{T}e^{-\int_0^s Y d\sigma} \\
 &= -Y \mathbb{T}e^{-\int_0^s Y d\sigma} + \hat{K}_\alpha \mathbb{T}e^{-\int_0^s Y d\sigma} - \mathbb{T}e^{-\int_0^s Y d\sigma} \hat{K}_\alpha. \tag{91}
 \end{aligned}$$

We have then $Y = i\hbar^{-1}T\Lambda_\alpha + \eta_\alpha^{(1)} + \hat{K}_\alpha - \mathbb{T}e^{-\int_0^s Y d\sigma} \hat{K}_\alpha \left(\mathbb{T}e^{-\int_0^s Y d\sigma} \right)^{-1}$ and by comparison with the definition of X we have $Y = X$ and then

$$\sum_{b,d} \left[\mathbb{T}e^{-\int_0^s X d\sigma} \right]_{bd} \left| \zeta_{b\alpha}^{(1)} \right\rangle \left\langle \zeta_{d\alpha}^{(1)} \right| = \mathbb{T}e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(1)} d\sigma}. \tag{92}$$

- Let $Z \in \mathfrak{M}_{n \times n}(\mathbb{C})$ be such that $\mathbb{T}e^{-\int_0^s A_\alpha^{(1)} d\sigma} = \sum_{f,c} \left[\mathbb{T}e^{-\int_0^s Z d\sigma} \right]_{fc} \left| \zeta_{f\alpha}^{(1)} \right\rangle \left\langle \zeta_{c\alpha}^{(1)} \right|$.

$$\left(\mathbb{T}e^{-\int_0^s A_\alpha^{(1)} d\sigma} \right)' = -\mathbb{T}e^{-\int_0^s A_\alpha^{(1)} d\sigma} A_\alpha^{(1)} \tag{93}$$

implies that

$$\begin{aligned}
 -\mathbb{T}e^{-\int_0^s Z d\sigma} \hat{K}_\alpha &= -Z \mathbb{T}e^{-\int_0^s Z d\sigma} \\
 &+ \hat{K}_\alpha \mathbb{T}e^{-\int_0^s Z d\sigma} - \mathbb{T}e^{-\int_0^s Z d\sigma} \hat{K}_\alpha \tag{94}
 \end{aligned}$$

$Z = \hat{K}_\alpha$ and then

$$\sum_{f,c} \left[\mathbb{T}e^{-\int_0^s \hat{K}_\alpha d\sigma} \right]_{fc} \left| \zeta_{f\alpha}^{(1)} \right\rangle \left\langle \zeta_{c\alpha}^{(1)} \right| = \mathbb{T}e^{-\int_0^s A_\alpha^{(1)} d\sigma}. \tag{95}$$

Finally we have

$$\mathcal{U}_\alpha = \mathbb{T}e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(1)} d\sigma} \mathbb{T}e^{-\int_0^s A_\alpha^{(1)} d\sigma} + \mathcal{O}(\epsilon^2). \tag{96}$$

This concludes the proof by injecting this expression into equation (83). \square

We note that we have used the Wigner–Brillouin method for the perturbation theory ($\zeta_{b\alpha}^{(1)}(s) = \zeta_b(s) + \epsilon \sum_{d \neq b} \frac{V_{da,ba}(s)}{\mu_b(s) - \mu_d(s) + \epsilon V_{ba,ba}(s)} \zeta_d(s)$) because the weak adiabatic regime does not need $\tau_S \ll T$, and permits crossings of eigenvalues of S . The Wigner–Brillouin method permits us to avoid some divergences in the perturbation expansion induced by these possible crossings.

We can remark that the off-diagonal part of $E_\alpha^{(1)}$ includes in fact a geometric phase generator associated with $\mathcal{E}(\eta_\alpha^{(1)})$. This is not surprising since $E_\alpha^{(1)}$ takes the role of an effective Hamiltonian of \mathcal{S} dressed by \mathcal{E} (see below). Such a dynamical phase generator is similar to the one generated by quasi-energies in adiabatic Floquet theory (see for example [25]) where the role of \mathcal{S} is played by an atom or a molecule interacting with a strong laser field described by $L^2(S^1, \frac{d\theta}{2\pi})$ (the space of square integrable functions on the circle S^1 , θ being the laser phase) which plays the role of $\mathcal{H}_\mathcal{E}$.

3.4. Second order weak adiabatic regime

The case of the second order perturbative approximation is more difficult. Indeed the second order approximation of the eigenvectors

$$\begin{aligned} \phi_{b\beta} &= \zeta_b \otimes \xi_\beta \\ &+ \epsilon \sum_{(c\gamma) \neq (b\beta)} \frac{V_{c\gamma, b\beta}}{\mu_b - \mu_c + \nu_\beta - \nu_\gamma} \zeta_c \otimes \xi_\gamma \\ &+ \epsilon^2 \sum_{\substack{(d\delta) \neq (b\beta) \\ (c\gamma) \neq (b\beta)}} \frac{V_{d\delta, c\gamma} V_{c\gamma, b\beta} - V_{c\gamma, b\beta} V_{b\beta, d\delta}}{(\mu_b - \mu_d + \nu_\beta - \nu_\delta)(\mu_b - \mu_c + \nu_\beta - \nu_\gamma)} \zeta_d \otimes \xi_\delta \\ &+ \mathcal{O}(\epsilon^3) \end{aligned} \quad (97)$$

is not normalized (at the order ϵ^3). This induces some difficulties in defining an adiabatic transport formula, especially for the definition of the generator of the geometric phase. A normalization factor could be very complicated and difficult to use. We prefer to use a biorthonormal basis $\{\phi_{b\beta}^*\}_{b\beta}$ defined such that

$$\langle\langle \phi_{c\gamma}^* | \phi_{b\beta} \rangle\rangle = \delta_{cb} \delta_{\gamma\beta} + \mathcal{O}(\epsilon^3). \quad (98)$$

Such an approach is able to define a correct geometric phase generator [23, 24]. In the present context, the biorthonormal eigenvectors are

$$\langle\langle \phi_{b\beta}^* | = \langle\langle \phi_{b\beta} | - \epsilon^2 \sum_{(c\gamma)} X_{b\beta, c\gamma} \langle\langle \zeta_c \otimes \xi_\gamma | \quad (99)$$

with

$$\begin{aligned} X_{b\beta, c\gamma} &= \sum_{(d\delta) \neq (c\gamma)} \frac{V_{b\beta, d\delta} V_{d\delta, c\gamma} - V_{d\delta, c\gamma} V_{c\gamma, d\delta}}{(\mu_c - \mu_b + \nu_\gamma - \nu_\beta)(\mu_c - \mu_d + \nu_\gamma - \nu_\delta)} (1 - \delta_{bc} \delta_{\beta\gamma}) \\ &+ \sum_{(d\delta) \neq (b\beta)} \frac{V_{d\delta, c\gamma} V_{b\beta, d\delta} - V_{b\beta, d\delta} V_{b\beta, c\gamma}}{(\mu_b - \mu_c + \nu_\beta - \nu_\gamma)(\mu_b - \mu_d + \nu_\beta - \nu_\delta)} (1 - \delta_{bc} \delta_{\beta\gamma}) \\ &+ \sum_{(d\delta) \neq (b\beta)} \frac{V_{d\delta, c\gamma} V_{b\beta, d\delta}}{(\mu_c - \mu_d + \nu_\gamma - \nu_\delta)(\mu_b - \mu_d + \nu_\beta - \nu_\delta)} (1 - \delta_{dc} \delta_{\delta\gamma}). \end{aligned} \quad (100)$$

Proposition 4. *In the conditions of the weak adiabatic theorem (theorem 2) we have $\forall s \in [0, 1]$*

$$\begin{aligned}
\rho(s) &= \mathfrak{A} \mathfrak{D} [\mathcal{U}_\alpha(s)] \rho_{aa}^{(2)}(s) \\
&+ \epsilon^2 \sum_{\delta \neq \alpha} \mathfrak{A} \mathfrak{D} [\mathcal{W}_{\delta\alpha}(s) \mathcal{U}_\alpha(s)] |\zeta_\alpha(s)\rangle \langle \zeta_\alpha(s)| \\
&+ \mathcal{O} \left(\max \left(\frac{1}{T}, \epsilon^3 \right) \right)
\end{aligned} \tag{101}$$

$$\mathcal{U}_\alpha(s) = \overleftarrow{\mathbb{T}} e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(2)}(\sigma) d\sigma} \overrightarrow{\mathbb{T}} e^{-\int_0^s A_\alpha^{(2)}(\sigma) d\sigma} \tag{102}$$

$$\mathcal{W}_{\delta\alpha}(s) = \sum_d \sum_{c \neq d} \frac{V_{d\delta, c\alpha}(s)}{\Delta_{c\alpha, d\delta}(s)} |\zeta_d(s)\rangle \langle \zeta_c(s)| \tag{103}$$

with $\Delta_{c\alpha, d\delta} = \mu_c - \mu_d + \nu_\alpha - \nu_\delta + \epsilon V_{c\alpha, c\alpha}$. The first order dynamical phase generator is defined as being

$$E_\alpha^{(2)}(s) = \sum_{b,c} \left(\lambda_{ba}(s) \delta_{bc} - \frac{i\hbar}{T} \eta_{abc}^{(2)}(s) \right) |\zeta_{ba}^{(2)}(s)\rangle \langle \zeta_{ca}^{*(2)}(s)| \in \mathcal{L}(\mathcal{H}_S) \tag{104}$$

and the first order geometric phase generator is defined as being

$$\begin{aligned}
A_\alpha^{(2)}(s) &= \sum_{b,c} \left(\langle \zeta_{ba}^{*(2)}(s) | \zeta_{ca}^{(2)'}(s) \rangle \right. \\
&+ \epsilon^2 \sum_{\substack{d \neq c \\ f \neq b \\ \delta \neq \alpha}} \frac{V_{d\delta, c\alpha}(s) V_{ba, f\delta}(s)}{\Delta_{c\alpha, d\delta}(s) \Delta_{ba, f\delta}(s)} \langle \zeta_f(s) | \zeta_d'(s) \rangle \left. \right) \\
&\times |\zeta_{ba}^{(2)}(s)\rangle \langle \zeta_{ca}^{*(2)}(s)| \in \mathcal{L}(\mathcal{H}_S)
\end{aligned} \tag{105}$$

with

$$\begin{aligned}
\zeta_{ba}^{(2)} &= \zeta_b + \epsilon \sum_{d \neq b} \frac{V_{d\alpha, ba}}{\Delta_{ba, d\alpha}} \zeta_d \\
&+ \epsilon^2 \sum_{\substack{d \neq b \\ e \neq b}} \frac{V_{d\alpha, e\alpha} V_{e\alpha, ba} - V_{e\alpha, ba} V_{d\alpha, e\alpha}}{\Delta_{ba, d\alpha} \Delta_{ba, e\alpha}} \zeta_d
\end{aligned} \tag{106}$$

