IOP Publishing Journal of Physics A: Mathematical and Theoretical
J. Phys. A: Math. Theor **47** (2014) 295301 (28pp) doi:10.1088/1751-8113/47/29/295301

Adiabatic quantum control hampered by entanglement

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Received 15 October 2013, revised 30 May 2014
Accepted for publication 13 June 2014
Published 9 July 2014

Abstract

We study the defects in adiabatic control of a quantum system caused by the entanglement of the system with its environment. Such defects can be related to decoherence processes due to perturbative couplings between the system and the environment. We propose, for analysing these effects, a geometric approach, based on a field theory on the control manifold issuing from the higher gauge theory associated with the C^*-geometric phases. We study a visualization method for analysing the defects of the adiabatic control, based on plotting the field strengths of the gauge theory. To illustrate the present methodology, we consider the example of atomic STIRAP (stimulated Raman adiabatic passage), where the controlled atom is entangled with another atom. We study the robustness of the STIRAP effect when the controlled atom is entangled with another one.

Keywords: quantum control, entanglement, decoherence, geometric phase, adiabatic approximation

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

1. Introduction

Quantum control is one of the main research subjects in modern physics. One quantum control problem is that of finding how the external parameters (for example, the parameters of strong laser fields) vary in the course of a quantum system (a spin, an atom or a molecule) evolving to a predetermined target state satisfying the control goal. Such problems can offer very important applications in different fields: nanosciences (in driving molecular machines), quantum information (in yielding quantum logic gates), and physical chemistry (in performing vibrational cooling, or controlling chemical reactions). If the target state is an

eigenstate of the quantum system, an adiabatic approach [1] is a good strategy for solving quantum control problems, since external parameters are usually slowly varied with respect to the response of the quantum system and since the adiabatic approximation predicts that the wavefunction remains projected onto an eigenstate during the dynamics. Adiabatic schemes of quantum control have been proposed for quantum computation by holonomic approaches [2, 3] or by quantum annealing [4], and for atomic control by strong laser fields [5].

Real quantum systems are never isolated. The coupling between the quantum system and its environment, even if it is perturbative, can induce defects of the control result with respect to the idealized isolated quantum system. The system and the environment are entangled and the dynamics can be characterized by decoherence processes. The goal of the present paper is the characterization of these defects. Some adiabatic quantum control methods are based on geometric approaches (the geometry of fibre bundles [3] or the topology of eigensurfaces [5]). We want a geometric characterization of the defects induced by the entanglement. Recently, we have proposed a generalization of the geometric phase concept for open and composite quantum systems [6, 7]. This geometric phase takes its values in the C^*-algebra of the operators of the quantum system. In contrast with the usual geometric phase which is associated with a simple gauge theory [8], the C^*-geometric phase is associated with a higher gauge theory (a generalization of gauge theory to a category theory context; see for example [9]). This higher gauge theory involves some fields on the manifold spanned by the control external parameters, which are introduced in [6]. In this paper, we do not wish to recall the mathematical structure associated with this higher gauge theory (it can be found in [6]), but we do wish to interpret physically the fields involved from the viewpoint of quantum control hampered by entanglement.

This paper is organized as follows. Section 2 is devoted to a brief review of the adiabatic quantum control for an idealized isolated quantum system. The goal of this section is the introduction of some notation and concepts. Section 3 studies the theoretical properties of the fields associated with the higher gauge theory for control hampered by entanglement. We study the physical meaning of these fields with respect to the quantum control problem. Section 4 is devoted to a simple but instructive example. The stimulated Raman adiabatic passage (STIRAP) is a solution of a quantum control problem involving changing the state of a three-level atom from the bound state to an excited state via passage through a 'dark' state, by using two laser Gaussian pulses. We study the robustness of this solution for when the atom is entangled with another one which 'feels' the laser fields. We interpret the results by plotting the field strengths of the higher gauge theory, to confirm the physical meanings of these fields. Section 5 gives a discussion concerning the application of the methodology presented in this paper to a system entangled with a larger environment (by using small effective Hamiltonians to represent this environment or by working only at the stage of the density matrices). In this paper we use the word 'environment' in a broad sense. It can signify the large environment of an open quantum system, as for the discussion in section 5, or it can signify the (small) second part of a bipartite quantum system, as for the example treated in section 4. We focus on the effect of the entanglement on the control. We have chosen an example with a small environment (a bipartite quantum system) in order to avoid the possible effects of the dissipation induced by large environments and shed light on the effects associated only with the entanglement.

2. Adiabatic quantum control

In this section, we consider an idealized isolated quantum system controlled by external parameters denoted by x. The set of all configurations of x is assumed to form a C^∞-manifold M called the control manifold. We denote by $\mathcal{H}_S$ the Hilbert space of the states of the system (for the sake of simplicity, throughout this paper we suppose that $\mathcal{H}_S$ is finite dimensional). The dynamics of the controlled quantum system is governed by the self-adjoint Hamiltonian $H(x) \in \mathcal{L}(\mathcal{H}_S)$ ($\mathcal{L}(\mathcal{H}_S)$ denotes the C^*-algebra of the operators of $\mathcal{H}_S$). A control solution is a path C: $t \mapsto x(t) \in M$ such that the wavefunction $\psi(t) \in \mathcal{H}_S$, a solution of the Schrödinger equation

$$\mathrm{i}\hbar \frac{\mathrm{d}\psi}{\mathrm{d}t} = H(x(t))\psi(t) \qquad \psi(0) = \psi_0 \in \mathcal{H}_S, \tag{1}$$

becomes, at $t = T$ (the end of the control), $\psi(T) = \psi_{target}$. $\psi_{target} \in \mathcal{H}_S$ is the predetermined target state satisfying the goal of the control. We will suppose that the path C is closed (this is a generic situation; we start and we stop with a control system off).

2.1. The adiabatic approximation

Let $\{\lambda_a(x)\}_a$ be the instantaneous eigenvalues of $H(x)$ that we suppose to be non-degenerate for all $x \in M$, except eventually for some isolated points in M at first. Let $\{\phi_a(x)\}_a$ be the associated normalized eigenvectors;

$$H(x)\phi_a(x) = \lambda_a(x)\phi_a(x). \tag{2}$$

If $\psi(0) = \phi_a(x(0))$ and if

$$\forall\, b \neq a, \quad \hbar \sup_{t\in[0,T]} \left| \frac{\left\langle \phi_a \middle| \partial_\mu \phi_b \right\rangle \dot{x}^\mu}{\lambda_b - \lambda_a} \right| \ll 1, \tag{3}$$

then the wavefunction satisfies the adiabatic approximation (see for example [1])

$$\psi(T) \simeq \mathrm{e}^{-\mathrm{i}\hbar^{-1}\int_0^T \lambda_a(x(t))\mathrm{d}t} \mathrm{e}^{-\oint_C A_a(x)} \phi_a(x(T)) \tag{4}$$

where the geometric phase $\mathrm{e}^{-\oint_C A_a(x)}$ discovered by Berry [10] is generated by

$$A_a(x) = \left\langle \phi_a(x) \middle| \mathrm{d}\phi_a(x) \right\rangle \in \Omega^1 M. \tag{5}$$

d is the exterior differential of M and $\Omega^n M$ denotes the set of differential n-forms of M. The adiabatic condition (3) implies that the control parameter variations ($\dot{x}^\mu$; the dot denotes the time derivative) are slow, the non-adiabatic couplings ($\langle \phi_a | \partial_\mu \phi_b \rangle$) are small, and a gap condition between the eigenvalue λ_a and the other eigenvalues is satisfied.

If C passes through a point $x_* \in M$ where λ_a and λ_b cross, $\lambda_a(x_*) = \lambda_b(x_*)$, with a rapid passage in the neighbourhood of x_*, and with the adiabatic condition (3) satisfied elsewhere, then we have

$$\begin{aligned}\psi(T) \simeq\ & \mathrm{e}^{-\mathrm{i}\hbar^{-1}\int_0^{t_*} \lambda_a(x(t))\mathrm{d}t} \mathrm{e}^{-\int_{C:x(0)\to x_*} A_a(x)} \\ & \times \mathrm{e}^{-\mathrm{i}\hbar^{-1}\int_{t_*}^T \lambda_b(x(t))\mathrm{d}t} \mathrm{e}^{-\int_{C:x_*\to x(T)} A_b(x)} \psi_b(x(T)).\end{aligned} \tag{6}$$

The rapid adiabatic passage method of quantum control [5] is based on this equation. To reach $\psi_{target} = \phi_b(x(T))$, it needs to find a path C passing through a crossing point of λ_a and λ_b (we can also pass by several crossing points with some intermediate eigenstates).

2.2. The geometric approach

As shown by Simon [8], the geometric phase of the adiabatic approximation is associated with a gauge theory described by a connection on a principal $U(1)$-bundle ($U(1)$ is the set of unit-modulus complex numbers). $A_a \in \Omega^1 M$ plays the role of a gauge potential which defines a gauge field

$$F_a = \mathrm{d}A_a = \left\langle \mathrm{d}\phi_a \right| \wedge \left| \mathrm{d}\phi_a \right\rangle \in \Omega^2 M. \tag{7}$$

$\wedge$ denotes the exterior product of differential forms. F_a is called the adiabatic curvature.

Property 1. *The adiabatic curvature $F_a(x)$ is a measure at the point x of the non-adiabaticity involving the state ϕ_a.*

Proof. $\{\phi_b\}_b$ constitutes an orthonormal basis of $\mathcal{H}_S$. By using the closure relation we have

$$F_a = \left\langle \mathrm{d}\phi_a \right| \wedge \left| \mathrm{d}\phi_a \right\rangle \tag{8}$$

$$= \sum_b \left\langle \mathrm{d}\phi_a \middle| \phi_b \right\rangle \wedge \left\langle \phi_b \middle| \mathrm{d}\phi_a \right\rangle \tag{9}$$

$$= -\sum_b \left\langle \phi_a \middle| \mathrm{d}\phi_b \right\rangle \wedge \left\langle \phi_b \middle| \mathrm{d}\phi_a \right\rangle. \tag{10}$$

$\langle \phi_a | \mathrm{d}\phi_a \rangle \wedge \langle \phi_a | \mathrm{d}\phi_a \rangle = 0$ and, moreover, we have for $b \neq a$

$$H\phi_a = \lambda_a \phi_a \Rightarrow \left\langle \phi_b \middle| \mathrm{d}H \middle| \phi_a \right\rangle + \lambda_b \left\langle \phi_b \middle| \mathrm{d}\phi_a \right\rangle = \lambda_a \left\langle \phi_b \middle| \mathrm{d}\phi_a \right\rangle. \tag{11}$$

We have then

$$F_a = \sum_{b \neq a} \frac{\left\langle \phi_a \middle| \mathrm{d}H \middle| \phi_b \right\rangle \wedge \left\langle \phi_b \middle| \mathrm{d}H \middle| \phi_a \right\rangle}{\left(\lambda_a - \lambda_b\right)^2}. \tag{12}$$

The adiabatic condition (3) is then equivalent to $\mathrm{i}\hbar^2 |i_v F_a| \ll 1$ where i is the interior product and $v = \dot{x}^\mu \frac{\partial}{\partial x^\mu}$ is the speed tangent vector of C.

F_a diverges at the crossing points of λ_a (which are the singularities of the Simon principal bundle) if the non-adiabatic couplings are different from zero. In the case where $\dim M = 2$, in place of plotting the eigenvalue surfaces like in [5] we can plot the field strength densities $F_{a\mu\nu}$ to locate the crossing points. The benefits of studying the adiabatic curvature in place of the eigenvalue surfaces are: F_a is zero at a crossing point where the adiabatic couplings are zero (such a crossing does not induce rapid transitions); F_a shows the distribution of the non-adiabatic couplings around the crossings [11]; and F_a can be generalized to some non-Hermitian cases where the eigenvalue surfaces are complex surfaces [12].

If now the eigenvalue is degenerate with the associated eigenvectors $\{\phi_a\}_{a \in I}$ (I is a set of indices), or if we consider a weaker adiabatic approximation consisting in assuming that the wavefunction remains projected onto a group of several eigenvectors $\{\phi_a\}_{a \in I}$, then the gauge potential becomes

$$A_I \in \Omega^1(M, \mathfrak{u}(n)) \qquad A_{I,ab} = \left\langle \phi_a \middle| \mathrm{d}\phi_b \right\rangle \qquad \forall\, a, b \in I, \tag{13}$$

where $\mathfrak{u}(n)$ is the set of anti-self-adjoint matrices of order n (the number of elements in I) and $A_{I,ab}$ denotes the matricial element of A_I in row a and column b. The adiabatic approximation becomes (for a single degenerate eigenvalue)

$$\psi(T) \simeq \mathrm{e}^{-\mathrm{i}\hbar^{-1}\int_0^T \lambda_a(x(t))\mathrm{d}t} \sum_{b\in I} \left[\mathbb{P}\mathrm{e}_{\leftarrow}^{-\oint_C A_I(x)} \right]_{ba} \phi_b(x(T)) \tag{14}$$

where $\mathbb{P}\mathrm{e}_{\leftarrow}$ denotes the path-ordered exponential, i.e. the Dyson series along a path:

$$\frac{\mathrm{d}}{\mathrm{d}t} \mathbb{P}\mathrm{e}_{\leftarrow}^{-\int_{C:x(0)\to x(t)} A_I(x)} = -A_{I\mu}(x(t))\dot{x}^\mu(t) \mathbb{P}\mathrm{e}_{\leftarrow}^{-\int_{C:x(0)\to x(t)} A_I(x)}. \tag{15}$$

The 'non-Abelian' geometric phase is the Wilson loop $\mathbb{P}\mathrm{e}_{\leftarrow}^{-\oint_C A_I(x)} \in U(n)$ ($U(n)$ is the group of unitary matrices of order n) which is associated with a connection on a principal $U(n)$-bundle. In holonomic quantum computation [2, 3], the Wilson loops are used to provide quantum logic gates. The non-Abelian adiabatic curvature is

$$F_I = \mathrm{d}A_I + A_I \wedge A_I \in \Omega^2(M, \mathfrak{u}(n)). \tag{16}$$

Property 2. *The non-Abelian adiabatic curvature $F_I(x)$ is a measure at the point x of the non-adiabaticity between the space spanned by $\{\phi_a\}_{a\in I}$ and its orthogonal supplement, but it is not sensitive to the non-adiabaticity inside the space spanned by $\{\phi_a\}_{a\in I}$.*

Proof. After some algebra similar to that for the non-degenerate case, we find

$$F_{I,ab} = \left(\left\langle \partial_\mu \phi_a \middle| \partial_\nu \phi_b \right\rangle + \sum_{c\in I} \left\langle \phi_a \middle| \partial_\mu \phi_c \right\rangle \left\langle \phi_c \middle| \partial_\nu \phi_b \right\rangle \right) \mathrm{d}x^\mu \wedge \mathrm{d}x^\nu \tag{17}$$

$$= \sum_{d\notin I} \frac{\left\langle \phi_a \middle| \mathrm{d}H \middle| \phi_d \right\rangle \wedge \left\langle \phi_d \middle| \mathrm{d}H \middle| \phi_b \right\rangle}{(\lambda_a - \lambda_d)(\lambda_b - \lambda_d)}. \tag{18}$$

Remark: if the set of vectors is complete, i.e. $I = \{1, \ldots, \dim \mathcal{H}_S\}$, then $F_I = 0$.