$$\begin{aligned}
\langle \zeta_{ca}^{*(2)} | &= \langle \zeta_c | \\
&+ \epsilon \sum_{f \neq c} \frac{V_{c\alpha, f\alpha}}{\Delta_{c\alpha, f\alpha}} \langle \zeta_f | \\
&+ \epsilon^2 \sum_{\substack{d \neq c \\ e \neq c}} \frac{V_{e\alpha, d\alpha} V_{c\alpha, e\alpha} - V_{c\alpha, e\alpha} V_{e\alpha, d\alpha}}{\Delta_{c\alpha, d\alpha} \Delta_{c\alpha, e\alpha}} \langle \zeta_d | \\
&- \epsilon^2 \sum_{\substack{e \\ k \neq e}} \frac{(V_{c\alpha, k\alpha} V_{k\alpha, e\alpha} - V_{k\alpha, e\alpha} V_{c\alpha, k\alpha})(1 - \delta_{ce})}{\Delta_{c\alpha, c\alpha} \Delta_{c\alpha, k\alpha}} \langle \zeta_e |
\end{aligned}$$

$$\begin{aligned}
 & -\epsilon^2 \sum_{\substack{e \\ k \neq c}} \frac{(V_{ka,ea} V_{ca,ka} - V_{ca,ka} V_{ca,ca})(1 - \delta_{ce})}{\Delta_{ca,ea} \Delta_{ca,ka}} \langle \zeta_e | \\
 & -\epsilon^2 \sum_{\substack{e \\ k \neq c \\ \gamma \neq \alpha}} \frac{V_{k\gamma,ea} V_{ca,k\gamma} (1 - \delta_{ke})}{\Delta_{ea,k\gamma} \Delta_{ca,k\gamma}} \langle \zeta_e |
 \end{aligned} \tag{107}$$

$$\begin{aligned}
 \eta_{abc}^{(2)} &= \langle \xi_\alpha | \xi'_\alpha \rangle \delta_{bc} \\
 &+ \epsilon \sum_{\delta \neq \alpha} \frac{V_{b\delta,ca} \langle \xi_\alpha | \xi'_\delta \rangle (1 - \delta_{bc})}{\Delta_{ca,b\delta}} \\
 &+ \epsilon \sum_{\gamma \neq \alpha} \frac{V_{ba,c\gamma} \langle \xi_\gamma | \xi'_\alpha \rangle (1 - \delta_{bc})}{\Delta_{ba,c\gamma}} \\
 &+ \epsilon^2 \sum_{\substack{d \neq c \\ \delta \neq \alpha \\ \gamma}} \frac{V_{d\delta,ca} V_{ba,d\gamma} (1 - \delta_{db}) \langle \xi_\gamma | \xi'_\delta \rangle}{\Delta_{ca,d\delta} \Delta_{ba,d\gamma}} \\
 &+ \epsilon^2 \sum_{\substack{\delta \neq \alpha \\ e \neq c \\ \phi \neq a}} \frac{(V_{b\delta,c\phi} V_{e\phi,ca} - V_{e\phi,ca} V_{ca,ca})(1 - \delta_{bc}) \langle \xi_\alpha | \xi'_\delta \rangle}{\Delta_{ca,b\delta} \Delta_{ca,e\phi}} \\
 &+ \epsilon^2 \sum_{\substack{\gamma \neq \alpha \\ d \neq c}} \frac{V_{ba,d\gamma} V_{da,ca} (1 - \delta_{db}) \langle \xi_\gamma | \xi'_\alpha \rangle}{\Delta_{ba,d\gamma} \Delta_{da,ca}} \\
 &+ \epsilon^2 \sum_{\substack{\delta \neq \alpha \\ e \neq b \\ \phi \neq \alpha}} \frac{(V_{e\phi,c\delta} V_{ba,e\phi} - V_{ba,e\phi} V_{ba,ba})(1 - \delta_{bc}) \langle \xi_\delta | \xi'_\alpha \rangle}{\Delta_{ba,c\delta} \Delta_{ba,e\phi}} \\
 &- \epsilon^2 \sum_{\substack{\phi \neq \alpha \\ k \neq c \\ \gamma \neq \phi, \alpha}} \frac{(V_{ba,k\gamma} V_{k\gamma,c\phi} - V_{k\gamma,c\phi} V_{c\phi,ba})(1 - \delta_{(ba),(c\phi)}) \langle \xi_\phi | \xi'_\alpha \rangle}{\Delta_{c\phi,ba} \Delta_{c\phi,k\gamma}} \\
 &- \epsilon^2 \sum_{\substack{\phi \neq \alpha \\ k \neq b \\ \gamma \neq \alpha}} \frac{(V_{k\gamma,c\phi} V_{ba,k\gamma} - V_{ba,k\gamma} V_{ba,ba})(1 - \delta_{(ba),(c\phi)}) \langle \xi_\phi | \xi'_\alpha \rangle}{\Delta_{ba,c\phi} \Delta_{ba,k\gamma}} \\
 &- \epsilon^2 \sum_{\substack{\phi \neq \alpha \\ k \neq b \\ \gamma \neq \alpha}} \frac{V_{k\gamma,c\phi} V_{ba,k\gamma} (1 - \delta_{(k\gamma),(c\phi)}) \langle \xi_\phi | \xi'_\alpha \rangle}{\Delta_{c\phi,k\gamma} \Delta_{ba,k\gamma}}
 \end{aligned} \tag{108}$$

$\rho_{aa}^{(2)}$ is the corrected density matrix defined as

$$\begin{aligned}
 \rho_{aa}^{(2)} = & \rho_{aa} \\
 & + e^2 \sum_c \frac{V_{c\alpha, d\gamma} V_{d\gamma, a\alpha} (1 - \delta_{ad})}{\Delta_{c\alpha, d\gamma} \Delta_{aa, d\gamma}} |\zeta_c\rangle \langle \zeta_a| \\
 & \quad d \neq c \\
 & \quad \gamma \neq \alpha \\
 & + e^2 \sum_f \frac{V_{d\gamma, f\alpha} V_{aa, d\gamma} (1 - \delta_{ad})}{\Delta_{f\alpha, d\gamma} \Delta_{aa, d\gamma}} |\zeta_a\rangle \langle \zeta_f| \\
 & \quad d \neq c \\
 & \quad \gamma \neq \alpha \\
 & - e^2 \sum_{c, f} \frac{V_{aa, f\delta} V_{c\delta, aa} (1 - \delta_{ac})(1 - \delta_{af})}{\Delta_{aa, f\delta} \Delta_{aa, c\delta}} |\zeta_c\rangle \langle \zeta_f|. \tag{109} \\
 & \quad \delta \neq \alpha
 \end{aligned}$$

The proof is very long but its development is very similar to the first order case except that we need to take into account the biorthonormality and that some second order extra terms involve indices $\delta \neq \alpha$ of \mathcal{E} , which are not killed by the partial trace. The significance of these extra terms and of the higher complexity of the adiabatic transport formula is discussed in the following section.

3.5. Discussion of the operator-valued phases

Operator-valued geometric phases were introduced in [16–18] for density matrices. We recall rapidly the motivation of such geometric phases. The quantum control problems are characterized by the condition $H(1) = H(0)$ (we start and we end with the control system off). This induces $\phi_{aa}(1) = \phi_{aa}(0)$ and then $\rho_{aa}(1) = \rho_{aa}(0)$. But to solve a quantum control problem, we need $\|\rho(1) - \rho_{\text{target}}\|$ to be minimal (with ρ_{target} the control goal and $\rho(s)$ the density matrix of the dynamics such that $\rho(0) = \rho_{aa}(0)$). But if $\rho(1) = \rho_{aa}(1)$ (strong adiabatic regime) it is impossible to solve a quantum control problem by an adiabatic scheme (unless the initial condition is already the control target). In adiabatic quantum control, it is necessary that $\rho(1) = U\rho_{aa}(1)U^\dagger$ with U an operator of \mathcal{S} associated with the adiabatic transport of the mixed state ρ_{aa} , and transforming $\rho_{aa}(1)$ such that $\rho(1)$ is close to ρ_{target} . In comparison with the adiabatic transport of pure states of closed systems ($\psi(1) = e^{i\varphi}\phi_a(1)$, where ϕ_a is an instantaneous eigenvector and $e^{i\varphi}$ is the product of a dynamical and a geometric phase); U plays the role of the product of a dynamical phase and a geometric phase. But these phases are operator valued since U is an operator. This is what we find with the adiabatic transport formula of ρ_{aa} in the weak adiabatic regime.

In [17] by an analysis based on a generalization of the geometric structure describing the usual adiabatic geometric phases (using a noncommutative Hilbert space—a C^* -module—and a categorical principal bundle) the generator of an operator-valued geometric phase has been defined by (we use the present notations)

$$A_\alpha = \text{tr}_{\mathcal{E}} \left(|P_\alpha \phi'_{aa}\rangle \rangle \langle \langle \phi_{aa} | \right) \rho_{aa}^{-1} \tag{110}$$

where ρ_{aa}^{-1} is the pseudo-inverse of ρ_{aa} ($\rho_{aa}\rho_{aa}^{-1} = 1 - P_{\text{ker}\rho_{aa}}$ where $P_{\text{ker}\rho_{aa}}$ is the orthogonal projection onto the kernel of ρ_{aa}). By considering the perturbative expansions we find that

$$A_\alpha = A^{(0)} + \langle \xi_\alpha | \xi'_\alpha \rangle + \mathcal{O}(\epsilon) \quad (111)$$

$$= A_\alpha^{(1)} + \langle \xi_\alpha | \xi'_\alpha \rangle + \mathcal{O}(\epsilon^2). \quad (112)$$

Up to a $U(1)$ -gauge change leaving invariant the density matrix $\rho(s)$ ($e^{-\int_0^s \langle \xi_\alpha | \xi'_\alpha \rangle d\sigma} \in U(1)$), the operator-valued geometric phases found in the present paper coincide with the definition introduced in [17], which is a generalization of the geometric phases introduced in [13–16].

The role of the operator-valued dynamical phase is interesting. Suppose temporarily that $\zeta_{ba}^{(1)}$ is constant (independent of s) but not $\lambda_{ba}(s)$. In this assumption we have

$$\rho(s) \simeq \mathfrak{A} \mathfrak{d} \left[\mathbb{T} e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(1)}(\sigma) d\sigma} \right] \rho_{aa} \quad (113)$$

This induces

$$i\hbar\dot{\rho} \simeq [E_\alpha^{(1)}, \rho]. \quad (114)$$

This expression is very similar to the Liouville–von Neumann equation of an isolated system ([9]): if S is isolated and governed by the self-adjoint Hamiltonian $H_S \in \mathcal{L}(\mathcal{H}_S)$, we have

$$i\hbar\dot{\rho} = [H_S, \rho]. \quad (115)$$

$E_\alpha^{(1)}$ plays then the role of an effective Hamiltonian of S taking into account effects induced by \mathcal{E} . We can consider $E_\alpha^{(1)}$ as the effective Hamiltonian of S dressed by \mathcal{E} , as the Floquet Hamiltonian of an atom interacting with a strong laser field is the effective Hamiltonian of the atom dressed by the photons [25, 26].

In reality $\zeta_{ba}^{(1)}$ depends on the reduced time s , and $E_\alpha^{(1)}$ is described by using a moving basis. The operator-valued geometric phase (as for all geometric phases) is just a correction to take into account the movement of the basis (as for the simpler example, the inertial forces are corrections in Newtonian mechanics to take into account a description in a noninertial frame).

Concerning the second order adiabatic transport formula, we suppose temporarily again that $\zeta_{ba}^{(2)}$ and $\mathcal{W}_{\delta\alpha}$ are constant. By using the expression (101), $\rho(s) \simeq \mathfrak{A} \mathfrak{d} [U_\alpha] \rho_{aa}^{(2)} + \epsilon^2 \sum_{\delta \neq \alpha} \mathfrak{A} \mathfrak{d} [\mathcal{W}_{\delta\alpha} U_\alpha] \rho_{aa}^{(2)}$ satisfies

$$i\hbar\dot{\rho} \simeq E_\alpha^{(2)} \rho - \rho E_\alpha^{(2)\dagger} + \epsilon^2 \sum_{\delta \neq \alpha} \mathcal{W}_{\delta\alpha} (E_\alpha^{(2)} \rho - \rho E_\alpha^{(2)\dagger}) \mathcal{W}_{\delta\alpha}^\dagger \quad (116)$$

$$\begin{aligned} &\simeq [E_{\alpha+}^{(2)}, \rho] + \mathfrak{I} \{ E_{\alpha-}^{(2)}, \rho \} \\ &\quad + \epsilon^2 \sum_{\delta \neq \alpha} \mathcal{W}_{\delta\alpha} \left([E_{\alpha+}^{(2)}, \rho] + \mathfrak{I} \{ E_{\alpha-}^{(2)}, \rho \} \right) \mathcal{W}_{\delta\alpha}^\dagger \end{aligned} \quad (117)$$

where $E_{\alpha+}^{(2)} = \frac{1}{2}(E_\alpha^{(2)} + E_\alpha^{(2)\dagger})$ and $E_{\alpha-}^{(2)} = \frac{1}{2i}(E_\alpha^{(2)} - E_\alpha^{(2)\dagger})$; the braces denote the anticommutator ($\mathfrak{I}\{A, B\} = AB + BA$). The dynamical phase generator has the form $E_\alpha^{(2)} = E_{\alpha 0}^{(2)} - \epsilon^2 \sum_{\delta \neq \alpha} E_{\alpha 0}^{(2)} \mathcal{W}_{\delta\alpha}^\dagger \mathcal{W}_{\delta\alpha}$, and then $E_{\alpha+}^{(2)} = E_{\alpha 0}^{(2)} - \frac{\epsilon^2}{2} \sum_{\delta \neq \alpha} \{E_{\alpha 0}^{(2)}, \mathcal{W}_{\delta\alpha}^\dagger \mathcal{W}_{\delta\alpha}\}$ and $E_{\alpha-}^{(2)} = -\frac{\epsilon^2}{2i} \sum_{\delta \neq \alpha} [E_{\alpha 0}^{(2)}, \mathcal{W}_{\delta\alpha}^\dagger \mathcal{W}_{\delta\alpha}]$. This implies that

$$\begin{aligned} i\hbar\dot{\rho} &\simeq [E_{\alpha+}^{(2)}, \rho] - \frac{\epsilon^2}{2} \sum_{\delta \neq \alpha} \left\{ [E_{\alpha 0}^{(2)}, \mathcal{W}_{\delta\alpha}^\dagger \mathcal{W}_{\delta\alpha}], \rho \right\} \\ &\quad + \epsilon^2 \sum_{\delta \neq \alpha} \mathcal{W}_{\delta\alpha} [E_{\alpha 0}^{(2)}, \rho] \mathcal{W}_{\delta\alpha}^\dagger \end{aligned} \quad (118)$$

Let $\Gamma_{\alpha\delta 0} = \mathcal{W}_{\delta\alpha} + 1\mathcal{W}_{\delta\alpha}E_{\alpha 0}^{(2)}$, $\Gamma_{\alpha\delta 1} = \mathcal{W}_{\delta\alpha}$ and $\Gamma_{\alpha\delta 2} = \mathcal{W}_{\delta\alpha}E_{\alpha 0}^{(2)}$; we have then

$$\begin{aligned} i\hbar\dot{\rho} \simeq & \left[E_{\alpha+}^{(2)}, \rho \right] - \frac{1\epsilon^2}{2} \sum_{\delta \neq \alpha} \sum_k \gamma^k \left\{ \Gamma_{\alpha\delta k}^\dagger \Gamma_{\alpha\delta k}, \rho \right\} \\ & + 1\epsilon^2 \sum_{\delta \neq \alpha} \sum_k \gamma^k \Gamma_{\alpha\delta k} \rho \Gamma_{\alpha\delta k}^\dagger \end{aligned} \quad (119)$$

with $\gamma^0 = 1$ and $\gamma^1 = \gamma^2 = -1$. This last equation is similar to the Lindblad equation of an open quantum system in the Markovian approximation [9] (except that in the strict Lindblad theory $\gamma^k > 0$ for all k). $E_{\alpha}^{(2)}$ and $\mathcal{W}_{\alpha\delta}$ then generate an effective Lindblad equation for \mathcal{S} in contact with \mathcal{E} . The extra terms involving indices of \mathcal{E} different from α in equation (101) are then associated with the ‘quantum jumps’ (see [9]). The geometric phase is again a correction to take into account that the biorthonormal basis $\{\zeta_{b\alpha}^{(2)}, \zeta_{b\alpha}^{*(2)}\}_b$ is moving.

3.6. The thermal bath case

When \mathcal{E} is a large subsystem, it can be interesting to consider it at $s = 0$ as being a thermal bath, i.e. \mathcal{E} is described by the density matrix

$$\rho_B = \frac{e^{-\beta H_{\mathcal{E}}(0)}}{Z} = \sum_{\alpha} \frac{e^{-\beta \nu_{\alpha}(0)}}{Z} \left| \xi_{\alpha}(0) \right\rangle \left\langle \xi_{\alpha}(0) \right| \quad (120)$$

where $\beta = \frac{1}{k_B \underline{T}}$ (\underline{T} being the temperature of the bath and k_B being the Boltzmann constant; the underline is just a notation to avoid confusion with state indices or with the duration of the evolution). The partition function is $Z = \text{tr}_{\mathcal{E}} e^{-\beta H_{\mathcal{E}}(0)}$. Let $\rho_{\mathcal{V}} \in \mathcal{L}(\mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{E}})$ be the density matrix of the complete bipartite system solution of the Liouville–von Neumann equation:

$$\frac{1\hbar}{T} \rho'_{\mathcal{V}}(s) = \left[H_{\mathcal{S}}(s) \otimes 1_{\mathcal{E}} + 1_{\mathcal{S}} \otimes H_{\mathcal{E}}(s) + \epsilon V(s), \rho_{\mathcal{V}}(s) \right] \quad (121)$$

$$\rho_{\mathcal{V}}(0) = \sum_{\alpha} \frac{e^{-\beta \nu_{\alpha}(0)}}{Z} \left| \phi_{\alpha\alpha}(0) \right\rangle \left\langle \phi_{\alpha\alpha}(0) \right|. \quad (122)$$

We have $\text{tr}_{\mathcal{S}} \rho_{\mathcal{V}}(0) = \rho_B + \mathcal{O}(\epsilon^2)$, implying that \mathcal{E} is a good thermal bath (moreover $\rho_{\mathcal{V}}$ is a steady state of $H(0)$). The solution of the Liouville–von Neumann equation is

$$\rho_{\mathcal{V}}(s) = \sum_{\alpha} \frac{e^{-\beta \nu_{\alpha}(0)}}{Z} \left| \psi_{(\alpha\alpha)}(s) \right\rangle \left\langle \psi_{(\alpha\alpha)}(s) \right| \quad (123)$$

where $\psi_{(\alpha\alpha)}$ is the solution of the Schrödinger equation $\frac{1\hbar}{T} \psi'_{(\alpha\alpha)} = H \psi_{(\alpha\alpha)}$ with the initial condition $\psi_{(\alpha\alpha)}(0) = \phi_{\alpha\alpha}(0)$. At the weak adiabatic limit we have then

$$\rho(s) = \text{tr}_{\mathcal{E}} \rho_{\mathcal{V}}(s) \quad (124)$$

$$\begin{aligned} &= \sum_{\alpha} \frac{e^{-\beta \nu_{\alpha}(0)}}{Z} \mathfrak{A} \mathfrak{D} \left[\overleftarrow{\mathbb{T}} e^{-1\hbar^{-1}T \int_0^s E_{\alpha}^{(1)}(\sigma) d\sigma} \overrightarrow{\mathbb{T}} e^{-\int_0^s A_{\alpha}^{(1)}(\sigma) d\sigma} \right] \rho_{\alpha\alpha}(s) \\ &+ \mathcal{O} \left(\max \left(\frac{1}{T}, \epsilon^2 \right) \right). \end{aligned} \quad (125)$$