3. Adiabatic quantum control hampered by entanglement

We consider now that the quantum system is in 'contact' with another quantum 'object' that we call the 'environment'. We call the composite system constituted by the quantum system and the environment the 'universe'. We denote by $\mathcal{H}_\mathcal{E}$ the Hilbert space of the environment and by $\mathcal{H}_S \otimes \mathcal{H}_\mathcal{E}$ the Hilbert space of the universe. The dynamics of the universe is governed by the self-adjoint Hamiltonian

$$H_\mathcal{U}(x) = H_S(x) \otimes 1_{\mathcal{H}_\mathcal{E}} + 1_{\mathcal{H}_S} \otimes H_\mathcal{E}(x) + V(x) \tag{19}$$

where $H_S \in \mathcal{L}(\mathcal{H}_S)$ and $H_\mathcal{E} \in \mathcal{L}(\mathcal{H}_\mathcal{E})$ are the Hamiltonians of the system and of the environment when they are separated, and $V(x) \in \mathcal{L}(\mathcal{H}_S \otimes \mathcal{H}_\mathcal{E})$ is the coupling operator. Let $\psi(t) \in \mathcal{H}_S \otimes \mathcal{H}_\mathcal{E}$ be the solution of the Schrödinger equation of the universe. We are interested by the state 'reduced' to the system which is represented by the density matrix

$$\rho_\psi(t) = \mathrm{tr}_{\mathcal{H}_\mathcal{E}} \left| \psi(t) \right\rangle\!\!\rangle \left\langle\!\!\left\langle \psi(t) \right| \right. \tag{20}$$

where $\langle\!\langle . \,|\, . \rangle\!\rangle$ denotes the scalar product of $\mathcal{H}_S \otimes \mathcal{H}_\mathcal{E}$ and $\mathrm{tr}_{\mathcal{H}_\mathcal{E}}$ denotes the partial trace on $\mathcal{H}_\mathcal{E}$. If ρ_ψ has a rank equal to 1, there exists $\varphi \in \mathcal{H}_S$ such that $\rho_\psi = |\varphi\rangle\langle\varphi|$ (ρ_ψ is said to be a pure state), and φ is the single state which can be attributed to the system. If the rank of ρ_ψ is larger that 1, we cannot attribute a single state to the system (ρ_ψ is said to be a mixed state);

the system and the environment are entangled. If $V \neq 0$, the dynamics transforms pure states into mixed states.

The role of the partial trace on $\mathcal{H}_{\mathcal{E}}$ is to lose information concerning the environment. Indeed, the 'experimentalist' controls only the system, and not directly the environment (even if this environment 'feels' the control). The adiabatic regime is assumed for the system, not for the universe. We consider then a weaker adiabatic assumption consisting in assuming an adiabatic evolution for the system but not necessarily for the environment. The C^*-geometric phases have been introduced in [6] as a framework for describing this situation.

3.1. C^*-geometric phases

Let $\{\lambda_a(x)\}_a$ be the instantaneous eigenvalues of the universe (we suppose that they are not degenerate for all $x \in M$ except for some isolated points) and $\{\phi_a\}$ be the associated eigenvectors;

$$H_{\mathcal{U}}(x)\phi_a(x) = \lambda_a(x)\phi_a(x). \tag{21}$$

Following [6] we can define a geometric phase with values in the C^*-algebra $\mathfrak{s} = \mathcal{L}(\mathcal{H}_{\mathcal{S}})$ as being

$$\mathbb{P}\mathrm{e}_{\rightarrow}^{-\oint_C \mathcal{A}_a(x)} \in \mathfrak{s} \tag{22}$$

where $\mathbb{P}\mathrm{e}_{\rightarrow}$ is the path anti-ordered exponential, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbb{P}\mathrm{e}_{\rightarrow}^{-\int_{C:x(0)\to x(t)} \mathcal{A}_a(x)} = -\mathbb{P}\mathrm{e}_{\rightarrow}^{-\int_{C:x(0)\to x(t)} \mathcal{A}_a(x)} \mathcal{A}_{a\mu}(x(t))\dot{x}^{\mu}(t). \tag{23}$$

Let $\rho_a(x) = \mathrm{tr}_{\mathcal{H}_{\mathcal{E}}}|\phi_a(x)\rangle\rangle\langle\langle\phi_a(x)|$ be the density eigenmatrix. The generator of the C^*-geometric phase is defined by

$$\mathcal{A}_a = \mathrm{tr}_{\mathcal{H}_{\mathcal{E}}}\left(\left|\mathrm{d}\phi_a\right\rangle\rangle\langle\langle\phi_a\right|\right)\rho_a^{-1} \in \Omega^1(M, \mathfrak{s}) \tag{24}$$

where ρ_a^{-1} is the pseudo-inverse of ρ_a, i.e. $\rho_a^{-1}\rho_a = 1_{\mathcal{H}_S} - P_{\ker\rho_a}$ ($P_{\ker\rho_a}$ is the orthogonal projector onto the kernel of ρ_a).

3.2. Adiabatic fields

In [6] we have shown that the C^*-geometric phases are associated with an higher gauge theory (a connective structure on a 2-bundle [9]) which is characterized by two fields:

- the adiabatic curving:

$$B_a = \mathrm{d}\mathcal{A}_a - \mathcal{A}_a \wedge \mathcal{A}_a \in \Omega^2(M, \mathfrak{s}). \tag{25}$$

- the adiabatic fake curvature:

$$F_a = \mathrm{d}A_a - A_a \wedge A_a - B_a \in \Omega^2(M, \mathfrak{s}), \tag{26}$$

where the reduced potential is defined by

$$A_a = \mathrm{tr}_{\mathcal{H}_{\mathcal{E}}}\left(P_a\left|\mathrm{d}\phi_a\right\rangle\rangle\langle\langle\phi_a\right|\right)\rho_a^{-1} \tag{27}$$

where P_a is the projection onto the eigensubspace associated with λ_a which is considered as a 'non-commutative eigenvalue' (see [6]); usually we can expect that P_a is simply $|\phi_a\rangle\rangle\langle\langle\phi_a|$ (A_a is then P_a multiplied by the usual geometric phase generator of the universe). Since these

fields are $\mathfrak{s}$-valued, they have statistical interpretations with respect to mixed states associated with the entanglement. More precisely, the physical meaning is not directly supported by these fields, but by their statistical averages:

$$\mathrm{tr}_{\mathcal{H}_S}\left(\rho_a B_a\right) \in \Omega^2 M, \tag{28}$$

$$\mathrm{tr}_{\mathcal{H}_S}\left(\rho_a F_a\right) \in \Omega^2 M. \tag{29}$$

Since the entanglement of the quantum system with the environment is responsible for a loss of information in the partial trace $\mathrm{tr}_{\mathcal{H}_\mathcal{E}}$, it is interesting to consider also the von Neumann entropy of the density eigenmatrix:

$$-\mathrm{tr}_{\mathcal{H}_S}\left(\rho_a \ln \rho_a\right) \in \Omega^0 M, \tag{30}$$

which can be viewed as a measure of the information lack for the system where its mixed state is described by the density eigenmatrix ρ_a.

By construction, the average adiabatic fake curvature seems to have the same interpretation as the usual adiabatic curvature of isolated systems. It measures the local non-adiabaticity. It is also the fake curvature which must be considered and not $\mathrm{d}A_a - A_a \wedge A_a$ (the correction by B_a is necessary). This is induced by the mathematical structure of a higher gauge theory (see [9]) but, with a more pragmatic approach, we will justify this via the examples which follow in the rest of this paper.

The role of the adiabatic curving is revealed by the following property.

Property 3. The average adiabatic curving $\mathrm{tr}_{\mathcal{H}_S}(\rho_a(x)B_a(x))$ is a measure of the entropy variation associated with ϕ_a and which is induced by variations of the control parameters in the neighbourhood of x.

Proof. Let C_x be an infinitesimal closed loop in M, starting and ending at $x \in M$. Let $\mathcal{S}_x$ be a surface in M having C_x as boundary. We denote by Δ the area of $\mathcal{S}_x$ which is in the neighbourhood of zero. Let $\mathrm{e}^{\int\int_{S_x} B_a}\rho_a(x) \simeq \mathrm{e}^{\oint_{C_x}\mathcal{A}_a}\rho_a(x)$ be the density matrix obtained by the 'parallel transport' of $\rho_a(x)$ along C_x (since the loop C_x is infinitesimal, the path-ordered exponential is approximately equal to the matrix exponential, and the Wilson loop $\mathrm{e}^{\oint_{C_x}\mathcal{A}_a}$ is approximately equal to $\mathrm{e}^{\int\int_{S_x} B_a}$ by a Stokes theorem). By using the Baker–Campbell–Hausdorff formula [13], we have

$$\begin{aligned}\ln\left(\mathrm{e}^{\int\int_{S_x} B_a}\rho_a\right) = {} & \int\int_{S_x} B_a + \ln\rho_a + \frac{1}{2}\left[\int\int_{S_x} B_a, \ln\rho_a\right] \\ & + \frac{1}{12}\left[\int\int_{S_x} B_a, \left[\int\int_{S_x} B_a, \ln\rho_a\right]\right] \\ & - \frac{1}{12}\left[\ln\rho_a, \left[\int\int_{S_x} B_a, \ln\rho_a\right]\right] \\ & + \cdots.\end{aligned} \tag{31}$$

We have then

$$\begin{aligned}\mathrm{tr}_{\mathcal{H}_S}\left(\rho_a \ln\left(\mathrm{e}^{\int\int_{S_x} B_a}\rho_a\right)\right) = {} & \mathrm{tr}_{\mathcal{H}_S}\left(\rho_a \int\int_{S_x} B_a\right) \\ & + \mathrm{tr}_{\mathcal{H}_S}\left(\rho_a \ln\rho_a\right) + O\left(\Delta^2\right)\end{aligned} \tag{32}$$

and because of the cyclicity of the trace we have $\mathrm{tr}\,(\rho[B, \rho]) = \mathrm{tr}\,(\rho B \ln\rho) - \mathrm{tr}\,(\rho \ln\rho B) = \mathrm{tr}\,(\ln\rho\rho B) - \mathrm{tr}\,(\rho \ln\rho B) = 0$ $(\rho \ln\rho = \ln\rho\rho)$.

We have similar calculations for higher orders. Finally we have

$$\mathrm{tr}_{\mathcal{H}_S}\left(\rho_a \iint_{\mathcal{S}_x} B_a\right) = -\mathrm{tr}_{\mathcal{H}_S}\left(\rho_a\left(\ln\rho_a - \ln\left(\mathrm{e}^{\iint_{\mathcal{S}_x} B_a}\rho_a\right)\right)\right) + O\left(\Delta^2\right) \tag{33}$$

$$= S\left(\rho_a \,\middle\|\, \mathrm{e}^{\iint_{\mathcal{S}_x} B_a}\rho_a\right) + O\left(\Delta^2\right) \tag{34}$$

where $S(\rho \parallel \tau) = -\mathrm{tr}\,(\rho(\ln\rho - \ln\tau))$ is the relative entropy (see [14]). $\mathrm{tr}_{\mathcal{H}_S}\left(\rho_a \iint_{\mathcal{S}_x} B_a\right)$ is then the relative entropy of $\rho_a(x)$ with respect to its parallel transport along an infinitesimal loop passing through x. On writing $\iint_{\mathcal{S}_x} B_a = B_{a;12}\Delta + O(\Delta^2)$ (the indices 12 being associated with local coordinates along $\mathcal{S}_x$), we see that $\mathrm{tr}_{\mathcal{H}_S}(\rho_a(x)B_a(x))$ is a measure of the entropy variation induced by the transport of ρ_a in the neighbourhood of x. □

The increase of the entropy is associated with an increase of the entanglement between the system and the environment (and dynamically it is associated with decoherence processes). In quantum control, we can define the decoherence as a dynamical process associated with an increase of the entropy and of the entanglement. We have two kinds of decoherence: a '*local decoherence*' associated with $-\mathrm{tr}_{\mathcal{H}_S}(\rho_a(x)\ln\rho_a(x))$ (decoherence induced by the point x) and a '*kinematic decoherence*' associated with $\mathrm{tr}_{\mathcal{H}_S}(\rho_a(x)B_a(x))$ (decoherence induced by loops passing through x).

3.3. Two reference cases

In order to illustrate the roles of the curving and of the fake curvature, and to shed light on their interpretations, we consider two simple cases where these fields can be expressed by using the curvatures of the system and of the environment.

3.3.1. A factorizable eigenstate. We suppose that an eigenvector of the universe is $\phi_a(x) = \zeta_i(x) \otimes \xi_\alpha(x)$ where $\zeta_i(x)$ is an eigenvector of $H_S(x)$ (associated with a non-degenerate eigenvalue) and $\xi_\alpha(x)$ is an eigenvector of $H_\mathcal{E}(x)$ (associated with a non-degenerate eigenvalue). We do not need to suppose that the other eigenvectors of the universe have the same decomposition. In that case, the density eigenmatrix is the projection (pure state) $\rho_a = |\zeta_i\rangle\langle\zeta_i| = P_{\zeta_i}$ and $P_a = P_{\zeta_i} \otimes P_{\xi_\alpha}$ ($P_{\xi_\alpha} = |\xi_\alpha\rangle\langle\xi_\alpha|$). Since the density matrix is a pure state, its von Neumann entropy is zero and no local decoherence associated with an adiabatic approximation involving only ϕ_a occurs. The gauge potential and the reduced potential are

$$\mathcal{A}_a = \tilde{\mathcal{A}}_i + A_{\mathcal{E},\alpha}P_{\zeta_i} \tag{35}$$

$$A_a = \left(A_{\mathcal{S},i} + A_{\mathcal{E},\alpha}\right)P_{\zeta_i} \tag{36}$$

where $\tilde{\mathcal{A}}_i = |\mathrm{d}\zeta_i\rangle\langle\zeta_i| \in \Omega^1(M, \mathfrak{s})$ is the C^*-geometric phase generator for the system without environment, $A_{\mathcal{S},i} = \langle\zeta_i|\mathrm{d}\zeta_i\rangle \in \Omega^1 M$ is the (usual) geometric phase generator for the isolated system, and $A_{\mathcal{E},\alpha} = \langle\xi_\alpha|\mathrm{d}\xi_\alpha\rangle \in \Omega^1 M$ is the (usual) geometric phase generator for the isolated environment.