3.7. Eigenvalue crossings of \mathcal{E} in the weak adiabatic regime

The weak adiabatic theorem (theorem 2) requires that the eigenvalue of \mathcal{E} , $\nu_\alpha(s)$, does not cross another eigenvalue. Although this requirement is natural for the control problem, it may not be realized in practice. Suppose that $\exists s_* \in [0, 1]$ such that $\nu_\alpha(s_*) = \nu_\beta(s_*)$ (no other crossings implying ν_α and ν_β occur). We suppose that the conditions of the weak adiabatic theorem are satisfied except in the neighbourhood of s_* . Due to the nonadiabatic transitions induced in the neighbourhood of s_* by this crossing, the density matrix becomes (for $s \gg s_*$)

$$\begin{aligned} \rho(s) = & (1-p) \mathfrak{A} \mathfrak{D} \left[\mathbb{T} e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(1)} d\sigma} \mathbb{T} e^{-\int_0^s A_\alpha^{(1)} d\sigma} \right] \rho_{\alpha\alpha}(s) \\ & + p \mathfrak{A} \mathfrak{D} \left[\mathbb{T} e^{-i\hbar^{-1}T \int_0^s E_\beta^{(1)} d\sigma} \mathbb{T} e^{-\int_0^s A_\beta^{(1)} d\sigma} \right] \rho_{\alpha\beta}(s) \\ & + \sqrt{(1-p)p} e^{i\varphi} \mathfrak{A} \mathfrak{D} \left[\mathbb{T} e^{-i\hbar^{-1}T \int_0^s E_\alpha^{(1)} d\sigma} \mathbb{T} e^{-\int_0^s A_\alpha^{(1)} d\sigma} \right] \tau_{\alpha\alpha\beta}(s) \\ & + \sqrt{(1-p)p} e^{-i\varphi} \mathfrak{A} \mathfrak{D} \left[\mathbb{T} e^{-i\hbar^{-1}T \int_0^s E_\beta^{(1)} d\sigma} \mathbb{T} e^{-\int_0^s A_\beta^{(1)} d\sigma} \right] \tau_{\alpha\beta\alpha}(s) \\ & + \mathcal{O} \left(\max \left(\frac{1}{T}, \epsilon^2 \right) \right) \end{aligned} \quad (126)$$

where $\mathfrak{A} \mathfrak{D} [U] \tau = U_\alpha \tau U_\beta^\dagger$ and

$$\tau_{\alpha\alpha\beta} = \text{tr}_{\mathcal{E}} \left| \phi_{\alpha\alpha} \right\rangle \left\langle \left\langle \phi_{\alpha\beta} \right| \right. \quad (127)$$

$$\begin{aligned} & = \epsilon \sum_{d \neq \alpha} \frac{V_{d\beta, \alpha\alpha}}{\mu_\alpha - \mu_d + \nu_\alpha - \nu_\beta + \epsilon V_{\alpha\alpha, \alpha\alpha}} |\zeta_d\rangle \langle \zeta_\alpha| \\ & + \epsilon \sum_{d \neq \alpha} \frac{V_{\alpha\beta, d\alpha}}{\mu_\alpha - \mu_d + \nu_\beta - \nu_\alpha + \epsilon V_{\alpha\beta, \alpha\beta}} |\zeta_\alpha\rangle \langle \zeta_d| + \mathcal{O}(\epsilon^2). \end{aligned} \quad (128)$$

p is the probability of the nonadiabatic transition from ξ_α to ξ_β induced by the passage through the crossing, and φ is a phase difference accumulated during the nonadiabatic transition. It is clear that the crossing of eigenenergies of \mathcal{E} generates a decoherence effect in the density matrix of S that we call *kinematic decoherence* since it is induced by the variation of the control system with respect to time. In practice it can be difficult to compute p explicitly, but if we suppose that $\forall s \in \mathcal{V}(s_*)$, $\nu_\beta(s) - \nu_\alpha(s) = \mathfrak{N}(s - s_*)$ (\mathfrak{N} being a constant) and that $V_{\alpha\alpha, \alpha\beta}$ is independent of s , then p can be estimated by the Landau–Zener formula [27, 28], i.e.

$$p = e^{-2\pi \frac{\tau_{\alpha\alpha, \alpha\beta}^2}{\hbar |\mathfrak{N}|}}.$$

4. Examples

In this section we present two examples of bipartite quantum systems and we study their adiabatic dynamics. We want to compare their real dynamics (numerically computed using a split operator method without another approximation) to the prediction of the usual adiabatic transport formula for S alone (by neglecting the influence of \mathcal{E} , an approximation currently considered in adiabatic control methods), and to the prediction of the adiabatic transport formulae with operator-valued phases, which considers S dressed by states of \mathcal{E} (the operator-valued phases are numerically computed by the same split operator method with the same

time discretization; nevertheless, the dimension of the matrices— $\dim\mathcal{H}_S$ —is reduced in comparison with the ‘exact’ computation— $\dim\mathcal{H}_S \times \dim\mathcal{H}_E$).

4.1. Control of atomic qubits

4.1.1. The model. We consider a two level atom S interacting with a laser field which is governed in the rotating wave approximation with one photon by the Hamiltonian

$$H_S(s) = \frac{\hbar}{2} \begin{pmatrix} 0 & \Omega(s)e^{i\varphi(s)} \\ \Omega(s)e^{-i\varphi(s)} & 2\Delta(s) \end{pmatrix} \quad (129)$$

$$= \frac{\hbar}{2} \left(\Omega(s) \cos \varphi(s) \sigma_x + \Omega(s) \sin \varphi(s) \sigma_y + \Delta(s) (\text{id} - \sigma_z) \right) \quad (130)$$

where $\Omega(s)$ is the product between the electric field strength and the dipolar moment of the atom, φ is the dephasing of the laser field, and Δ is the detuning (the energy gap between the two atomic states minus the energy of one photon of the laser field). This system can be viewed like a model of one qubit where the laser field is the control system performing a one input/output logic gate on it. (σ_x , σ_y , σ_z) are the Pauli matrices.

A second atom (qubit) \mathcal{E} is in contact with the first one and is governed by the following Hamiltonian:

$$H_E = \begin{pmatrix} 0 & 0 \\ 0 & \hbar\omega_e \end{pmatrix} = \frac{\hbar\omega_e}{2} (\text{id} - \sigma_z). \quad (131)$$

The interaction between the two atoms is chosen as being

$$\epsilon V = \epsilon \begin{pmatrix} V_0 & V_1 & 0 & V_3 \\ V_1 & V_0 & V_3 & 0 \\ 0 & V_3 & 2V_0 & V_2 \\ V_3 & 0 & V_2 & 2V_0 \end{pmatrix} \quad (132)$$

$$= \epsilon \left(\left(\frac{V_0}{2} \text{id} \otimes (\text{id} + \sigma_z) + V_0 \text{id} \otimes (\text{id} - \sigma_z) \right) \right. \\ \left. + \frac{V_1}{2} \sigma_x \otimes (\text{id} + \sigma_z) + \frac{V_2}{2} \sigma_x \otimes (\text{id} - \sigma_z) + V_3 \sigma_x \otimes \sigma_x \right) \quad (133)$$

in a matrix representation where the two first inputs are associated with both states of S and the ground state of \mathcal{E} , and the two last inputs are associated with both states of S and the excited state of \mathcal{E} . $\epsilon \ll 1$ is the perturbative parameter.

Let $r(s) = \sqrt{\Omega(s)^2 + \Delta(s)^2}$ and $\theta(s) = \arctan \frac{\Omega(s)}{\Delta(s)}$ be variable changes of the control parameters. The eigenvalues and the eigenvectors of both components of the bipartite system are

$$\mu_0(s) = \frac{\hbar}{2} r(s) (\cos \theta(s) - 1) \quad \zeta_0(s) = \begin{pmatrix} -\cos \frac{\theta(s)}{2} \\ e^{-i\varphi(s)} \sin \frac{\theta(s)}{2} \end{pmatrix} \quad (134)$$

$$\mu_1(s) = \frac{\hbar}{2} r(s) (\cos \theta(s) + 1) \quad \zeta_1(s) = \begin{pmatrix} e^{i\varphi(s)} \sin \frac{\theta(s)}{2} \\ \cos \frac{\theta(s)}{2} \end{pmatrix} \quad (135)$$

$$\nu_0 = 0 \quad \xi_0 = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad (136)$$

$$\nu_1 = \hbar \omega_e \quad \xi_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (137)$$

The control is fixed by the following variation of the control parameters:

$$r(s) = r_{\max} + (r_{\min} - r_{\max}) e^{-25(s-0.5)^2} \quad (138)$$

$$\theta(s) = \theta_{\max} \sin(\pi s) \quad (139)$$

$$\varphi(s) = 2\pi s \quad (140)$$

corresponding to laser pulses and a laser frequency modulation represented in figure 1 and with a drifting phase.

4.1.2. Adiabatic transport. We start with both qubits in the ground state, $\phi_{00}(0)$ with $\Omega(0) = 0$ (the control laser is off). The adiabatic transport of the density matrix for S alone is

$$\rho_{\text{alone-ad}}(s) = |\zeta_0(s)\rangle\langle\zeta_0(s)|. \quad (141)$$

If the dynamics of both qubits is strongly adiabatic the adiabatic transport of the density matrix is

$$\begin{aligned} \rho_{\text{strong-ad}}(s) &= \rho_{00}(s) \quad (142) \\ &= |\zeta_0(s)\rangle\langle\zeta_0(s)| \\ &\quad + \frac{\epsilon V_1}{-\hbar r(s) + \epsilon(V_0 - V_1 \cos \varphi(s) \sin \theta(s))} \\ &\quad \times \left(\left(e^{2i\varphi(s)} \sin^2 \frac{\theta(s)}{2} - \cos^2 \frac{\theta(s)}{2} \right) |\zeta_0(s)\rangle\langle\zeta_1(s)| \right. \\ &\quad \left. + \left(e^{-2i\varphi(s)} \sin^2 \frac{\theta(s)}{2} - \cos^2 \frac{\theta(s)}{2} \right) |\zeta_1(s)\rangle\langle\zeta_0(s)| \right) \end{aligned} \quad (143)$$

and if the dynamics is weakly adiabatic the adiabatic transport of the density matrix is

$$\rho_{\text{weak-ad}}(s) = \mathfrak{A} \mathfrak{D} \left[\mathbb{T} e^{-i\hbar^{-1}T \int_0^s E_0^{(1)}(\sigma) d\sigma} \mathbb{T} e^{-\int_0^s A_0^{(1)}(\sigma) d\sigma} \right] \rho_{00}(s) \quad (144)$$

with

$$E_0^{(1)} = \lambda_{00} |\zeta_{00}^{(1)}\rangle\langle\zeta_{00}^{(1)}| + \lambda_{10} |\zeta_{10}^{(1)}\rangle\langle\zeta_{10}^{(1)}| \quad (145)$$

$(\eta^{(1)} = 0$ because (ξ_{β}) are independent of s), and

$$A_0^{(1)} = \sum_{b,c=0}^1 \left\langle \zeta_{b0}^{(1)} \left| \zeta_{c0}^{(1)'} \right. \right\rangle \zeta_{b0}^{(1)} \left\langle \zeta_{c0}^{(1)} \right| \quad (146)$$

where

$$\lambda_{00} = \frac{\hbar}{2} r (\cos \theta - 1) + \epsilon (V_0 - V_1 \cos \varphi \sin \theta) + \mathcal{O}(\epsilon^2) \quad (147)$$

$$\lambda_{10} = \frac{\hbar}{2} r (\cos \theta + 1) + \epsilon (V_0 + V_1 \cos \varphi \sin \theta) + \mathcal{O}(\epsilon^2) \quad (148)$$

$$\lambda_{01} = \frac{\hbar}{2} r (\cos \theta - 1) + \hbar \omega_e + \epsilon (2V_0 - V_2 \cos \varphi \sin \theta) + \mathcal{O}(\epsilon^2) \quad (149)$$

$$\lambda_{11} = \frac{\hbar}{2} r (\cos \theta + 1) + \hbar \omega_e + \epsilon (2V_0 + V_2 \cos \varphi \sin \theta) + \mathcal{O}(\epsilon^2) \quad (150)$$

and

$$\zeta_{00}^{(1)} = \zeta_0 + \frac{\epsilon V_1 \left(e^{-2i\varphi} \sin^2 \frac{\theta}{2} - \cos^2 \frac{\theta}{2} \right)}{-\hbar r + \epsilon (V_0 - V_1 \cos \varphi \sin \theta)} \zeta_1 \quad (151)$$

$$\zeta_{10}^{(1)} = \zeta_1 + \frac{\epsilon V_1 \left(e^{2i\varphi} \sin^2 \frac{\theta}{2} - \cos^2 \frac{\theta}{2} \right)}{\hbar r + \epsilon (V_0 + V_1 \cos \varphi \sin \theta)} \zeta_0 \quad (152)$$

$$\zeta_{01}^{(1)} = \zeta_0 + \frac{\epsilon V_2 \left(e^{-2i\varphi} \sin^2 \frac{\theta}{2} - \cos^2 \frac{\theta}{2} \right)}{-\hbar r + \epsilon (2V_0 - V_1 \cos \varphi \sin \theta)} \zeta_1 \quad (153)$$

$$\zeta_{11}^{(1)} = \zeta_1 + \frac{\epsilon V_2 \left(e^{2i\varphi} \sin^2 \frac{\theta}{2} - \cos^2 \frac{\theta}{2} \right)}{\hbar r + \epsilon (2V_0 + V_1 \cos \varphi \sin \theta)} \zeta_0. \quad (154)$$

The energies of both qubits are represented in figure 2.

4.1.3. Strong adiabatic regime. We study a strong adiabatic regime where $T = 20000$ au, $\tau_S = \inf_{s \in [0,1]} \frac{\hbar}{|\mu_1(s) - \mu_0(s)|} = 2$ au and $\theta^\epsilon = \frac{\hbar}{\epsilon \|V\|} = 21$ au (au: atomic unit). We have $T \gg \theta^\epsilon \sim \tau_S$ and do not have resonance between transitions of S and \mathcal{E} involving ϕ_{00} as shown in figure 2. The assumptions of theorem 1 are then satisfied. The population of qubit state 0 $\langle \zeta_0(0) | \rho(s) | \zeta_0(0) \rangle$ and the coherence of the controlled atom $|\langle \zeta_0(0) | \rho(s) | \zeta_1(0) \rangle|$ (note that $(\zeta_0(0), \zeta_1(0))$ is the eigenstate of the bare atom S since the laser is off at $s = 0$) are represented in figure 3. The errors between the different adiabatic transport formulae and the exact dynamics are plotted in figure 4. The errors concerning the population reach 10^{-2} with the prediction of the adiabatic transport formula for S alone (in accordance with the fact that the order of the coupling between S and \mathcal{E} is $\epsilon = 1.6 \times 10^{-2}$), while the errors concerning the coherence reach 2.5×10^{-2} . The strong adiabatic transport formula permits us to gain more than one order of magnitude on the errors in accordance with the theoretical error $\frac{\theta^\epsilon}{T} = 10^{-3}$.

4.1.4. Weak adiabatic regime. We study a weak adiabatic regime where $T = 200$ au, $\tau_S = \inf_{s \in [0,1]} \frac{\hbar}{|\mu_1(s) - \mu_0(s)|} = 50$ au, $\theta^\epsilon = \frac{\hbar}{\epsilon \|V\|} = 667$ au and $\tau_{\mathcal{E}} = \frac{1}{\omega_e} = 2$ au (au: atomic unit).

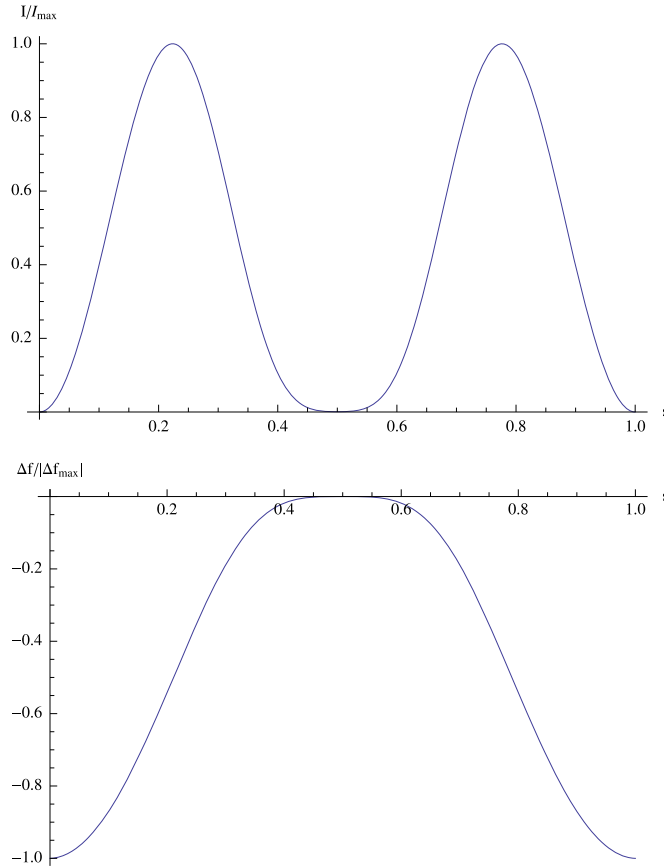


Figure 1. Intensity of the laser pulses applied on the atom with respect to the reduced time (top) and difference of the modulated laser frequency with the frequency of the atomic transition with respect to the reduced time (bottom).

We have $\theta^\epsilon \sim \tau_S \sim T$ and $T \gg \tau_\epsilon$ and there is no quasi-resonance between transitions of S and \mathcal{E} . The assumptions of theorem 2 are then satisfied. The population of qubit state 0 $\langle \zeta_0(0) | \rho(s) | \zeta_0(0) \rangle$ and the coherence of the controlled atom $|\langle \zeta_0(0) | \rho(s) | \zeta_1(0) \rangle|$ are represented in figure 5. The errors between the different adiabatic transport formulae and the exact dynamics are plotted in figure 6. The errors of the prediction of the adiabatic transport formula with S alone are now very large in accordance with the very small gap between the two eigenvalues of $H_S(s)$ during the dynamics. The weak adiabatic transport formula provides a very good approximation with an error smaller than $\frac{\tau_\epsilon}{T} = 10^{-3}$ in accordance with the theoretical error $\max\left(\frac{\tau_\epsilon}{T}, \epsilon^2\right)$.

4.2. Control of a spin in the middle of a chain

4.2.1. The model. We consider a Heisenberg line chain of $2N + 1$ spins with nearest neighbour interaction. A constant and uniform magnetic field $\vec{B}_{\text{Zeeman}} = -\frac{\omega_e}{2} \vec{e}_z$ is applied on all the spins of the chain in order to split the energy levels of the spins by a Zeeman effect. A time dependent magnetic field $\vec{B}_{\text{control}}(s)$ is applied only on the middle spin denoted by S to

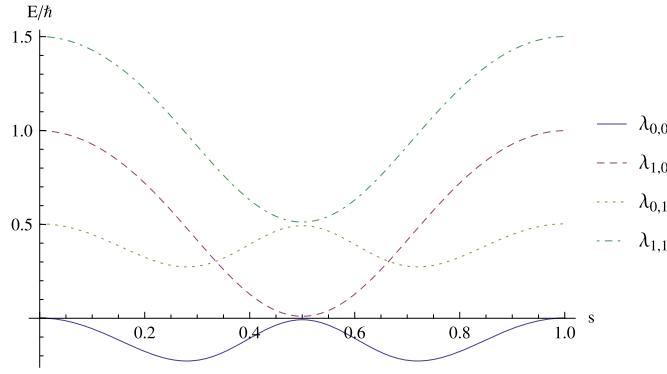


Figure 2. Instantaneous energies of both atoms during the control with respect to the reduced time (with $\hbar\omega_e = 0.5$ au, $r_{\max} = 1$ au, $r_{\min} = 0.02$ au, $V_0 = 3$ au, $V_1=1.5$ au, $V_2=0.5$ au, $V_3=2.5$ au, $\theta_{\max} = \frac{\pi}{2}$ and $\epsilon = 5 \times 10^{-4}$ (au: atomic unit)).

control it. S is governed by the Hamiltonian

$$H_S(s) = \vec{B}(s) \cdot \vec{S} \quad (155)$$

$$= \frac{\hbar}{2} (B_x(s)\sigma_x + B_y(s)\sigma_y + B_z(s)\sigma_z). \quad (156)$$

$\vec{S} = \frac{\hbar}{2}(\sigma_x, \sigma_y, \sigma_z)$ is the spin operator ($\{\sigma_i\}_i$ are the Pauli matrices) and $\vec{B}(s) = \vec{B}_{\text{control}}(s) + \vec{B}_{\text{Zeeman}}$. The rest of the chain is denoted by \mathcal{E} and is described by the Hilbert space $\mathcal{H}_{\mathcal{E}} = \mathcal{H}_{\mathcal{E}l} \otimes \mathcal{H}_{\mathcal{E}r}$ where $\mathcal{H}_{\mathcal{E}l/r} = (\mathbb{C}^2)^{\otimes N}$ are the Hilbert spaces of the half chains on the left and on the right of the controlled spin. \mathcal{E} is governed by the Hamiltonian

$$H_{\mathcal{E}} = H_C \otimes \text{id}^{\otimes N} + \text{id}^{\otimes N} \otimes H_C \quad (157)$$

$$H_C = \sum_{n=1}^N \text{id}^{\otimes(n-1)} \otimes \vec{B}_{\text{Zeeman}} \cdot \vec{S} \otimes \text{id}^{\otimes(N-n)} - J \sum_{n=1}^{N-1} \text{id}^{\otimes(n-1)} \otimes \vec{S} \otimes \vec{S} \otimes \text{id}^{\otimes(N-n-1)} \quad (158)$$

where id denotes the identity operator for one spin, $\vec{S} \otimes \vec{S} = \sum_{i=x,y,z} S_i \otimes S_i$, and J is the coupling constant. The interaction between S and \mathcal{E} is described by

$$V_{S-\mathcal{E}} = -J\vec{S} \otimes (\text{id}^{\otimes(N-1)} \otimes \vec{S} \otimes \text{id}^{\otimes N} + \text{id}^{\otimes N} \otimes \vec{S} \otimes \text{id}^{\otimes(N-1)}) \quad (159)$$

with $V_{S-\mathcal{E}} \in \mathcal{H}_S \otimes \mathcal{H}_{\mathcal{E}}$. The coupling constant $J \ll 1$ is the perturbative parameter.