The curving and the fake curvature are

$$B_a = \tilde{B}_a + F_{\mathcal{E},\alpha}P_{\zeta_i} - A_{\mathcal{E},\alpha} \wedge P_{\zeta_i}\left(\tilde{\mathcal{A}}_i + \tilde{\mathcal{A}}_i^\dagger\right) \tag{37}$$

$$F_a = \left(F_{S,i} + F_{\mathcal{E},\alpha}\right)P_{\zeta_i} - \left(A_{S,i} + A_{\mathcal{E},\alpha}\right) \wedge \left(\mathcal{A}_a + \mathcal{A}_a^\dagger\right) - B_a \tag{38}$$

where $F_{S,i} = \mathrm{d}A_{S,i} \in \Omega^2 M$ is the adiabatic curvature of the isolated system, $F_{\mathcal{E},\alpha} = \mathrm{d}A_{\mathcal{E},\alpha} \in \Omega^2 M$ is the adiabatic curvature of the isolated environment, and $\tilde{B}_a = \mathrm{d}\tilde{\mathcal{A}}_i - \tilde{\mathcal{A}}_i \wedge \tilde{\mathcal{A}}_i = -|\mathrm{d}\zeta_i\rangle \wedge \langle \mathrm{d}\zeta_i| + A_{S,i} \wedge \mathcal{A}_a \in \Omega^2(M, \mathfrak{s})$ is the curving associated with the C^*-geometric phase generator of the system without environment. These expressions seem to contain complicated terms, but in fact the averages are very simple:

$$\mathrm{tr}_{\mathcal{H}_S}\left(\rho_a F_a\right) = F_{S,i} \tag{39}$$

$$\mathrm{tr}_{\mathcal{H}_\mathcal{E}}\left(\rho_a B_a\right) = F_{\mathcal{E},\alpha}. \tag{40}$$

The average fake curvature is the curvature of the isolated system, in accordance with their common interpretation. Because the system and the environment are not entangled, if the universe is in the state ϕ_a, the non-adiabatic processes are the same one for the system in contact with the environment and for the isolated system.

The average curving is the curvature of the environment. It is this curvature which measures the kinematic decoherence processes. The explanation of this fact is the following. We assume an adiabatic approximation for the system in contact with the environment, but we do not assume that the dynamics of the environment is adiabatic. Indeed if we assume a total adiabaticity (system and environment), the evolution of the universe is 'strongly' adiabatic and is characterized by the universe geometric phase generator $\langle\langle \phi_a | \mathrm{d}\phi_a \rangle\rangle$. This is not in accordance with the problem of quantum control of a system in contact with an environment. We directly control only the system (and we can only assume the adiabaticity for the system). The environment feels the control, but the 'experimentalist' does not know the environment and its dynamics. This is the sense of the partial trace $\mathrm{tr}_{\mathcal{H}_\mathcal{E}}$; the information concerning the environment is lost. The dynamics of the universe under the control is then 'weakly' adiabatic and is characterized by the C^*-geometric phase generator $|\mathrm{d}\phi_a\rangle\rangle\langle\langle\phi_a|\rho_a^{-1}$. If the universe is in the state $\zeta_i \otimes \xi_\alpha$, and if the control path C passes through a region of M with a strong curvature of the environment, then non-adiabatic transitions occur from ξ_α to another state ξ_β. But $\zeta_i \otimes \xi_\beta$ is not necessarily an eigenvector of the universe (we have not supposed that all eigenstates of the universe are factorizable). $\zeta_i \otimes \xi_\beta$ can be a superposition of eigenstates of the universe, and the dynamics will induce Rabi oscillations between these states. These oscillations will destroy the factorization, and the system and the environment will become entangled.

3.3.2. An eigenstate as a Schmidt decomposition. We suppose that an eigenvector of the universe has a Schmidt decomposition:

$$\phi_a(x) = \sum_{i\in I} \sqrt{p_i}\,\zeta_i(x) \otimes \xi_i(x) \qquad \sum_{i\in I} p_i = 1 \tag{41}$$

where I is a subset of $\{1, \ldots, \dim \mathcal{H}_S\}$ and $0 < p_i < 1$ are occupation probabilities independent of x. $\{\zeta_i\}_i$ and $\{\xi_i\}_i$ are eigenvectors of the system and of the environment (associated with non-degenerate eigenvalues). The density eigenmatrix is $\rho_a = \sum_{i\in I} p_i |\zeta_i\rangle\langle\zeta_i|$ and $P_a = \sum_{i\in I} P_{\zeta_i} \otimes P_{\xi_i}$. The von Neumann entropy is the same on the whole of M: $-\mathrm{tr}_{\mathcal{H}_S}(\rho_a \ln \rho_a) = -\sum_{i\in I} p_i \ln p_i$.

The gauge potential and the reduced potential are

$$\mathcal{A}_a = \sum_{i\in I}\tilde{A}_i + \sum_{i,j\in I}\hat{A}_{\mathcal{E},I,ij}\left|\zeta_i\right\rangle\left\langle\zeta_j\right| \tag{42}$$

$$A_a = \sum_{i\in I}\left(A_{S,I,ii} + A_{\mathcal{E},I,ii}\right)P_{\zeta_i} \tag{43}$$

where $\tilde{\mathcal{A}}_i = |\mathrm{d}\zeta_i\rangle\langle\zeta_i| \in \Omega^1(M, \mathfrak{s})$ is the C^*-geometric phase generator for the system without environment, $A_{S,I} \in \Omega^1(M, \mathfrak{u}(n))$ ($A_{S,I,ij} = \langle\zeta_i|\mathrm{d}\zeta_j\rangle$ and $n = \mathrm{card}I$) is the non-Abelian geometric phase generator for the isolated system, $A_{\mathcal{E},I} \in \Omega^1(M, \mathfrak{u}(n))$ ($A_{\mathcal{E},I,ij} = \langle\xi_i|\mathrm{d}\xi_j\rangle$) is the non-Abelian geometric phase generator for the isolated environment, and $\hat{A}_{\mathcal{E},I} = \varpi^{-1}A_{\mathcal{E},I}\varpi$ with $\varpi_{ij} = \sqrt{p_i}\,\delta_{ij}$.

The average fake curvature and the average curving are

$$\mathrm{tr}_{\mathcal{H}_S}\left(\rho_a F_a\right) = \mathrm{tr}_{\mathbb{C}^n}\left(\varpi^2\left(F_{S,I} + \left[A_{S,I}, \hat{A}^{t}_{\mathcal{E},I}\right]\right)\right) \tag{44}$$

$$\mathrm{tr}_{\mathcal{H}_S}\left(\rho_a B_a\right) = \mathrm{tr}_{\mathbb{C}^n}\left(\varpi^2\left(F_{\mathcal{E},I} - A_{S,I}\wedge A_{S,I}\right)\right) \tag{45}$$

where $F_{S,I} = \mathrm{d}A_{S,I} + A_{S,I}\wedge A_{S,I} \in \Omega^2(M, \mathfrak{u}(n))$ is the non-Abelian curvature of the isolated system and $F_{\mathcal{E},I} = \mathrm{d}A_{\mathcal{E},I} + A_{\mathcal{E},I}\wedge A_{\mathcal{E},I} \in \Omega^2(M, \mathfrak{u}(n))$ is the non-Abelian curvature of the isolated environment (A^t denotes the transposition of the matrix A).

The average fake curvature is then essentially the statistical average of the non-Abelian curvature of the isolated system. In the same way, the average curving is essentially the statistical average of the non-Abelian curvature of the isolated environment. The interpretations are then the same as for the previous example, but with an average associated with the superposition of factorized states of the Schmidt decomposition. The additional term in the average curving $\mathrm{tr}\,(\varpi^2 A_{S,I}\wedge A_{S,I}) = \sum_{i,j\in I}p_i A_{S,I,ij}\wedge A_{S,I,ji}$ characterizes the non-adiabatic transitions of the system inside the space spanned by $\{\zeta_i\}_{i\in I}$. These transitions can modify the superposition coefficients and induce Rabi oscillations between ϕ_a and other eigenvectors of the universe (and induce modifications of the entanglement). The additional term in the average fake curvature $\mathrm{tr}\,(\varpi^2[A_{S,I}, \hat{A}^{t}_{\mathcal{E},I}])$ characterizes non-adiabatic transitions for the system induced by its entanglement with the environment.

Remark: if the probabilities p_i depend on x, we have a new gauge potential $\breve{\mathcal{A}}_a = \mathcal{A}_a + \sum_i \mathrm{d}\ln\sqrt{p_i}P_{\zeta_i} = \mathcal{A}_a + \sum_i(\mathrm{d}\varpi\varpi^{-1})_{ii}P_{\zeta_i}$; ϖ plays the role of a usual gauge change and the results for the average fake curvature and for the average curving are similar to those for the case where the probabilities are independent of x.

4. An example: STIRAP

In this section, we illustrate the role of the fields associated with the higher gauge theory with a concrete example. We want also show that a geometric representation of the field strengths can be used to interpret the hampering of the quantum control induced by the entanglement of the system with its environment. Then it can be used to analyse the robustness of a control solution found by considering solely the system. We have chosen a very simple quantum control problem in order to avoid unnecessary complications which could hide the fundamental behaviours of the universe.

We consider a three-level atom controlled by two laser Gaussian pulses. The first one, called the 'pump' pulse, is quasi-resonant with the transition $|1\rangle \to |2\rangle$; and the second one, called the 'Stokes' pulse, is quasi-resonant with the transition $|2\rangle \to |3\rangle$ $((|i\rangle)_{i=1,2,3}$ being the

atomic bare states). A second three-level atom interacts with the first one and feels the laser pulses but with attenuated intensities (we set the attenuation as being a division by a factor 2). This second atom constitutes the environment for the controlled atom. In the rotating wave approximation (see [5]), the Hamiltonian of the universe is

$$H_{\mathcal{U}}(x) = H_{\mathcal{S}}(x) \otimes 1_{\mathcal{H}_{\mathcal{E}}} + 1_{\mathcal{H}_{\mathcal{S}}} \otimes H_{\mathcal{E}}(x) + V(x) \tag{46}$$

with, in the basis $(|i\rangle)_{i=1,2,3}$ for the first atom,

$$H_{\mathcal{S}}(x) = \frac{\hbar}{2}\begin{pmatrix} 0 & \Omega_P & 0 \\ \Omega_P & 2\Delta_P & \Omega_S \\ 0 & \Omega_S & 2\big(\Delta_P - \Delta_S\big) \end{pmatrix} \tag{47}$$

and, in the basis $(|i\rangle)_{i=1,2,3}$ for the second atom,

$$H_{\mathcal{E}}(x) = \frac{\hbar}{2}\begin{pmatrix} 0 & \frac{1}{2}\Omega_P & 0 \\ \frac{1}{2}\Omega_P & 2\Delta_P & \frac{1}{2}\Omega_S \\ 0 & \frac{1}{2}\Omega_S & 2\big(\Delta_P - \Delta_S\big) \end{pmatrix}. \tag{48}$$

$\Omega_P = |\langle 1|\vec{\mu} \cdot \vec{\mathcal{E}}_P|2\rangle|$ where $\vec{\mu}$ is the electric dipole moment of an atom and $\vec{\mathcal{E}}_P$ is the electric field of the pump pulse, $\Omega_S = |\langle 2|\vec{\mu} \cdot \vec{\mathcal{E}}_S|3\rangle|$ where $\vec{\mathcal{E}}_S$ is the electric field of the Stokes pulse, $\hbar\Delta_P = (\epsilon_2 - \epsilon_1) - \hbar\omega_P$ and $\hbar\Delta_S = (\epsilon_3 - \epsilon_2) - \hbar\omega_S$ where $(\epsilon_i)_{i=1,2,3}$ are the atomic bare energies and ω_P and ω_S are the laser frequencies. The laser frequencies (and thus the detuning $\Delta_{P/S}$) are fixed; and the $x = (\Omega_P, \Omega_S)$ constitute the control parameters. The control manifold is $M = \mathbb{R}^+ \times \mathbb{R}^+$.

For the sake of simplicity, we choose a simple operator V to model the coupling between the two atoms. We consider two cases:

- a static coupling:

$$V = g\,(|2,\,3\rangle\rangle\langle\langle 3,\,2| + |3,\,2\rangle\rangle\langle\langle 2,\,3|) \tag{49}$$

  where $|i,\,j\rangle\rangle = |i\rangle \otimes |j\rangle \in \mathcal{H}_{\mathcal{S}} \otimes \mathcal{H}_{\mathcal{E}}$;
- a dynamical coupling:

$$\begin{aligned} V(x) = g\Big(&\big|\zeta_2(x) \otimes \xi_3(x)\big\rangle\big\rangle\big\langle\big\langle\zeta_3(x) \otimes \xi_2(x)\big| \\ &+ \big|\zeta_3(x) \otimes \xi_2(x)\big\rangle\big\rangle\big\langle\big\langle\zeta_2(x) \otimes \xi_3(x)\big|\Big) \end{aligned} \tag{50}$$

  where $\{\zeta_i(x)\}_{i=1,2,3}$ are the eigenvectors of $H_{\mathcal{S}}(x)$ (continuous with respect to x) such that $|\zeta_i(0)\rangle = |i\rangle$; and $\{\xi_i(x)\}_{i=1,2,3}$ are the eigenvectors of $H_{\mathcal{E}}(x)$ (continuous with respect to x) such that $|\xi_i(0)\rangle = |i\rangle$ ($x = 0$ is the point corresponding to off lasers, $\Omega_S = \Omega_P = 0$).

$g \geqslant 0$ is the coupling strength. We consider only perturbative couplings between the system and the environment ($g \ll 1$).

Let $\{\phi_a(x)\}_{a=1,\ldots,9}$ be the eigenvectors of $H_{\mathcal{U}}(x)$, continuous with respect to x and such that

$$\lim_{g\to 0} \phi_1 = \zeta_1 \otimes \xi_1 \qquad \lim_{g\to 0} \phi_2 = \zeta_2 \otimes \xi_1 \qquad \lim_{g\to 0} \phi_3 = \zeta_3 \otimes \xi_1 \tag{51}$$

$$\lim_{g\to 0}\phi_4=\zeta_1\otimes\xi_2 \qquad \lim_{g\to 0}\phi_5=\zeta_2\otimes\xi_2 \qquad \lim_{g\to 0}\phi_6=\zeta_3\otimes\xi_2 \tag{52}$$

$$\lim_{g\to 0}\phi_7=\zeta_1\otimes\xi_3 \qquad \lim_{g\to 0}\phi_8=\zeta_2\otimes\xi_3 \qquad \lim_{g\to 0}\phi_9=\zeta_3\otimes\xi_3. \tag{53}$$

The quantum control problem is that of reaching the pure target state $\rho_{target}=|3\rangle\langle 3|$ with the system initially in the pure state $\rho_0=|1\rangle\langle 1|$. First, we recall the classical solution of the problem (the STIRAP solution) when the controlled atom is alone. Secondly, we study the robustness of this solution where the controlled atom is in contact with the second one, without coupling, with the static coupling and with the dynamical coupling.