Let $B(s) = \|\vec{B}(s)\|$, $\theta(s) = \arccos \frac{B_z(s)}{B(s)}$ and $\varphi(s) = \arctan \frac{B_y(s)}{B_x(s)}$. The eigenvalues and the eigenvectors of S are

$$\mu_0(s) = -\frac{\hbar}{2}B(s) \quad \zeta_0(s) = \begin{pmatrix} -\sin \frac{\theta(s)}{2} \\ e^{i\varphi(s)} \cos \frac{\theta(s)}{2} \end{pmatrix} \quad (160)$$

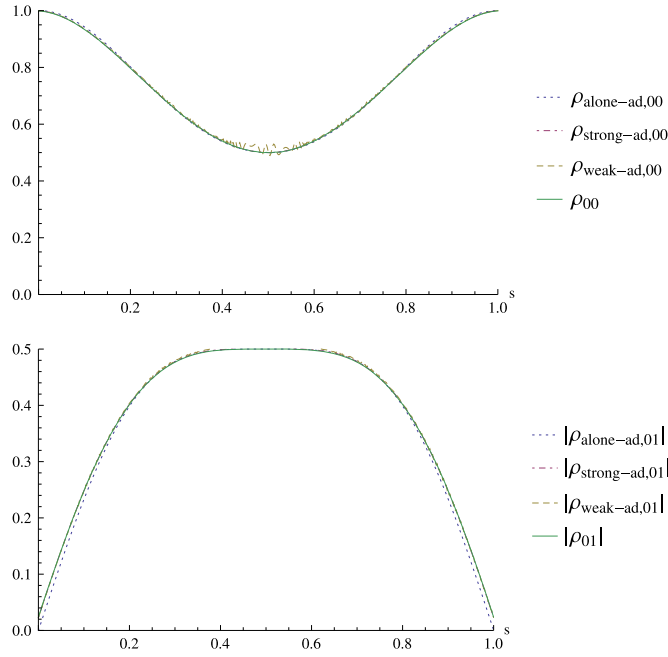


Figure 3. Population of qubit state 0 $\rho_{*,00} = \langle \zeta_0(0) | \rho_*(s) | \zeta_0(0) \rangle$ (top) and coherence $\rho_{*,01} = |\langle \zeta_0(0) | \rho_*(s) | \zeta_1(0) \rangle|$ (bottom) for the exact dynamics ($\bullet = \emptyset$), the adiabatic transport formula with S alone ($\bullet = \text{alone-ad}$), the strong adiabatic transport formula ($\bullet = \text{strong-ad}$) and the weak adiabatic transport formula ($\bullet = \text{weak-ad}$), in conditions corresponding to a strong adiabatic regime (with $\hbar\omega_e = 1.5$ au, $r_{\max} = 1$ au, $r_{\min} = 0.5$ au, $V_0 = 3$ au, $V_1 = 1.5$ au, $V_2 = 0.5$ au, $V_3 = 2.5$ au, $\theta_{\max} = \frac{\pi}{2}$ and $\epsilon = 1.6 \times 10^{-2}$ (au: atomic unit)).

$$\mu_1(s) = +\frac{\hbar}{2}B(s) \quad \zeta_1(s) = \begin{pmatrix} e^{-i\varphi(s)} \cos \frac{\theta(s)}{2} \\ \sin \frac{\theta(s)}{2} \end{pmatrix}. \quad (161)$$

The eigenvalues of \mathcal{E}_l or \mathcal{E}_r for $N = 3$ are

$$\nu_{(000)} = -3\frac{\hbar\omega_e}{4} - J\frac{\hbar^2}{2} + \mathcal{O}(J^2) \quad (162)$$

$$\nu_{(100)-(001)} = -\frac{\hbar\omega_e}{4} + \mathcal{O}(J^2) \quad (163)$$

$$\nu_{(001)+(010)+(100)} = -\frac{\hbar\omega_e}{4} - J\frac{\hbar^2}{2} + \mathcal{O}(J^2) \quad (164)$$

$$\nu_{(001)-2(010)+(100)} = -\frac{\hbar\omega_e}{4} + J\hbar^2 + \mathcal{O}(J^2) \quad (165)$$

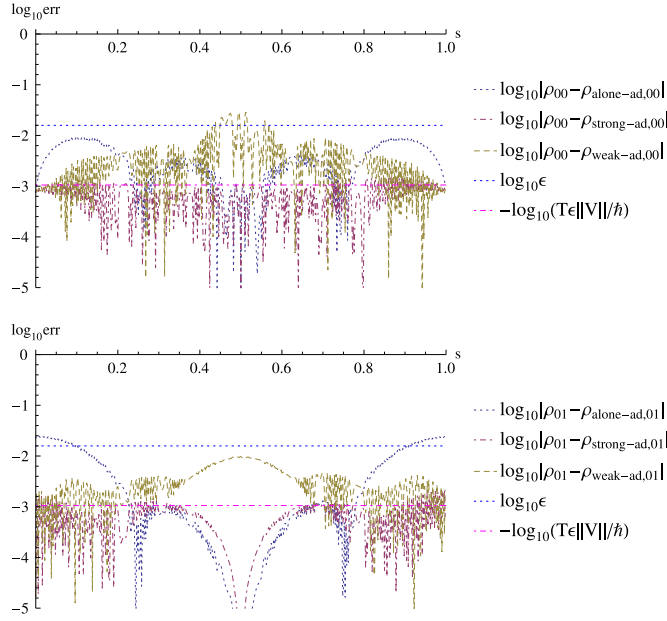


Figure 4. Errors in logarithmic scale between the approximations of the adiabatic transport formulae and the exact dynamics for the population of qubit state 0 (top) and the coherence (bottom) in conditions corresponding to a strong adiabatic regime (with $\hbar\omega_e = 1.5$ au, $r_{\max} = 1$ au, $r_{\min} = 0.5$ au, $V_0 = 3$ au, $V_1 = 1.5$ au, $V_2 = 0.5$ au, $V_3 = 2.5$ au, $\theta_{\max} = \frac{\pi}{2}$ and $\epsilon = 1.6 \times 10^{-2}$ (au: atomic unit)).

$$\nu_{(110)-(011)} = \frac{\hbar\omega_e}{4} + \mathcal{O}(J^2) \quad (166)$$

$$\nu_{(011)+(101)+(110)} = \frac{\hbar\omega_e}{4} - J\frac{\hbar^2}{2} + \mathcal{O}(J^2) \quad (167)$$

$$\nu_{(011)-2(101)+(110)} = \frac{\hbar\omega_e}{4} + J\hbar^2 + \mathcal{O}(J^2) \quad (168)$$

$$\nu_{(111)} = 3\frac{\hbar\omega_e}{4} - J\frac{\hbar^2}{2} + \mathcal{O}(J^2) \quad (169)$$

which are associated with the eigenvectors

$$\xi_{(ijk)} = |i\rangle \otimes |j\rangle \otimes |k\rangle \quad (170)$$

$$\xi_{a(ijk)+b(lmn)+c(opq)} = \frac{1}{\sqrt{a^2 + b^2 + c^2}} (a\xi_{ijk} + b\xi_{lmn} + c\xi_{opq}) \quad (171)$$

$(|i\rangle)_{i=0,1}$ being the eigenstates of an isolated spin.

The control is fixed by the following variation of the control parameters:

$$B(s) = B_0 \left(1 - e^{-(s-0.5)^2/\Delta s^2} \right) + B_{\min} \quad (172)$$

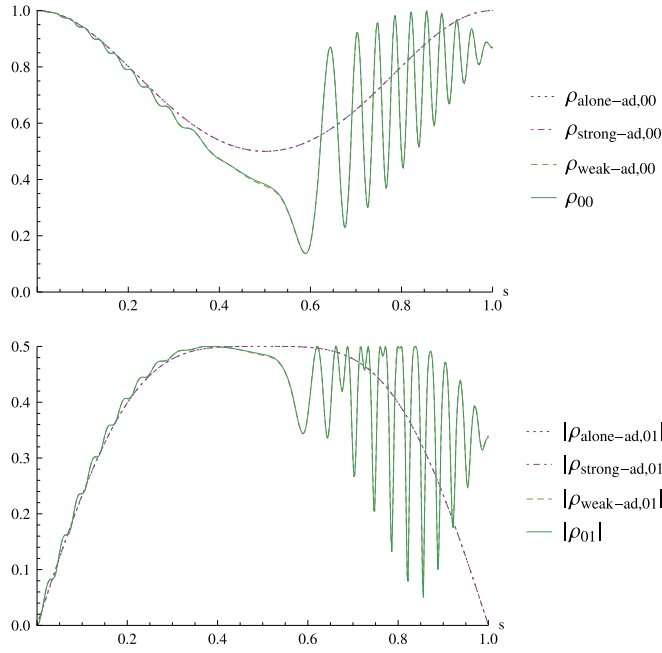


Figure 5. Population of qubit state 0 $\rho_{*,00} = \langle \zeta_0(0) | \rho_{*,(s)} | \zeta_0(0) \rangle$ (top) and coherence $\rho_{*,01} = |\langle \zeta_0(0) | \rho_{*,(s)} | \zeta_1(0) \rangle|$ (bottom) for the exact dynamics ($\bullet = \emptyset$), the adiabatic transport formula with S alone ($\bullet = \text{alone - ad}$), the strong adiabatic transport formula ($\bullet = \text{strong - ad}$) and the weak adiabatic transport formula ($\bullet = \text{weak - ad}$), in conditions corresponding to a weak adiabatic regime (with $\hbar\omega_e = 0.5$ au, $r_{\text{max}} = 1$ au, $r_{\text{min}} = 0.02$ au, $V_0 = 3$ au, $V_1 = 1.5$ au, $V_2 = 0.5$ au, $V_3 = 2.5$ au, $\theta_{\text{max}} = \frac{\pi}{2}$ and $\epsilon = 5 \times 10^{-4}$ (au: atomic unit)). Remark: the alone and the strongly adiabatic cases are graphically merged; the weak adiabatic and the exact cases are graphically merged.