The results of the control are computed by numerical integrations of the Schrödinger equation of the universe based on a second-order differential scheme (see for example [15]). The different field strengths (F_S, $\mathrm{tr}_{\mathcal{H}_S}(\rho_a F_a)$, $\mathrm{tr}_{\mathcal{H}_S}(\rho_a B_a)$) are numerically computed by using methods coming from lattice gauge theory [16, 17] after a triangulation of the control manifold M with a sufficiently thin triangular lattice.

4.1. A single isolated atom

The STIRAP solution [5] consists in the path C on M defined by

$$t\mapsto x(t)=\left(\Omega_0 \mathrm{e}^{-\frac{(t-t_P)^2}{\tau_P^2}},\ \Omega_0 \mathrm{e}^{-\frac{(t-t_S)^2}{\tau_S^2}}\right) \tag{54}$$

with $\Omega_0=3.5$ au, $t_P=70$ au, $t_S=20$ au, $\tau_P=\tau_S=30$ au (with $t_0=-60$ au and $T=140$ au; au = atomic units). This solution is counter-intuitive since it consists in starting the Stokes pulse (which is quasi-resonant with the transition $|2\rangle\to|3\rangle$) before the pump pulse (which is quasi-resonant with the transition $|1\rangle\to|2\rangle$). To shed light on this control solution, we numerically integrate the Schrödinger equation for the system alone, and we consider the density matrix $\rho_\psi(t)=|\psi(t)\rangle\langle\psi(t)|$ with $\psi(t)$ the solution of the Schrödinger equation. The occupation probabilities of the bare states $\rho_{\psi,ii}(t)=\langle i|\rho_\psi(t)|i\rangle$ and the occupation probabilities of the instantaneous eigenstates $\mathrm{tr}_{\mathcal{H}_S}(\rho_\psi(t)P_i(x(t)))$ with $P_i(x)=|\zeta_i(x)\rangle\langle\zeta_i(x)|$ are shown in figure 1. We can interpret the solution by using the adiabatic curvatures $F_{S,i}=\mathrm{d}A_{S,i}$ with $A_{S,i}=\langle\zeta_i|\mathrm{d}\zeta_i\rangle$. Figure 2 shows the densities of the field strengths $F_{S,i,12}=\langle\frac{\partial\zeta_i}{\partial x^1}|\wedge|\frac{\partial\zeta_i}{\partial x^2}\rangle$. Starting from P_1, the dynamics passes to P_2 at • which corresponds to the singularity common to $F_{S,1}$ and $F_{S,2}$ (the crossing of the two associated eigenvalues). The dynamics passes from P_2 to P_3 at ■, the singularity common to $F_{S,2}$ and $F_{S,3}$. This is in accordance with the adiabatic quantum control method based on rapid adiabatic passages (see also [5]).

In the following, we do not change the path C (the STIRAP solution of the control problem), but we study the robustness of this solution with the entanglement of the controlled atom with the atom constituting the environment.

4.2. Two atoms without coupling

We begin by studying the case without coupling between the two atoms ($g=0$). The eigenvectors ϕ_a are then factorizable, and the rank of the density eigenmatrices $\rho_a=\mathrm{tr}_{\mathcal{H}_\mathcal{E}}|\phi_a\rangle\rangle\langle\langle\phi_a|$ is equal to 1. The von Neumann entropy $-\mathrm{tr}_{\mathcal{H}_S}(\rho_a\ln\rho_a)$ is then 0 for all states.

We integrate the Schrödinger equation of the universe with two initial conditions: the first one is without state superposition $\psi(t_0)=\phi_1(0)$ and the second one, with initial environment state superposition $\psi(t_0)=\frac{1}{\sqrt{2}}(\phi_1(0)+\phi_7(0))$. In the two cases we have

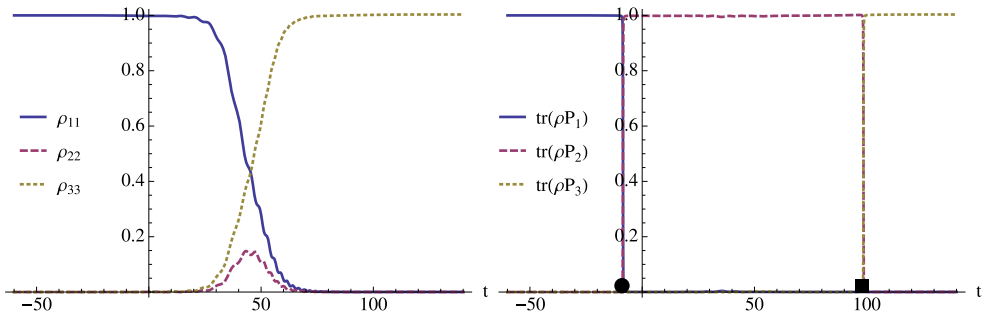

Figure 1. Left: occupation probabilities of the bare states $\rho_{\psi,ii}$ with respect to t. Right: occupation probabilities of the instantaneous eigenstates $\mathrm{tr}_{\mathcal{H}_S}(\rho_\psi P_i)$ with respect to t. The event • is the transition $\zeta_1 \to \zeta_2$ and the event ■ is the transition $\zeta_2 \to \zeta_3$.

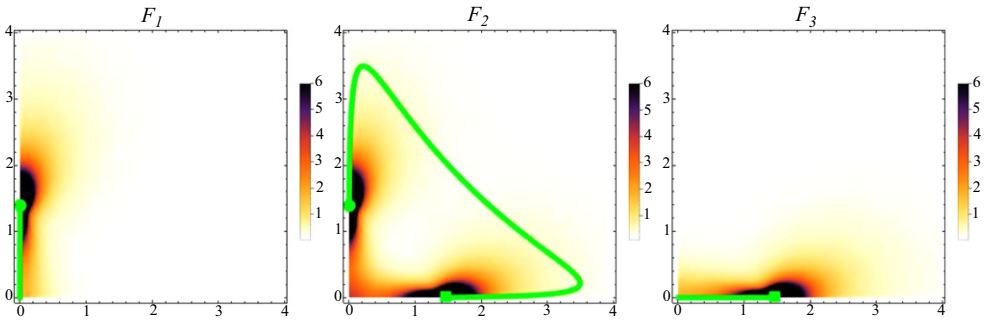

Figure 2. Densities of the adiabatic curvatures $F_{S,i}$ in M, with the path C and the events • (transition $\zeta_1 \to \zeta_2$) and ■ (transition $\zeta_2 \to \zeta_3$).

$\rho_\psi(t_0) = \mathrm{tr}_{\mathcal{H}_S}|\psi(0)\rangle\rangle\langle\langle\psi(0)| = |1\rangle\langle 1|$. The occupation probabilities of the bare states $\rho_{\psi,ii}$, the occupation probabilities of the instantaneous eigenvectors of the system $\mathrm{tr}_{\mathcal{H}_S}(\rho_\psi P_i)$ ($P_i = |\zeta_i\rangle\langle\zeta_i|$) and the occupation probabilities of the eigenvectors of the universe $|\langle\langle\phi_a|\psi\rangle\rangle|^2$ are shown in figure 3. In the two cases, we see that the adiabaticity is satisfied for the system, whereas this is not completely the case for the universe. But since all states of the universe are factorizable, no decoherence significantly occurs on the controlled dynamics (for the first case the entropy remains equal to 0 and it increases to a very small value in the second case, as shown in figure 4). We can interpret the results by plotting the densities in M of the average adiabatic fake curvatures $\mathrm{tr}_{\mathcal{H}_S}(\rho_a F_a)$ (figure 5) and of the average adiabatic curving $\mathrm{tr}_{\mathcal{H}_S}(\rho_a B_a)$ (figure 6). As shown in section 3.3.1, the average fake curvature is equal to the curvature of the system and the average curving is equal to the curvature of the environment. To summarize we have:

- the path C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_1 F_1)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_2 F_2)$ which induces a transition $P_1 \to P_2$ for the system (and a transition $\phi_1 \to \phi_2$ for the universe);
- ▲ C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_2 B_2)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_5 B_5)$ which induces a transition $\phi_2 \to \phi_5$ (without a non-adiabatic effect for the system);
- ⋆ C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_5 B_5)$ and $\mathrm{tr}_S(\rho_8 B_8)$ which induces a transition $\phi_5 \to \phi_8$ (without a non-adiabatic effect for the system);

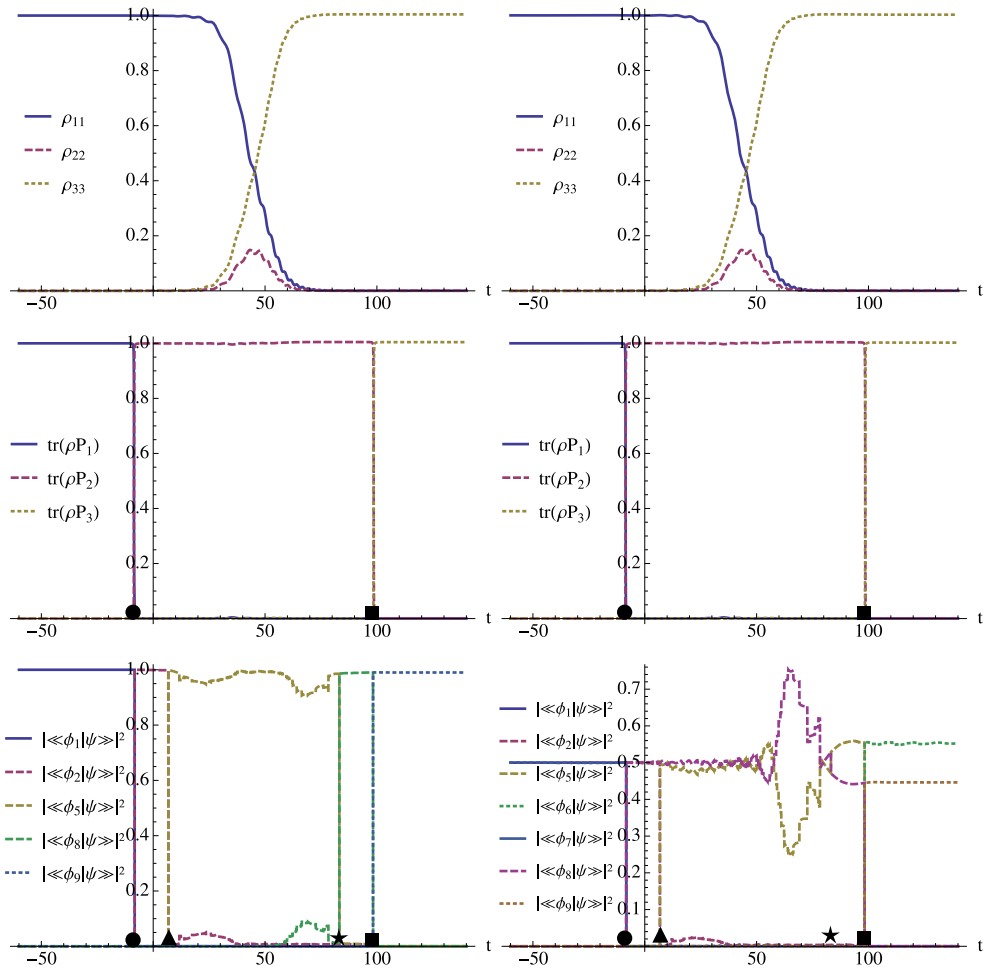

Figure 3. Upper: occupation probabilities of the bare states $\rho_{\psi,ii}$ with respect to t. Middle: occupation probabilities of the instantaneous eigenstates of the system $\mathrm{tr}_{\mathcal{H}_S}(\rho_\psi P_i)$ with respect to t. Lower: occupation probabilities of the instantaneous eigenstates of the universe $|\langle\langle \phi_a|\psi\rangle\rangle|^2$ with respect to t. Left: for the initial condition $\psi(t_0) = \phi_1(0)$. Right: for the initial condition $\psi(t_0) = \frac{1}{\sqrt{2}}(\phi_1(0) + \phi_7(0))$. The event • is the transition $\zeta_1 \to \zeta_2$ ($\phi_1 \to \phi_2$) and the event ■ is the transition $\zeta_2 \to \zeta_3$ ($\phi_5 \to \phi_9$). The event ▲ is the transition $\phi_2 \to \phi_5$ and the event ⋆ is the transition $\phi_5 \to \phi_8$.

■ C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_8 F_8)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_9 F_9)$ which induces a transition $P_2 \to P_3$ for the system (and a transition $\phi_8 \to \phi_9$ for the universe).

The passages by the singularities of the curving have no significant consequences for the control in this case (except the very small increase of the entropy associated with the non-adiabatic transitions in the environment for the case with a superposition of eigenstates).

4.3. Two atoms with a static coupling

We repeat the previous study with a static coupling ($g = 0.1$ au). In this case, all the density eigenmatrices ρ_a are invertible (their rank is equal to 3) for non-zero laser intensities. We

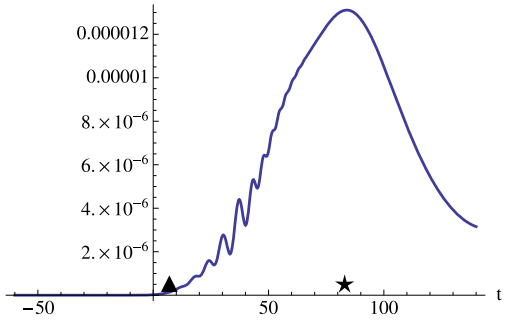

Figure 4. von Neumann entropy of the density matrix $-\mathrm{tr}_{\mathcal{H}_S}(\rho_\psi \ln \rho_\psi)$ with respect to t for the initial condition $\psi(0) = \frac{1}{\sqrt{2}}(\phi_1(0) + \phi_7(0))$.

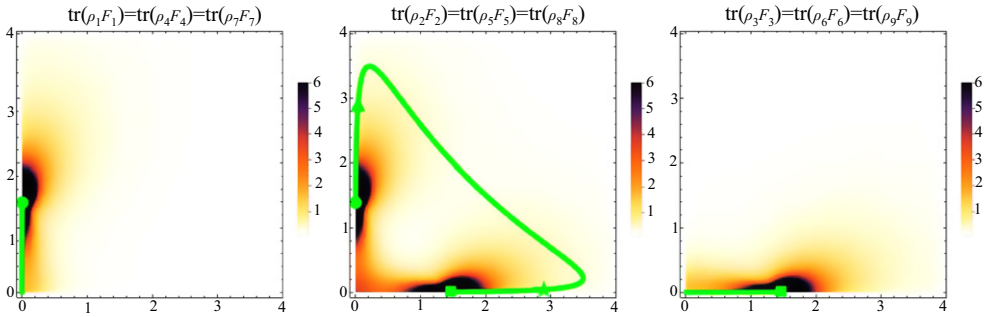

Figure 5. Densities of the average fake curvature $\mathrm{tr}_{\mathcal{H}_S}(\rho_a F_a)$ in M, with the path C and the events • (transition $\zeta_1 \to \zeta_2$), ▲ (transition $\phi_2 \to \phi_5$), ⋆ (transition $\phi_5 \to \phi_8$) and ■ (transition $\zeta_2 \to \zeta_3$).

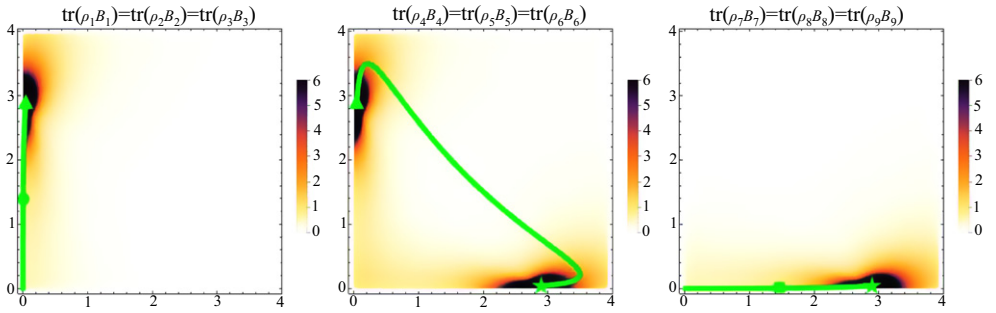

Figure 6. Densities of the average curving $\mathrm{tr}_{\mathcal{H}_S}(\rho_a B_a)$ in M, with the path C and the events • (transition $\zeta_1 \to \zeta_2$), ▲ (transition $\phi_2 \to \phi_5$), ⋆ (transition $\phi_5 \to \phi_8$) and ■ (transition $\zeta_2 \to \zeta_3$).

consider three initial conditions: $\psi(t_0) = \phi_1(0)$, $\psi(t_0) = \phi_4(0)$ and $\psi(t_0) = \phi_7(0)$. The occupation probabilities are plotted in figures 7 and 8, and the entropies of the density matrix are plotted in figure 9.

In the first case the control is imperfectly realized, in the second case the control quality is very low, and in the last case the control completely fails. We want to interpret

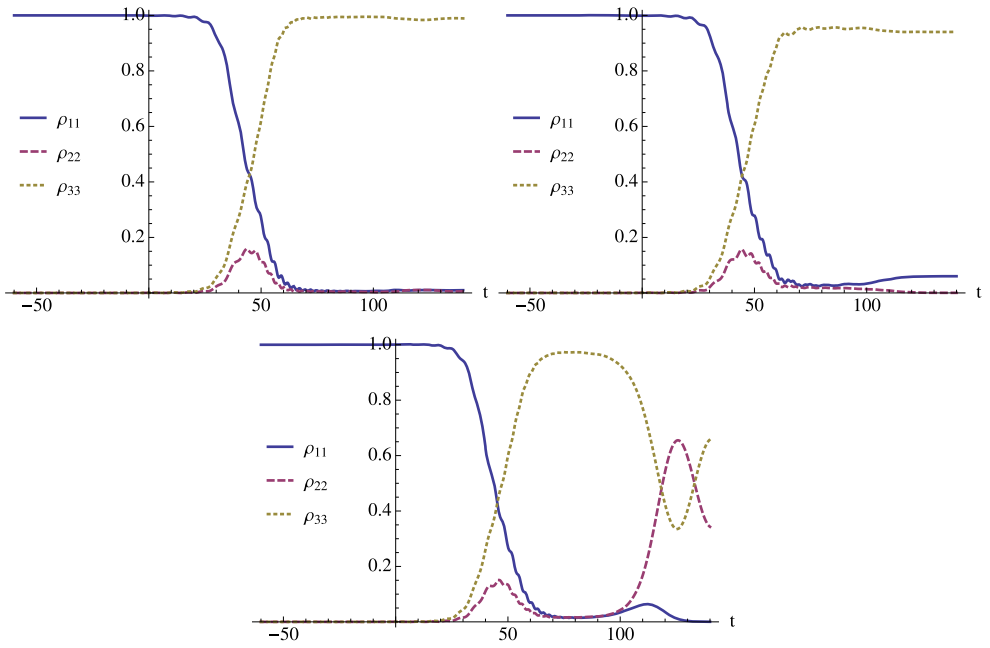

Figure 7. Occupation probabilities of the bare states $\rho_{\psi,ii}$ with respect to t, for the initial condition $\psi(t_0) = \phi_1(0)$, the initial condition $\psi(t_0) = \phi_4(0)$ and the initial condition $\psi(t_0) = \phi_7(0)$.

geometrically the different dynamical effects appearing in the previous figures. We first note that the average curving is zero for all states. Figure 10 shows the average fake curvatures and figure 11 shows the eigenentropies. We see in these figures that the regions with strong eigenentropies are correlated with some regions with strong fake curvature (which do not have the morphology of a point singularity). Because of their morphology, we call such a region an *entropic string*. We summarize the different events:

- the path C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_a F_a)$ and $\mathrm{tr}_S(\rho_{a+1}F_{a+1})$ (with $a = 1$ for the first case, $a = 4$ for the second one, and $a = 7$ for the last case) which induces a transition $P_1 \to P_2$ for the system;
- ▲ (not for the last case) C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_2 F_2)$ and $\mathrm{tr}_S(\rho_5 F_5)$ which induces a transition $\phi_2 \leftrightarrow \phi_5$ (without non-adiabatic effects for the system);
- ♦ (not for the second case) C passes through an entropic string (of $\mathrm{tr}_{\mathcal{H}_S}(\rho_5 F_5)$ for the first case, and of $\mathrm{tr}_{\mathcal{H}_S}(\rho_3 F_3)$ and $\mathrm{tr}_S(\rho_8 F_8)$ for the last case) which induces an increase of the entropy of the system (and non-adiabatic exchanges between ϕ_3 and ϕ_8 for the last case);
- ♣ C passes through an entropic string (of $\mathrm{tr}_{\mathcal{H}_S}(\rho_5 F_5)$ for the first case, of $\mathrm{tr}_{\mathcal{H}_S}(\rho_2 F_2)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_7 F_7)$ for the second case, and of $\mathrm{tr}_{\mathcal{H}_S}(\rho_3 F_3)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_5 F_5)$ for the last case) which induces oscillations of the entropy of the system (with non-adiabatic exchanges);
- ★ (not for the second case) C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_5 F_5)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_8 F_8)$ which induces a transition $\phi_5 \leftrightarrow \phi_8$;
- ■ C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_8 F_8)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_9 F_9)$ (first case), or of $\mathrm{tr}_{\mathcal{H}_S}(\rho_2 F_2)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_3 F_3)$ (second case), or of $\mathrm{tr}_{\mathcal{H}_S}(\rho_5 F_5)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_6 F_6)$ (last case), which induces a transition $P_2 \to P_3$ for the system; for the last case only C enters in a strong entropic string of $\mathrm{tr}_{\mathcal{H}_S}(\rho_6 F_6)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_8 F_8)$ which induces strong non-adiabatic exchanges;

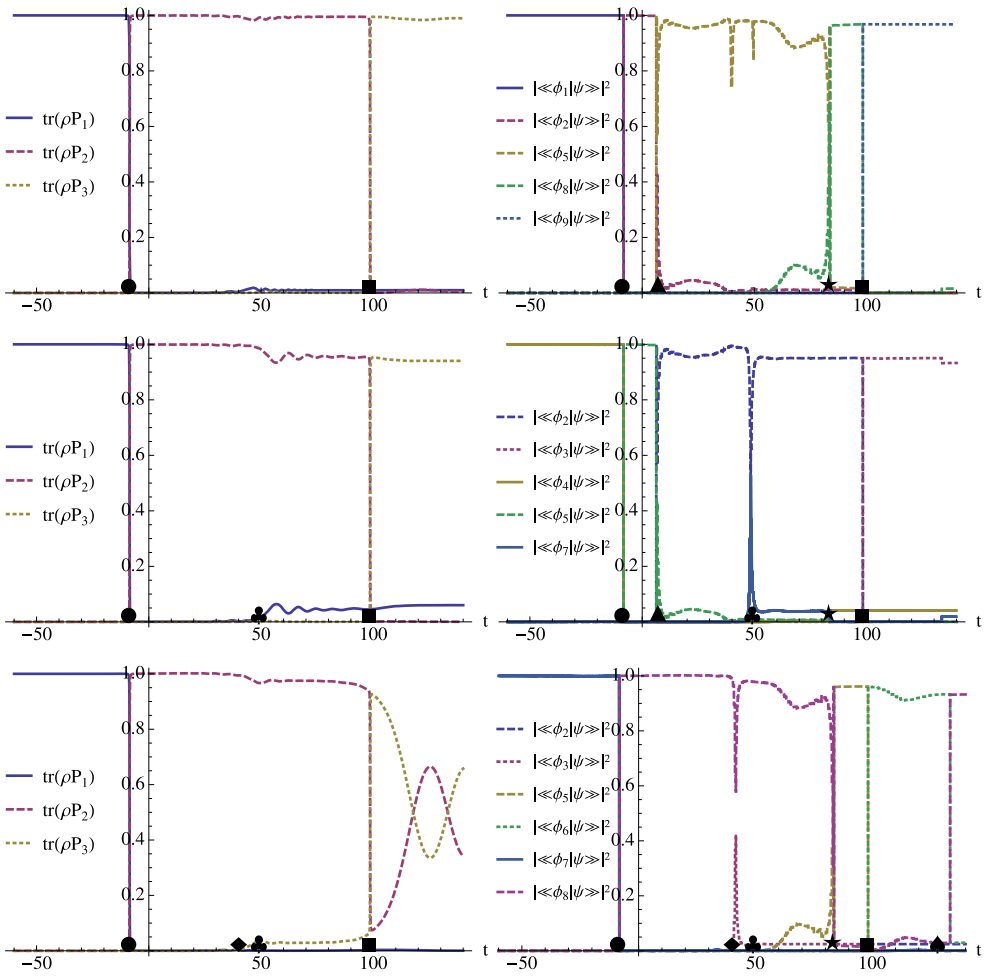

Figure 8. Left: occupation probabilities of the instantaneous eigenstates of the system $\mathrm{tr}_{\mathcal{H}_S}(\rho_\psi P_i)$ with respect to t. Right: occupation probabilities of the instantaneous eigenstates of the universe $|\langle\langle\phi_a|\psi\rangle\rangle|^2$ with respect to t. Upper: for the initial condition $\psi(t_0) = \phi_1(0)$. Middle: for the initial condition $\psi(t_0) = \phi_4(0)$. Lower: for the initial condition $\psi(t_0) = \phi_7(0)$. The event • is the transition $\zeta_1 \to \zeta_2$ and the event ■ is the transition $\zeta_2 \to \zeta_3$. The event ▲ is the transition $\phi_2 \leftrightarrow \phi_5$, the event ⋆ is the transition $\phi_5 \leftrightarrow \phi_8$, and the event ♠ is the transition $\phi_6 \to \phi_8$. The events ♦ and ♣ are the beginnings of non-adiabatic exchanges in the universe.

♠ (only for the last case) C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_6 F_6)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_8 F_8)$ which induces a transition $\phi_6 \to \phi_8$.

The passages by the entropic strings (♦, ♣ and ■ in the last case) are responsible of the failures of the adiabatic quantum control. We see two kinds of singularities of the fake curvature: the first one (• and ■) induces adiabatic passages for the system, and the second one (▲, ⋆ and ♠) induces adiabatic passages for the environment without effects on the system. The inactive and active singularities (from the viewpoint of the controlled system) seem not to be easily distinguishable without comparison with the singularities of the isolated system. The

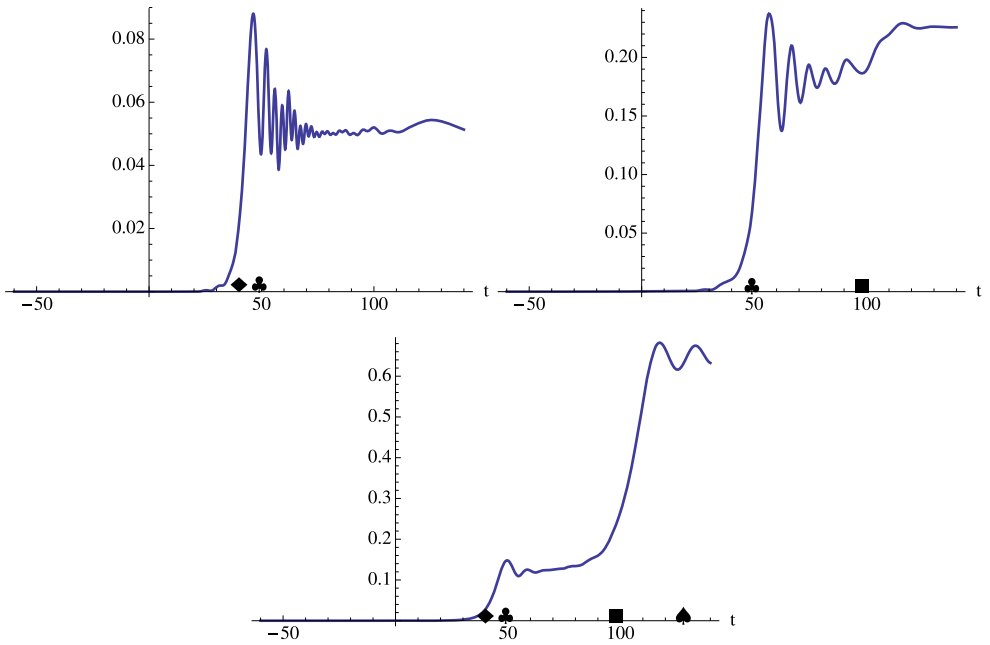

Figure 9. von Neumann entropy of the density matrix $-\mathrm{tr}_{\mathcal{H}_S}(\rho_\psi \ln \rho_\psi)$ with respect to t for the initial conditions $\psi(t_0) = \phi_1(0)$, $\psi(t_0) = \phi_4(0)$ and $\psi(t_0) = \phi_7(0)$.

average curving being equal to zero in this case, it does not eliminate the inactive singularities as in the previous case. This is clearly a drawback of an analysis based on adiabatic fields.