$$\theta(s) = \pi(1 - \sin(\pi s)) \tag{173}$$

$$\varphi(s) = 2\pi s. \tag{174}$$

4.2.2. Adiabatic transport. We start with the chain in a state $\phi_{0\alpha_l\alpha_d}$ where $\alpha_l, \alpha_g \in \{(000), (100) - (001), \dots, (011) - 2(101) + (110), (111)\}$ corresponding to the states of left and right half chains. The adiabatic transport of the density matrix for S alone is

$$\rho_{\text{alone-ad}}(s) = |\zeta_0(s)\rangle\langle\zeta_0(s)|. \tag{175}$$

If the dynamics of the chain is strongly adiabatic, the adiabatic transport of the density matrix is

$$\rho_{\text{strong-ad}}(s) = \rho_{0\alpha_l\alpha_r}(s) \tag{176}$$

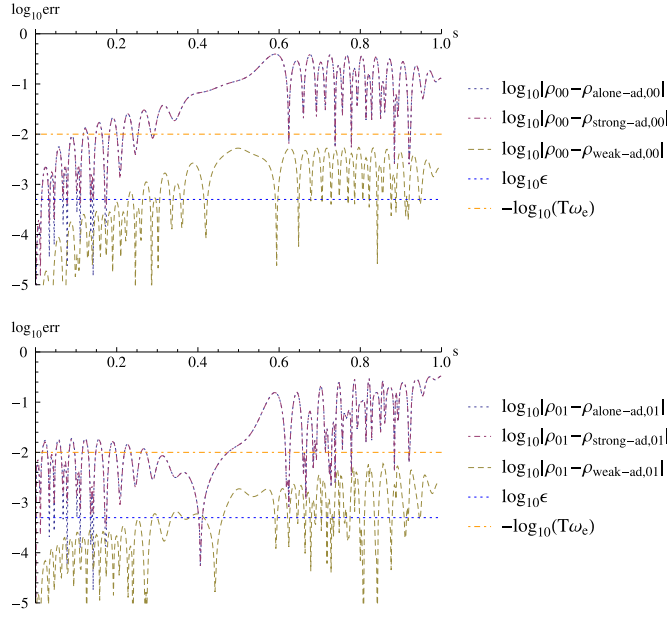


Figure 6. Errors in logarithmic scale between the approximations of the adiabatic transport formulae and the exact dynamics for the population of qubit state 0 (top) and the coherence (bottom) in conditions corresponding to a weak adiabatic regime (with $\hbar\omega_e = 0.5$ au, $r_{\text{max}} = 1$ au, $r_{\text{min}} = 0.02$ au, $V_0 = 3$ au, $V_1 = 1.5$ au, $V_2 = 0.5$ au, $V_3 = 2.5$ au, $\theta_{\text{max}} = \frac{\pi}{2}$ and $\epsilon = 5 \times 10^{-4}$ (au: atomic unit)). Remark: the alone and the strongly adiabatic cases are graphically merged.

$$\begin{aligned}
 &= |\zeta_0(s)\rangle\langle\zeta_0(s)| \\
 &+ \frac{J\hbar}{4}n_{\alpha_l\alpha_d} \frac{\sin\theta(s)}{-B(s) + \frac{J\hbar}{4}n_{\alpha_l\alpha_r} \cos\theta(s)} \\
 &\times (|\zeta_1(s)\rangle\langle\zeta_0(s)| + |\zeta_0(s)\rangle\langle\zeta_1(s)|)
 \end{aligned} \tag{177}$$

where $n_{\alpha_g\alpha_d} = n_{\alpha_g} + n_{\alpha_d}$ is a number defined by table 1.

If the dynamics is weakly adiabatic, the adiabatic transport of the density matrix is

$$\begin{aligned}
 &\rho_{\text{weak-ad}}(s) \\
 &= \mathfrak{A}\mathfrak{D} \left[\mathbb{T}e^{-\hbar^{-1}T \int_0^s E_{d|ar}^{(1)}(\sigma)d\sigma} \mathbb{T}e^{-\int_0^s A_{d|ar}^{(1)}(\sigma)d\sigma} \right] \rho_{0\alpha_l\alpha_r}(s)
 \end{aligned} \tag{178}$$

with

$$E_{\alpha_l\alpha_r}^{(1)} = \lambda_{0\alpha_l\alpha_r} \left| \zeta_{0\alpha_l\alpha_r}^{(1)} \right\rangle\left\langle \zeta_{0\alpha_l\alpha_r}^{(1)} \right| + \lambda_{1\alpha_l\alpha_r} \left| \zeta_{1\alpha_l\alpha_r}^{(1)} \right\rangle\left\langle \zeta_{1\alpha_l\alpha_r}^{(1)} \right| \tag{179}$$

Table 1. Values of the number n_α characterizing the coupling in a half chain in the state ξ_α .

α	n_α
(111)	-1
(110) - 2(101) + (011)	$-\frac{2}{3}$
(110) + (101) + (011)	$-\frac{1}{3}$
(110) - (011)	0
(100) - (001)	0
(100) + (010) + (001)	$\frac{1}{3}$
(100) - 2(010) + (001)	$\frac{2}{3}$
(000)	1

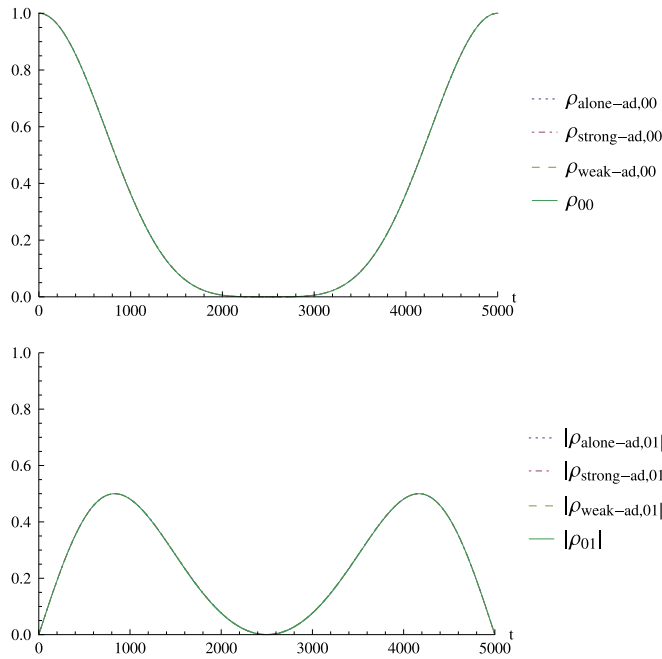


Figure 7. Population of spin state 0 $\rho_{*,00} = \langle \zeta_0(0) | \rho_*(s) | \zeta_0(0) \rangle$ (top) and coherence $\rho_{*,01} = |\langle \zeta_0(0) | \rho_*(s) | \zeta_1(0) \rangle|$ (bottom) for the exact dynamics ($\bullet = \emptyset$), the adiabatic transport formula with S alone ($\bullet = \text{alone - ad}$), the strong adiabatic transport formula ($\bullet = \text{strong - ad}$) and the weak adiabatic transport formula ($\bullet = \text{weak - ad}$), in conditions corresponding to a strong adiabatic regime (with $\hbar\omega_e = 2$ au, $B_0 = 1$ au, $B_{\min} = 0.67$ au and $J = 2 \times 10^{-2}$ au (au: atomic unit)).

$(\eta^{(1)} = 0$ because (ξ_β) are independent of s), and

$$A_{\alpha_1 \alpha_r}^{(1)} = \sum_{b,c=0}^1 \langle \zeta_{b\alpha_1 \alpha_r}^{(1)} | \zeta_{c\alpha_1 \alpha_r}^{(1)'} \rangle | \zeta_{b\alpha_1 \alpha_r}^{(1)} \rangle \langle \zeta_{c\alpha_1 \alpha_r}^{(1)} | \quad (180)$$

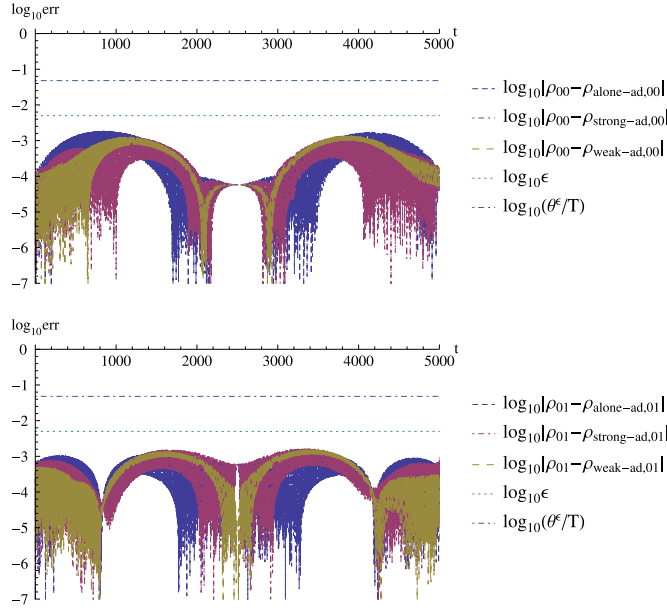


Figure 8. Errors in logarithmic scale between the approximations of the adiabatic transport formulae and the exact dynamics for the population of qubit state 0 (top) and the coherence (bottom) in conditions corresponding to a strong adiabatic regime (with $\hbar\omega_e = 2$ au, $B_0 = 1$ au, $B_{\min} = 0.67$ au and $J = 2 \times 10^{-2}$ au (au: atomic unit)).

where

$$\lambda_{0\alpha_l\alpha_r} = -\frac{\hbar}{2}B + \nu_{\alpha_l} + \nu_{\alpha_r} + \frac{J\hbar^2}{4}n_{\alpha_l\alpha_r} \cos \theta + \mathcal{O}(J^2) \quad (181)$$

$$\lambda_{1\alpha_l\alpha_r} = \frac{\hbar}{2}B + \nu_{\alpha_l} + \nu_{\alpha_r} - \frac{J\hbar^2}{4}n_{\alpha_l\alpha_r} \cos \theta + \mathcal{O}(J^2) \quad (182)$$

and

$$\zeta_{0\alpha_l\alpha_r}^{(1)} = \zeta_0 - \frac{J\hbar}{4}n_{\alpha_l\alpha_r} \frac{\sin \theta}{B - \frac{J\hbar}{4}n_{\alpha_l\alpha_r} \cos \theta} \zeta_1 \quad (183)$$

$$\zeta_{1\alpha_l\alpha_r}^{(1)} = \zeta_1 + \frac{J\hbar}{4}n_{\alpha_l\alpha_r} \frac{\sin \theta}{B - \frac{J\hbar}{4}n_{\alpha_l\alpha_r} \cos \theta} \zeta_0. \quad (184)$$

4.2.3. Strong adiabatic regime. We study a strong adiabatic regime where $T = 5 \times 10^3$ au, $\tau_S = \inf_{s \in [0,1]} \frac{\hbar}{|\mu_1(s) - \mu_0(s)|} = 1.5$ au and $\theta^J = \frac{\hbar}{\|V_{S-\varepsilon}\|} = 2 \times 10^2$ au (au: atomic unit). We have $T \gg \theta^J \gg \tau_S$ assuring that the assumptions of theorem 1 are satisfied. The population of spin state 0 $\langle \zeta_0(0) | \rho(s) | \zeta_0(0) \rangle$ and the coherence of the controlled spin $|\langle \zeta_0(0) | \rho(s) | \zeta_1(0) \rangle|$ (note that $(\zeta_0(0), \zeta_1(0))$ is the eigenstate of the ‘free’ spin S since the magnetic field of control is off at $s = 0$) are represented in figure 7. The errors between the different adiabatic transport formulae and the exact dynamics are plotted in figure 8. A numerical study shows that a purely strong adiabatic regime seems not to be present for this system, which presents rather