It is possible to give a heuristic explanation of these results. Write $\rho_a(x) = \sum_{i,j} p_{ij}(x) |\zeta_i(x)\rangle\langle\zeta_j(x)|$. The exact calculations of $p_{ij}(x)$ and of the different fields can be complicated. But we can heuristically suppose, in analogy with section 3.3.2, that $\mathrm{tr}_{\mathcal{H}_S}(\rho_a F_a)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_a B_a)$ have behaviours similar to those of $\mathrm{tr}_{\mathbb{C}^3}(\varpi^2(F_S + [A_S, \hat{A}_{\mathcal{E}}^t]))$ and $\mathrm{tr}_{\mathbb{C}^3}(\varpi^2(F_{\mathcal{E}} - A_S \wedge A_S))$ with $(\varpi^2)_{ij} = p_{ij}$. $A_S \in \Omega^1(M, \mathfrak{u}(3))$ is the non-Abelian generator of the geometric phase for all states of the system, and we have then $F_S = \mathrm{d}A_S + A_S \wedge A_S = 0$. In the same manner, we have $F_{\mathcal{E}} = 0$. The adiabatic transitions inside $\mathcal{H}_S$ do not induce decoherence processes; we can then expect that $\mathrm{tr}_{\mathbb{C}^3}(\varpi^2 A_S \wedge A_S)$ and, thus, $\mathrm{tr}_{\mathcal{H}_S}(\rho_a B_a)$ are zero. Moreover $\mathrm{tr}_{\mathbb{C}^3}(\varpi^2 [A_S, \hat{A}_{\mathcal{E}}^t])$ feels essentially the non-adiabatic couplings for the system (A_S) and for the environment ($A_{\mathcal{E}}$). Since the coupling is perturbative, we can expect that $\mathrm{tr}_{\mathcal{H}_S}(\rho_a F_a)$ presents essentially the singularities associated with the state $\lim_{g\to 0}\phi_a$ which characterizes non-adiabatic couplings for the system (active singularities) and for the environment (passive singularities). This argument is not a proof; it is just a heuristic argument showing the consistency of the numerical results with the interpretations of the adiabatic fields.

4.4. Two atoms with a dynamical coupling

We consider now a dynamical coupling ($g = 0.1$ au): $V(x) = g(|\zeta_2(x) \otimes \xi_3(x)\rangle\rangle\langle\langle\zeta_3(x) \otimes \xi_2(x)| + |\zeta_3(x) \otimes \xi_2(x)\rangle\rangle\langle\langle\zeta_2(x) \otimes \xi_3(x)|)$, i.e. the potential couples the dressed states in place of the bare states. In this case the density eigenmatrices have a rank equal to 1, except ρ_6 and ρ_8 which have a rank equal to 2 (for non-zero laser intensities). We consider two initial conditions: $\psi(t_0) = \phi_1(0)$ and $\psi(t_0) = \phi_7(0)$.

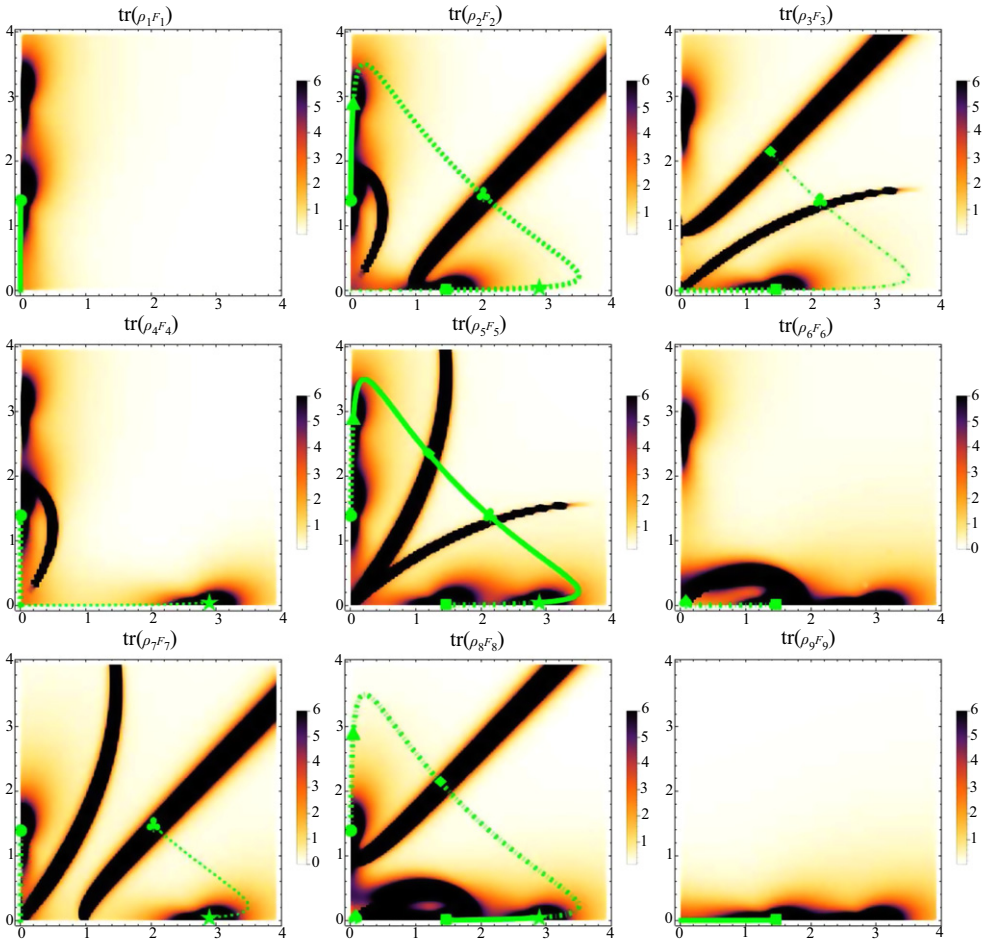

Figure 10. Densities of the average fake curvature $\mathrm{tr}_{\mathcal{H}_S}(\rho_a F_a)$ in M, with the path C (plain line for case 1, dashed line for case 2, dotted line for case 3; thick line for the states with a large occupation and thin line for the states with a small occupation). We show the events • (transition $\zeta_1 \to \zeta_2$), ▲ (transition $\phi_2 \leftrightarrow \phi_5$), ♦ and ♣ (beginnings of non-adiabatic exchanges), ★ (transition $\phi_5 \leftrightarrow \phi_8$), ■ (transition $\zeta_2 \to \zeta_3$), and ♠ (transition $\phi_6 \to \phi_8$).

The occupation probabilities are plotted in figure 12 and the entropies of the density matrix are plotted in figure 13. In these two cases, the control dramatically fails. The average fake curvatures are shown in figure 14, the average curvings are shown in figure 15 and the eigenentropies are shown in figure 16. We summarize the different events:

- the path C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_1 F_1)$ and $\mathrm{tr}_S(\rho_2 F_2)$ (or of $\mathrm{tr}_{\mathcal{H}_S}(\rho_7 F_7)$ and $\mathrm{tr}_S(\rho_8 F_8)$ for the second case) which induces a transition $P_1 \to P_2$ for the system;
- ▲ (only for the first case) C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_2 B_2)$ and $\mathrm{tr}_S(\rho_5 B_5)$ which induces a transition $\phi_2 \leftrightarrow \phi_5$ (without non-adiabatic effects for the system);
- ♦ (only for the second case) C approaches the region with large eigenentropies $-\mathrm{tr}\,(\rho_6 \ln \rho_6)$ and $-\mathrm{tr}\,(\rho_8 \ln \rho_8)$, which induces strong non-adiabatic oscillations between ϕ_6 and ϕ_8;

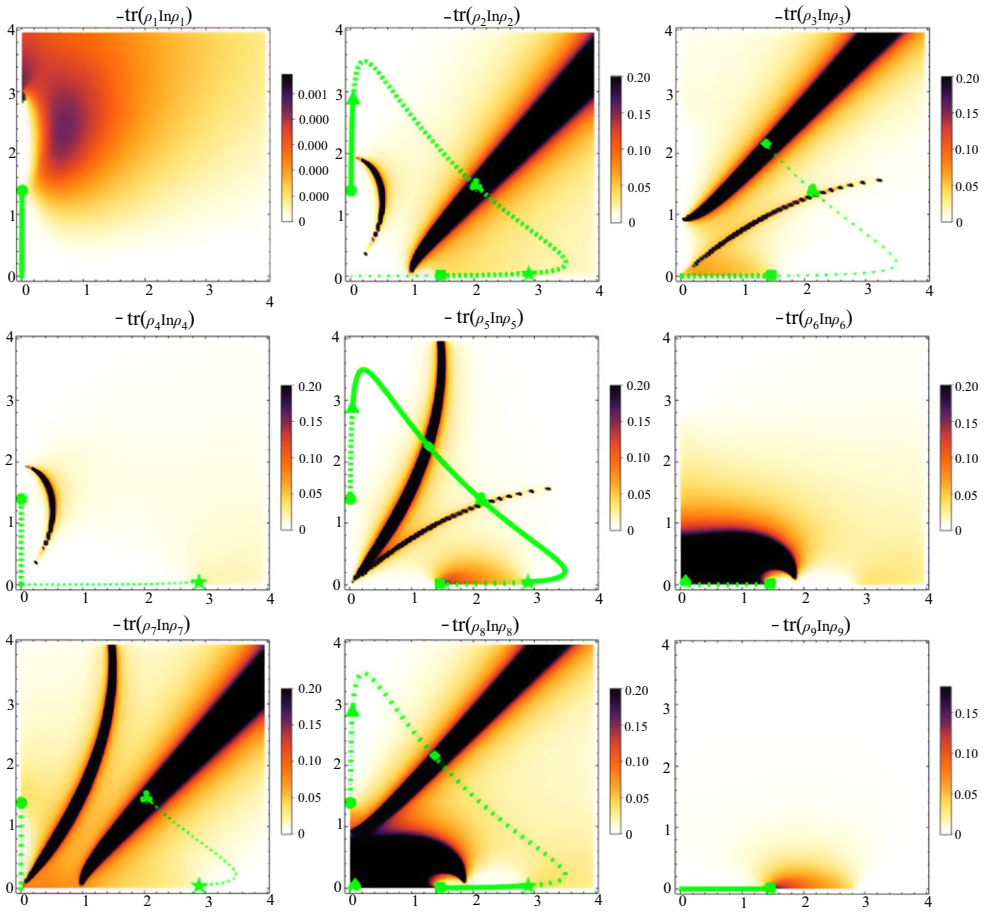

Figure 11. Eigenentropies $-\mathrm{tr}_{\mathcal{H}_S}(\rho_a \ln \rho_a)$ in M, with the path C (plain line for case 1, dashed line for case 2, dotted line for case 3; thick line for the states with a large occupation and thin line for the states with a small occupation). We show the events • (transition $\zeta_1 \to \zeta_2$), ▲ (transition $\phi_2 \leftrightarrow \phi_5$), ◆ and ♣ (beginnings of the increase of the entropy of the system), ⋆ (transition $\phi_5 \leftrightarrow \phi_8$), ■ (transition $\zeta_2 \to \zeta_3$), and ♠ (transition $\phi_6 \to \phi_8$).

♣ (only for the second case) C passes close to the region with large eigenentropies $-\mathrm{tr}\,(\rho_6 \ln \rho_6)$ and $-\mathrm{tr}\,(\rho_8 \ln \rho_8)$, and the non-adiabatic oscillations present a maximal amplitude;

⋆ C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_5 B_5)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_8 F_8)$ which induces a transition $\phi_5 \leftrightarrow \phi_8$; with the increase of the entropy of the system (with non-adiabatic exchanges) for the first case and with a modification of the entropy oscillations in the second case;

♡ (only for the first case) C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_6 F_6)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_8 F_8)$ which induces a transition $\phi_8 \to \phi_6$;

■ C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_5 F_5)$, $\mathrm{tr}_{\mathcal{H}_S}(\rho_6 F_6)$, $\mathrm{tr}_{\mathcal{H}_S}(\rho_8 F_8)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_9 F_9)$ (first case), or of $\mathrm{tr}_{\mathcal{H}_S}(\rho_7 F_7)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_8 F_8)$ (second case), which induces a transition $P_2 \to P_3$ for the system; for the second case C passes through the region with large eigenentropies

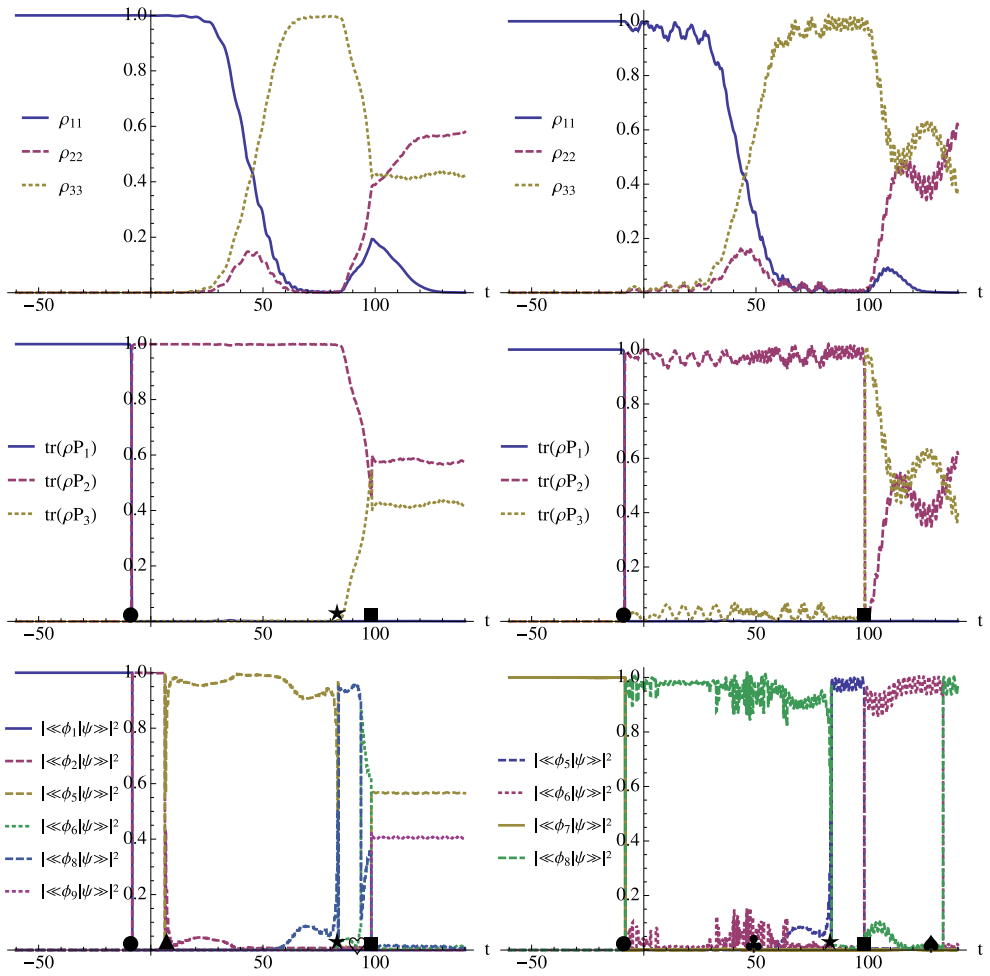

Figure 12. Upper: occupation probabilities of the bare states $\rho_{\psi,ii}$ with respect to t. Middle: occupation probabilities of the instantaneous eigenstates of the system $\mathrm{tr}_{\mathcal{H}_S}(\rho_\psi P_i)$ with respect to t. Lower: occupation probabilities of the instantaneous eigenstates of the universe $|\langle\langle\phi_a|\psi\rangle\rangle|^2$ with respect to t. Left: for the initial condition $\psi(t_0) = \phi_1(0)$. Right: for the initial condition $\psi(t_0) = \phi_7(0)$. The event • is the transition $\zeta_1 \to \zeta_2$ and the event ■ is the transition $\zeta_2 \to \zeta_3$. The event ▲ is the transition $\phi_2 \leftrightarrow \phi_5$, the event ⋆ is the transition $\phi_5 \leftrightarrow \phi_8$, and the events ♠ and ♡ are the transitions $\phi_6 \leftrightarrow \phi_8$. The events ♦ and ♣ are the beginnings of non-adiabatic exchanges in the universe.

$-\mathrm{tr}\,(\rho_6 \ln \rho_6)$ and $-\mathrm{tr}\,(\rho_8 \ln \rho_8)$ which induces a strong increase of the entropy of the system with strong non-adiabatic exchanges;

♠ (only for the second case) C passes through a singularity of $\mathrm{tr}_{\mathcal{H}_S}(\rho_6 F_6)$ and $\mathrm{tr}_{\mathcal{H}_S}(\rho_8 F_8)$ which induces a transition $\phi_6 \to \phi_8$.

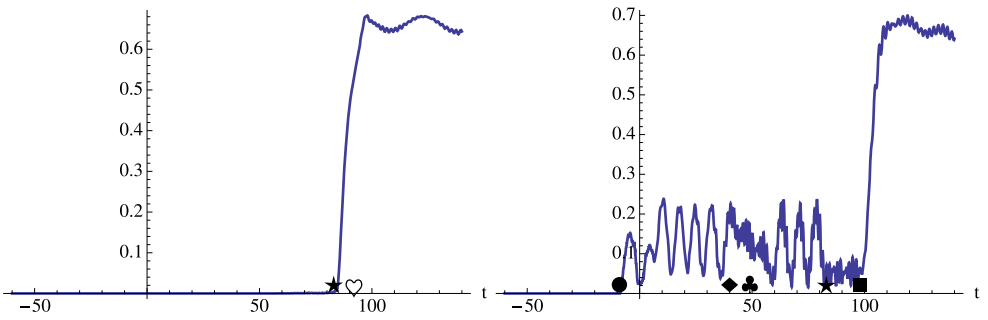

Figure 13. von Neumann entropy of the density matrix $-\mathrm{tr}_{\mathcal{H}_S}(\rho_\psi \ln \rho_\psi)$ with respect to t for the initial conditions $\psi(t_0) = \phi_1(0)$ (left) and $\psi(t_0) = \phi_7(0)$ (right).

5. Discussion and conclusion

5.1. Larger environments

The results presented in section 3 are independent of the dimensions of the Hilbert spaces of the system and of the environment. But the example treated in section 3 concerns a small system (a three-level atom) with a very small environment (another three-level atom). The restriction to a few levels for the system is not drastic. In principle, the adiabatic quantum control consists in controlling the probabilities of occupation of a few levels. For an N-level system (with N possibly very large), we can consider only a few parameter dependent eigenlevels linked by crossings or avoid crossings to the initial one. The adiabatic elimination of the other states is valid while the control path does not approach the crossings between a selected eigenlevel and an eliminated eigenlevel. By property 2, we know that the (fake) curvature presents a singularity at such a point for the selected eigenlevel involved, and which is not correlated with a singularity of another selected eigenlevel (since the crossing involved an eliminated eigenlevel). It is then easy to locate on the 'density charts' these forbidden regions (associated with cases of the adiabatic assumption failing).

For a complicated environment (with a lot of quantum levels), the analysis described in the present paper could be difficult to realize without other assumptions, because the number of 'density charts' of adiabatic field strengths to study becomes very large. Moreover, in a lot of situations, a complete and exact description of the environment (its Hamiltonian and the coupling operator) is unknown. To solve the first problem, we can consider the possibility of using effective small environments reproducing the effects of a large environment on the quantum system. For the second one, we can work only at the stage of the density matrices. We briefly discuss these two possibilities in this section.

5.1.1. Effective Hamiltonians for large environments. If $\dim \mathcal{H}_\mathcal{E}$ is very large, the number of 'density charts' to plot becomes too large for this to be realized. To solve this problem, we can proceed, in a first approximation, by adiabatic eliminations. Let $\{\xi_\alpha(x)\}_{\alpha\in\{1,\ldots,\dim\mathcal{H}_\mathcal{E}\}}$ be the parameter dependent eigenvectors of $H_\mathcal{E}(x)$. We assume that for physical reasons, only a few of these states $\{\xi_\alpha(x)\}_{\alpha\in I}$ are strongly involved at the starting point of the control $x_0 \in M$ (each control path considered starting and ending at x_0). We can then reduce the number of the environment states by projections onto the space spanned by $\{\xi_\alpha(x)\}_{\alpha\in I}$. In other words, we consider (for the eigenvector problem) the effective Hamiltonian $H_\mathcal{U}^{\mathit{eff},\,0}(x) = H_\mathcal{S}(x) \otimes 1_{\mathcal{H}_\mathcal{E}} + 1_{\mathcal{H}_\mathcal{S}} \otimes P_I(x)H_\mathcal{E}(x)P_I(x) + 1_{\mathcal{H}_\mathcal{S}} \otimes P_I(x)V(x)1_{\mathcal{H}_\mathcal{S}} \otimes P_I(x)$

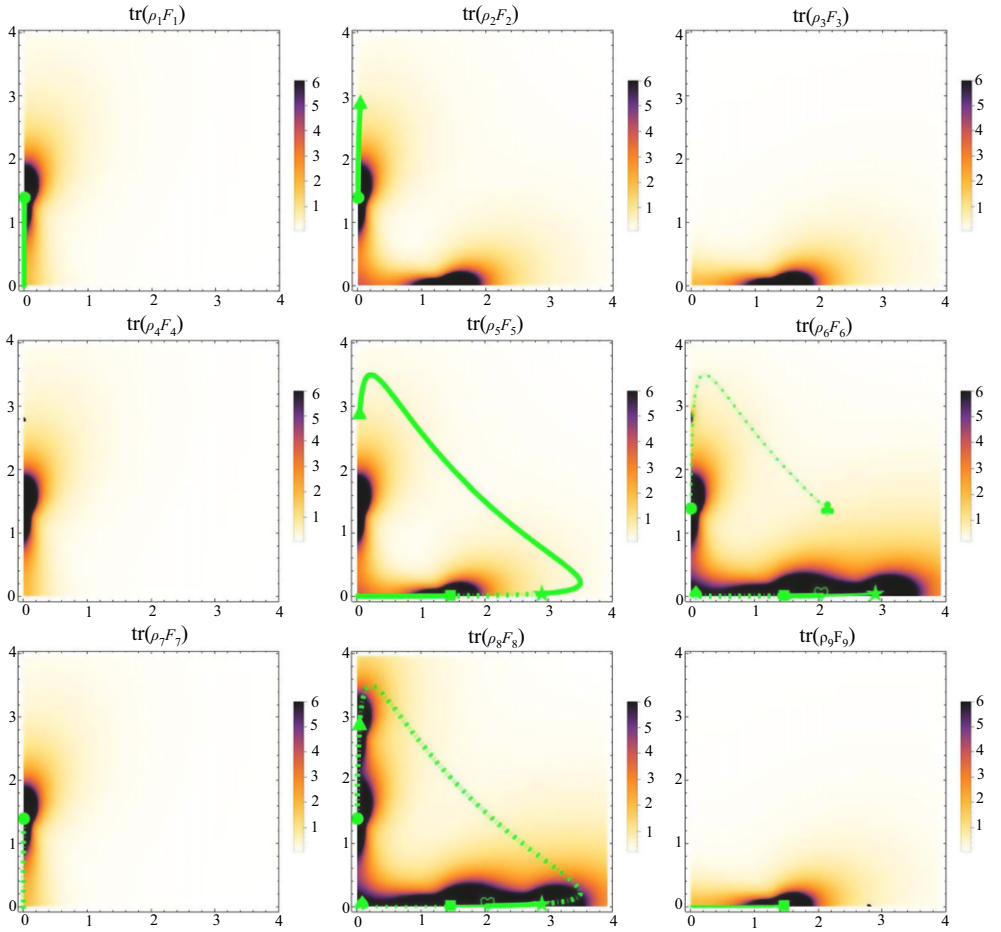

Figure 14. Densities of the average fake curvature $\mathrm{tr}_{\mathcal{H}_S}(\rho_a F_a)$ in M, with the path C (plain line for case 1 and dotted line for case 2; thick line for the states with a large occupation and thin line for the states with a small occupation). We show the events • (transition $\zeta_1 \to \zeta_2$), ▲ (transition $\phi_2 \leftrightarrow \phi_5$), ◆ and ♣ (beginnings of non-adiabatic exchanges), ★ (transition $\phi_5 \leftrightarrow \phi_8$), ■ (transition $\zeta_2 \to \zeta_3$), and ♠ and ♡ (transition $\phi_6 \leftrightarrow \phi_8$).

where $P_I(x)$ is the orthogonal projection onto the space spanned by $\{\xi_\alpha(x)\}_{\alpha \in I}$ (for the dynamics, it is associated with the effective Hamiltonian $H_{\mathcal{U}}^{eff-dyn,0} = H_{\mathcal{U}}^{eff,0} - \mathrm{i}\hbar 1_{\mathcal{H}_S} \otimes \dot{P}_I P_I$—the effective theories involve two effective Hamiltonians: one for the computation of the effective eigenvectors and the other for the computation of the effective dynamics). If the control is adiabatic with respect to the environment dynamics, this approximation is valid while the control path does not approach a crossing between a selected environment level and an eliminated one. The regions of M forbidden by this requirement are characterized by singularities of the curving (by the relation between the curving and the environment curvature and property 2). We can then locate these forbidden regions on the 'density charts'.

For example if we suppose that x_0 corresponds to the situation where the system and the environment are free (the control apparatus does not act on the quantum objects), then we can

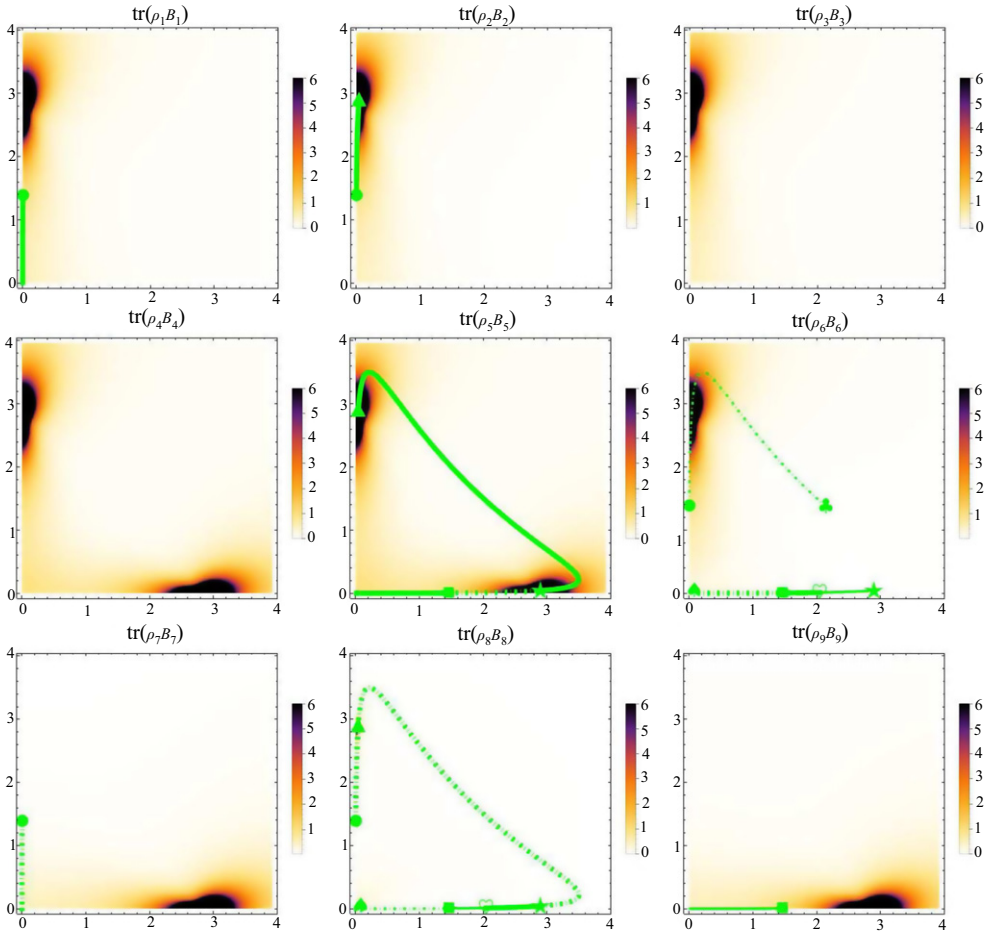

Figure 15. Densities of the average curving $\mathrm{tr}_{\mathcal{H}_S}(\rho_a B_a)$ in M,with the path C (plain line for case 1 and dotted line for case 2; thick line for the states with a large occupation and thin line for the states with a small occupation). We show the events • (transition $\zeta_1 \to \zeta_2$), ▲ (transition $\phi_2 \leftrightarrow \phi_5$), ◆ and ♣ (beginnings of non-adiabatic exchanges), ★ (transition $\phi_5 \leftrightarrow \phi_8$), ■ (transition $\zeta_2 \to \zeta_3$), ♠ and ♡ (transition $\phi_6 \leftrightarrow \phi_8$).

suppose that a very large environment is in a thermal equilibrium state: $\rho_{\mathcal{E}} = \frac{\mathrm{e}^{-\beta H_{\mathcal{E}}(x0)}}{Z}$ (where $\beta = \frac{1}{k_B T}$, T being the temperature and k_B the Boltzmann constant), with $Z = \mathrm{tr}_{\mathcal{H}_{\mathcal{E}}} \mathrm{e}^{-\beta H_{\mathcal{E}}(x_0)}$. The different initial conditions are then

$$\rho_{\mathcal{U},i}(0) = \sum_{\alpha=1}^{\dim \mathcal{H}_{\mathcal{E}}} \frac{\mathrm{e}^{-\beta \nu_\alpha(x_0)}}{Z} \left|\phi_{a(i,\alpha)}(x_0)\right\rangle\!\!\right\rangle \left\langle\!\!\left\langle \phi_{a(i,\alpha)}(x_0)\right| \tag{55}$$

where ν_α is the eigenvalue associated with ξ_α, and $\phi_{a(i,\alpha)}$ is the eigenstate of $H_{\mathcal{U}}$ such that

$$\lim_{g\to 0} \phi_{a(i,\alpha)} = \zeta_i \otimes \xi_\alpha \tag{56}$$

with $\{\zeta_i(x)\}$ the eigenstates of H_S, and g is the weak system–environment coupling amplitude. $\mathrm{tr}_{\mathcal{H}_{\mathcal{E}}} \rho_{\mathcal{U},i}(0) = \rho_{\mathcal{E}} + O(g)$. The density matrix of the system with respect to the time is then