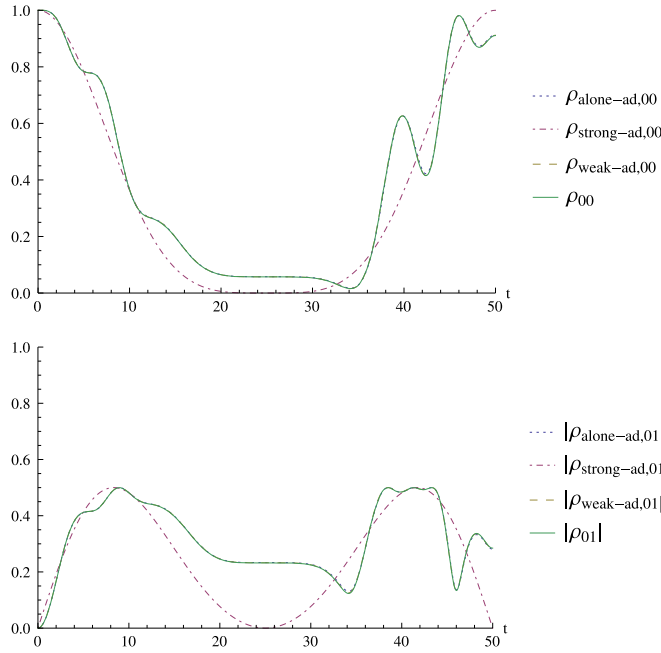


Figure 9. Population of spin state 0 $\rho_{*,00} = \langle \zeta_0(0) | \rho_*(s) | \zeta_0(0) \rangle$ (top) and coherence $\rho_{*,01} = |\langle \zeta_0(0) | \rho_*(s) | \zeta_1(0) \rangle|$ (bottom) for the exact dynamics ($\bullet = \emptyset$), the adiabatic transport formula with S alone ($\bullet = \text{alone - ad}$), the strong adiabatic transport formula ($\bullet = \text{strong - ad}$) and the weak adiabatic transport formula ($\bullet = \text{weak - ad}$), in conditions corresponding to a weak adiabatic regime (with $\hbar\omega_e = 2$ au, $B_0 = 1$ au, $B_{\min} = 10^{-2}$ au and $J = 2 \times 10^{-3}$ (au: atomic unit)). Remark: the alone and the strongly adiabatic cases are graphically merged; the weak adiabatic and the exact cases are graphically merged.

regimes where the adiabatic approximation without environment, the strong adiabatic approximation and the weak adiabatic approximation are not clearly distinguishable. Nevertheless we see in figure 8 that the strong adiabatic transport formula induces globally fewer errors.

4.2.4. Weak adiabatic regime. We study a weak adiabatic regime where $T = 50$ au, $\tau_S = \inf_{s \in [0,1]} \frac{\hbar}{|\mu_1(s) - \mu_0(s)|} = 10^2$ au, $\theta^J = \frac{\hbar}{\|V_{S-\mathcal{E}}\|} = 10^3$ au and $\tau_{\mathcal{E}} = \frac{1}{\omega_e} = 0.5$ au (au: atomic unit). We have $T \gg \tau_{\mathcal{E}}$ and $\theta^J \sim \tau_S \ll T$ assuring that the assumptions of theorem 2 are satisfied. The population of spin state 0 $\langle \zeta_0(0) | \rho(s) | \zeta_0(0) \rangle$ and the coherence of the controlled spin $|\langle \zeta_0(0) | \rho(s) | \zeta_1(0) \rangle|$ are represented in figure 9. The errors between the different adiabatic transport formulae and the exact dynamics are plotted in figure 10. The errors of the prediction of the adiabatic transport formula with S alone are now very large in accordance with the very small gap between the two eigenvalues of $H_S(s)$ during the dynamics. The weak adiabatic transport formula provides a very good approximation with an error smaller than $\frac{\tau_{\mathcal{E}}}{T} = 10^{-2}$ in accordance with theoretical error $\max\left(\frac{\tau_{\mathcal{E}}}{T}, e^2\right)$.

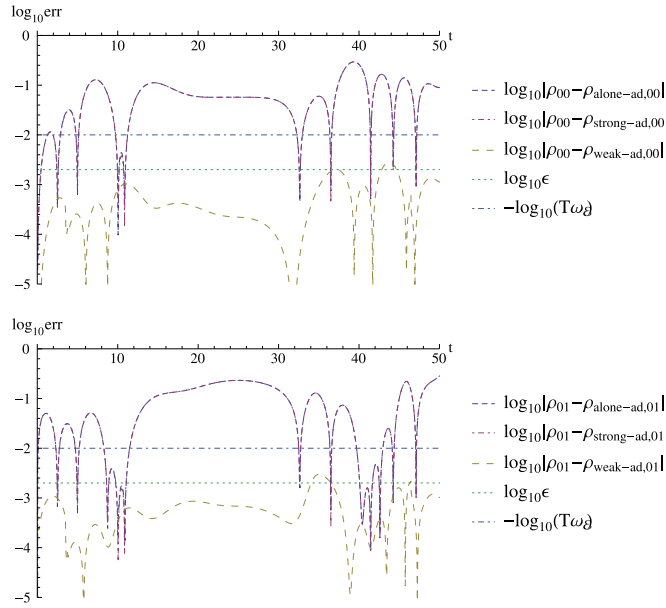


Figure 10. Errors in logarithmic scale between the approximations of the adiabatic transport formulae and the exact dynamics for the population of spin state 0 (top) and the coherence (bottom) in conditions corresponding to a weak adiabatic regime (with $\hbar\omega_e = 2$ au, $B_0 = 1$ au, $B_{\min} = 10^{-2}$ au and $J = 2 \times 10^{-3}$ (au: atomic unit)). Remark: the alone and the strongly adiabatic cases are graphically merged.

5. Conclusion

We have shown that operator-valued geometric phases as defined by [13–18] are exhibited by bipartite quantum systems in an adiabatic approximation with a perturbative coupling between the two parts of the system. This result remains valid if the bipartite system is constituted by a small subsystem and a large environment. Nevertheless, for a very large environment (a reservoir) the adiabatic theorem assumptions of no resonance or no quasi-resonance between transitions of S and \mathcal{E} may not be satisfied since the spectrum of a reservoir is assimilated to a continuum [9]. These adiabatic operator-valued geometric phases arise when the evolution of the environment is strongly adiabatic (the favorable case for a quantum control of the subsystem) but with a subsystem evolution not necessarily adiabatic with respect to the control and to the environment effects. The operator-valued dynamical phase generator arising with the geometric phase generator, is a kind of effective Hamiltonian representing the system dressed by environment states. The second order adiabatic transport satisfies a kind of effective Lindblad equation.

The perturbative assumption restricts the field of applications of the present result to special situations. It would be interesting to prove that the adiabatic transport of density matrices also exhibits an operator-valued geometric phase with a strong interaction between the two parts of a bipartite system.

Appendix. A corollary concerning the splitting of the time-ordered exponential

Corollary 1. Let $s \mapsto A(s) \in \mathcal{L}(\mathcal{V})$ be a family of bounded anti-self-adjoint operators of a Hilbert space \mathcal{V} . Let $s \mapsto U_A(s) \in \mathcal{U}(\mathcal{V})$ be the unitary operator strongly continuous with respect to s and solution of the equation

$$U'_A = -AU_A \quad U_A(0) = 1_{\mathcal{V}}. \quad (\text{A.1})$$

Let $s \mapsto B(s) \in \mathcal{L}(\mathcal{V})$ be another family of bounded anti-self-adjoint operators; with the same notations we have

$$U_{A+B} = U_X U_A \quad (\text{A.2})$$

with

$$X = A + B - U_X A U_X^{-1}. \quad (\text{A.3})$$

Proof. Let $X(s) \in \mathcal{L}(\mathcal{V})$ be such that $U_X = U_{A+B} U_A^{-1}$.

$$U_X U_A = U_{A+B} \Rightarrow U'_X U_A + U_X U'_A = U'_{A+B} \quad (\text{A.4})$$

$$\Rightarrow -X U_X U_A - U_X A U_A = -(A + B) U_X U_A \quad (\text{A.5})$$

$$\Rightarrow X = A + B - U_X A U_X^{-1}. \quad (\text{A.6})$$

□

We note that X is only implicitly defined.

References

- [1] Messiah A 1959 *Quantum Mechanics* (Paris: Dunod)
- [2] Zanardi P and Rasetti M 1999 *Phys. Lett. A* **264** 94
- [3] Lucarelli D 2005 *J. Math. Phys.* **46** 052103
- [4] Santoro G E and Tosatti E 2006 *J. Phys. A: Math. Gen.* **39** R393
- [5] Guérin S and Jauslin H R 2003 *Adv. Chem. Phys.* **125** 147
- [6] Fleischer A and Moiseyev N 2005 *Phys. Rev. A* **72** 032103
- [7] Sarandy M S and Lidar D A 2005 *Phys. Rev. A* **71** 012331
- [8] Sarandy M S and Lidar D A 2006 *Phys. Rev. A* **73** 062101
- [9] Breuer H P and Petruccione F 2002 *The Theory of Open Quantum Systems* (New York: Oxford University Press)
- [10] Nenciu G and Rasche G 1992 *J. Phys. A: Math. Gen.* **25** 5741
- [11] Abou Salem W K and Fröhlich J 2007 *Commun. Math. Phys.* **273** 651
- [12] Joye A 2007 *Commun. Math. Phys.* **275** 139
- [13] Sjöqvist A, Pati A K, Ekert A, Anandan J S, Ericsson M, Oi D K L and Vedral V 2000 *Phys. Rev. Lett.* **85** 2845
- [14] Tong D M, Sjöqvist E, Kwek L C, Oh C H and Ericsson M 2003 *Phys. Rev. A* **68** 022106
- [15] Dajka J, Łuczka J and Hänggi P 2011 *Quantum Inf. Process* **10** 85
- [16] Andersson O and Heydari H 2013 *New J. Phys.* **15** 053006
- [17] Viennot D and Lages J 2011 *J. Phys. A: Math. Theor.* **44** 365301
- [18] Viennot D and Lages J 2012 *J. Phys. A: Math. Theor.* **45** 365305
- [19] Nenciu G 1980 *J. Phys. A: Math. Gen.* **13** L15
- [20] Viennot D 2014 *J. Phys. A: Math. Theor.* **47** 295301
- [21] Viennot D 2005 *J. Math. Phys.* **46** 072102
- [22] Viennot D 2010 *J. Math. Phys.* **51** 103501
- [23] Viennot D 2007 *J. Math. Phys.* **48** 052102
- [24] Viennot D, Leclerc A, Jolicard J and Killingbeck J P 2012 *J. Phys. A: Math. Theor.* **45** 335301

- [25] Viennot D 2009 *J. Phys. A: Math. Theor.* **42** 395302
- [26] Guérin S, Monti F, Dupont J-M and Jauslin H R 1997 *J. Phys. A: Math. Gen.* **30** 7193
- [27] Landau L 1932 *Phys. Z. Sowjetunion* **2** 46
- [28] Zener C 1932 *Proc. R. Soc. London A* **137** 696