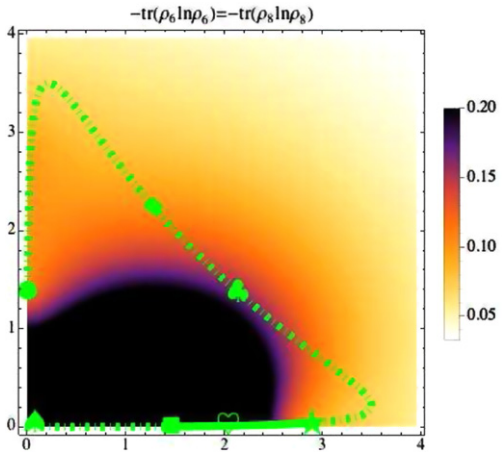

Figure 16. Eigenentropies $-\mathrm{tr}_{\mathcal{H}_S}(\rho_6 \ln \rho_6) = -\mathrm{tr}_{\mathcal{H}_S}(\rho_8 \ln \rho_8)$ in M (the other eigenentropies are zero), with the path C (plain line for case 1 and dotted line for case 2) and the events • (transition $\zeta_1 \to \zeta_2$), ▲ (transition $\phi_2 \leftrightarrow \phi_5$), ◆ and ♣ (beginnings of the increase of the entropy of the system), ★ (transition $\phi_5 \leftrightarrow \phi_8$) and ■ (transition $\zeta_2 \to \zeta_3$).

$$\rho_{S,i}(t) = \sum_{\alpha=1}^{\dim \mathcal{H}_\mathcal{E}} \frac{\mathrm{e}^{-\beta\nu_\alpha(x_0)}}{Z} \mathrm{tr}_{\mathcal{H}_\mathcal{E}} \left(U(t,0) \left| \phi_{a(i,\alpha)}(x_0) \right\rangle\!\right\rangle \left\langle\!\left\langle \phi_{a(i,\alpha)}(x_0) \right| U(t,0)^\dagger \right) \tag{57}$$

where $U(t,0)$ is the evolution operator of the universe, i.e. the solution of $\mathrm{i}\hbar \frac{\mathrm{d}U(t,0)}{\mathrm{d}t} = H_\mathcal{U}(x(t))U(t,0)$ with $U(0,0) = 1_{\mathcal{H}_S \otimes \mathcal{H}_\mathcal{E}}$. We can consider only the states $\{\xi_\alpha\}$ associated with the smallest energies (the Boltzmann factors $\mathrm{e}^{-\beta\nu_\alpha(x_0)}$ of the others being negligible) and, with the assumption that the control path does not approach crossings between the selected and the eliminated states, we have

$$\rho_{S,i}(t) \simeq \sum_{\alpha \in I} \frac{\mathrm{e}^{-\beta\nu_\alpha(x_0)}}{Z} \tag{58}$$

$$\times \mathrm{tr}_{\mathcal{H}_\mathcal{E}} \left(U^{eff,0}(t,0) \left| \phi_{a(i,\alpha)}(x_0) \right\rangle\!\right\rangle \left\langle\!\left\langle \phi_{a(i,\alpha)}(x_0) \right| U^{eff,0}(t,0)^\dagger \right) \tag{59}$$

with $\mathrm{i}\hbar \frac{\mathrm{d}U^{eff,0}(t,0)}{\mathrm{d}t} = H_\mathcal{U}^{eff,0}(x(t))U^{eff,0}(t,0)$. The control of $\rho_{S,i}(t)$ can then be deduced from the control of the states $\{U(t,0)\phi_{a(i,\alpha)}(x_0)\}_{i \in \{1,\ldots,\dim \mathcal{H}_S\}, \alpha \in I}$ at the adiabatic limit with a reasonable number of density charts to consider.

Nevertheless, the replacement of the universe Hamiltonian by $H_\mathcal{U}^{eff,0}$ is certainly too drastic for a lot of situations. We can indeed think that the requirement for the control to be strictly adiabatic with respect to the environment dynamics is difficult to achieve, since the 'experimentalist' controlling the system 'loses' the information concerning the environment (a loss of information which is mathematically modelled by the partial trace on $\mathcal{H}_\mathcal{E}$). Recently, we have proposed a framework in which to treat almost adiabatic dynamics [18]. It consists in considering (for the eigenvector problem) the effective Hamiltonian $H_\mathcal{U}^{eff,1} = 1_{\mathcal{H}_S} \otimes P_I H_\mathcal{U} \Omega$ where Ω (called the wave operator) is a solution of the Bloch equation $[H_\mathcal{U}, \Omega]\Omega = 0$ with $\Omega 1_{\mathcal{H}_S} \otimes P_I = \Omega$ (a complete exposition of the wave operator theory can be found in [19, 20], the effective Hamiltonian for the dynamics being $H_\mathcal{U}^{eff-dyn,1} = H_\mathcal{U}^{eff,1} - \mathrm{i}\hbar 1_S \otimes \dot{P}_I \Omega$). The interest of $H_\mathcal{U}^{eff,1}$ with respect to $H_\mathcal{U}^{eff,0}$ lies in $H_\mathcal{U}^{eff,1}$

taking into account non-adiabatic dynamical effects induced by the outside of the space spanned by $\{\xi_\alpha(x)\}_{\alpha\in I}$. It takes into account corrections of the strict adiabatic approximation. It is important to note that $H_{\mathcal{U}}^{eff,\,1}$ is not self-adjoint and generates then a non-unitary evolution. This is not an artefact, and it is one of the corrections of the strict adiabaticity. A decrease of the norm is associated with transitions from $\mathcal{H}_S \otimes \mathrm{Ran}P_I$ to $\mathcal{H}_S \otimes \ker P_I$ and an increase is associated with converse transitions. This effective Hamiltonian cannot include precise information about the eliminated states, but it includes information concerning 'quantum flows' entering and exiting from the $\mathcal{H}_S \otimes \mathrm{Ran}P_I$. We can compute the fake curvature and the curving by using the eigenstates of $H_{\mathcal{U}}^{eff,\,1}$ to plot a small number of 'density charts', which permit us to analyse the control problem (because of the non-self-adjointness of $H_{\mathcal{U}}^{eff,\,1}$, it is necessary to redefine the generator of the C^*-geometric phase as $\mathcal{A}_a = \mathrm{tr}_{\mathcal{H}_\mathcal{E}}(|\mathrm{d}\phi_a\rangle\rangle\langle\langle\phi_a^*|)\rho_a^{-1}$ with $\rho_a = \mathrm{tr}_{\mathcal{H}_\mathcal{E}}|\phi_a\rangle\rangle\langle\langle\phi_a^*|$ where $\{\phi_a^*\}_a$ are the eigenvectors of $H_{\mathcal{U}}^{eff,\,1^\dagger}$ to take into account the biorthogonality of the eigenbasis).

We note that the introduction of an effective Hamiltonian to reduce the size of the Hilbert space of the universe (needed to have a small number of density charts to consider) introduces a few approximations in the description of the system. But the consideration of the density charts of the curving and the fake curvature is used to obtain not quantitative results but just qualitative results. As in the example of section 4, we can use it *a posteriori* to analyse and to interpret the hampering of the control by the entanglement with the environment, and to understand the different processes occurring. And we can use it *a priori* to find the rough shape of a control solution path, taking into account the hampering by the environment (such a solution could be next optimized by specific numerical methods [21]).

5.1.2. Working directly at the stage of the density matrices. The density matrix of the system is a solution of the equation

$$\mathrm{i}\hbar\dot{\rho}_S(t) = \mathcal{L}_{x(t)}\Big(\rho_S(t)\Big) \tag{60}$$

where in the context used in this paper $\mathcal{L}_{x(t)}(\rho_S(t)) = \mathrm{tr}_{\mathcal{H}_\mathcal{E}}[H_\mathcal{U}(x(t)), |\psi(t)\rangle\rangle\langle\langle\psi(t)|]$. But in a lot of situations, a complete description of $H_\mathcal{U}$ is unknown or it is not practical to use. Under some assumptions (in particular with a Markovian approximation), the map $\mathcal{L}_x$ takes the Lindblad form [22]

$$\mathcal{L}_x(\rho) = \Big[\tilde{H}_S(x),\,\rho\Big] + \mathrm{i}\sum_k \gamma_k(x)\Gamma_k(x)\rho\Gamma_k(x)^\dagger - \frac{\mathrm{i}}{2}\sum_k \gamma_k(x)\Big\{\Gamma_k(x)^\dagger\Gamma_k(x),\,\rho\Big\}, \tag{61}$$

$\gamma_k \in \mathbb{R}$, $\Gamma_k \in \mathcal{L}(\mathcal{H}_S)$, $\tilde{H}_S$ being a system Hamiltonian possibly different from the free Hamiltonian H_S ($\{.,.\}$ being the anticommutator). It is interesting to note that the density eigenmatrix ρ_a, when it is induced by an eigenvector of $H_\mathcal{U}$, satisfies

$$\mathcal{L}_x\Big(\rho_a(x)\Big) = 0. \tag{62}$$

ρ_a is a steady state of the system. We postulate that even if $H_\mathcal{U}$ is unknown or forgotten, the density eigenmatrices are still parameter dependent steady states of the system governed by $\mathcal{L}_x$. Starting with a steady state $\rho_a(x(0))$, the dynamics, if it is sufficiently adiabatic, follows $\rho_a(x(t))$ except in the regions of rapid adiabatic passages (corresponding to the crossings of eigenlevels of $H_\mathcal{U}$) and in the regions inducing local or kinematic decoherence. Since we cannot use $H_\mathcal{U}$ which is unknown or forgotten, it is necessary to compute the curving and the fake curvature directly from ρ_a. Singularities and entropic strings of these fields indicate these

regions of M. The generator of the C^*-geometric phase is a solution of the equation [6]

$$\mathrm{d}\rho_a = \mathcal{A}_a\rho_a + \rho_a\mathcal{A}_a^\dagger. \tag{63}$$

After solving this equation, we have $B_a = \mathrm{d}\mathcal{A}_a - \mathcal{A}_a \wedge \mathcal{A}_a$. For eigenvectors ϕ_a of $H_\mathcal{U}$ associated with non-degenerate eigenvalues (as in the example of section 4), we have by construction $A_a = \langle\langle\phi_a|\mathrm{d}\phi_a\rangle\rangle 1_{\mathcal{H}_S}$. But $\langle\langle\phi_a|\mathrm{d}\phi_a\rangle\rangle = \mathrm{tr}_{\mathcal{H}_S}(\rho_a\mathcal{A}_a)$ (see [7]); we can then compute directly the reduced potential as

$$A_a = \mathrm{tr}_{\mathcal{H}_S}\left(\rho_a\mathcal{A}_a\right)1_{\mathcal{H}_S} \tag{64}$$

and then $F_a = \mathrm{d}\ \mathrm{tr}_{\mathcal{H}_S}(\rho_a\mathcal{A}_a)1_{\mathcal{H}_S} - B_a$.

Upon solving equations (62, 63 and 64, we can finally plot 'density charts' of the fields of the higher gauge structure by working only at the stage of the density matrix formalism.

Other approaches of adiabatic quantum control of open systems [23–25] are based on the consideration of a density matrix as being a Hilbert–Schmidt operator and $\mathcal{L}_x$ as being a non-self-adjoint operator on the Hilbert–Schmidt space (the Hilbert–Schmidt space is a so-called Liouville space and the operators on the Hilbert–Schmidt space are so-called 'super-operators'). We are interested in a comparison of these adiabatic approaches with the present one because they are also completely generic: like our approach, they do not require a particular form of the control Hamiltonian and they can be used with several independent control parameters (adiabatic approaches with a single control parameter have a trivial differential geometry and cannot be analysed by using a geometric framework since the problem is 'under-parametrized'; in other words, the Hamiltonian matrix of the problem is not 'versal' in the sense of the Arnold's theory [26]). It seems then pertinent to compare the present approach with the adiabatic quantum control methods based on the Hilbert–Schmidt representation because they have the same possibilities of geometric analyses. The density eigenmatrices considered in the works [23–25] are eigenvectors of $\mathcal{L}_x$ in the Hilbert–Schmidt sense. This approach induces a (usual) gauge theory with a single true curvature. We have seen in this paper that our approach with a higher gauge theory induces two fields (the fake curvature and the curving) which are complementary for describing non-adiabatic transition regions and kinematic decoherence. Our approach can be used to interpret the dynamical phenomenon occurring during the control, and to distinguish purely non-adiabatic effects (similar to non-adiabatic effects of closed quantum systems, which are essentially associated with the fake curvature) from kinematic decoherence effects (hampering of the adiabatic control by the entanglement, which is essentially associated with the curving). A single gauge field such as the one defined by the Hilbert–Schmidt analysis characterizes a mixing of these different dynamical processes, and does not provide clear interpretations.

5.2. Conclusion

The higher gauge structure ([9]) associated with the C^*-geometric phases [6] involves two fields. The average fake curvature is a measure of the non-adiabaticity of the system entangled with the environment (like the usual curvature for an isolated system). Nevertheless, for invertible eigenmatrices (corresponding to a strong information loss associated with the partial trace $\mathrm{tr}_{\mathcal{H}_\mathcal{E}}$), inactive singularities associated with the non-adiabaticity of the environment occur. This is a drawback of the interpretation of this field. The average curving is a measure of the 'kinematic decoherence' associated with variations of the entropy and of the entanglement between the system and the environment. It is essentially induced by the non-adiabaticity of the environment. In the example treated in this paper (the STIRAP system), it is zero for some invertible eigenmatrices. This seems to be the signature of the non-

adiabaticities of the environment not inducing increases of the entanglement and of the entropy in these cases. But in these cases, the curving does not play its second role, which consists in 'killing' the inactive singularities in the fake curvature. Finally, the von Neumann entropy of the eigenmatrices measures the 'local decoherence' induced by the 'non-dynamical' entanglement of the system with the environment appearing directly at the level of the eigenstates of the universe.

The method consisting in plotting the densities of the different field strengths can be used to interpret the hampering by entanglement of the adiabatic quantum control. It is also able to distinguish, in the geometric representation of the universe dynamics, the non-adiabatic effects concerning the system from the decoherence effects associated with the environment. The study of the adiabatic fields can then be a tool for establishing adiabatic control strategies for a system in contact with an environment. But as we can see for the example treated in the present paper (the STIRAP system entangled with another STIRAP system), it can be very difficult to completely avoid the decoherence regions (especially if an 'entropic string' splits the control manifold into two parts, as is the case for the example with a static coupling).

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