The energy minimization problem for two-level dissipative quantum systems

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***Abstract*— The objective of this article is to present developments of geometric optimal control to analyze the energy minimization problem of dissipative two-level quantum systems whose dynamics is governed by Kossakowski-Lindblad equations. This analysis completed by numerical simulations based on adapted algorithms allows a computation of the optimal control law whose robustness with respect to initial conditions and dissipative parameters is also detailed.**

I. INTRODUCTION

In this article, we consider the *energy minimization problem*: $\min \int_0^T (u_1^2(t) + u_2^2(t))dt$ with fixed transfer time T, for steering an initial state q_0 to a final state q_1, where $q = (x, y, z)$. The dynamics is governed by the following control system:

$$\begin{aligned} \dot{x} &= -\Gamma x + u_2 z \\ \dot{y} &= -\Gamma y - u_1 z \\ \dot{z} &= \gamma_- - \gamma_+ z + u_1 y - u_2 x. \end{aligned} \quad (1)$$

This system is deduced from *Kossakowski-Lindblad* equations [11], [16] describing the dynamics of two-level dissipative quantum systems in the Rotating Wave Approximation [3]. It correspond also to the dynamics of a dissipative spin 1/2 particle ruled by the Bloch equations [14], [15]. The set $\Lambda = (\Gamma, \gamma_+, \gamma_-)$ is the set of dissipative parameters satisfying the constraints $2\Gamma \geq \gamma_+ \geq |\gamma_-|$, the control is the complex function $u = u_1 + iu_2$ associated to the physical control which is an electromagnetic field. The cost corresponds to the energy transfer. The *Bloch ball* $|q| \leq 1$, which is the physical state space of the system, is invariant for the dynamics.

Such a control problem is motivated by a recent experimental research project which concerns the control of the spin dynamics by a magnetic field in Nuclear Magnetic Resonance (NMR) [15]. The dissipative parameters which can be determined experimentally with a great accuracy model the interaction of the system with the environment, mainly molecular interactions. This problem can be viewed as the ideal testbed for the application of our geometric optimal control techniques since the two-level case is physically relevant for a spin 1/2 particle [12], [13]. The use of recent geometric control techniques to analyze quantum control systems is a new challenge in optimal control. In this context, many articles are devoted to the conservative case, e.g. see [8], [9], [13]. The aim of our research program is to extend these works by including the dissipation effects.

Our work is related to a previous study concerning the time-minimal control problem with a control bound $|u| \leq M$, whose results were presented in a series of articles [3], [7], [18]. The departing framework for both problems is the same. Writing the control system in the form:

$$\dot{q} = F_0(q) + \sum_{i=1}^{2} u_i F_i(q),$$

the *Pontryagin's maximum principle* [17] tells us that, for the time-minimal control problem, outside a surface Σ: $H_i = 0$, $i = 1, 2$ where H_i denotes the Hamiltonian lift $\langle p, F_i(q) \rangle$ of the vector field F_i, the optimal trajectories are chosen among a set of *extremal curves* solutions of the Hamiltonian vector field $\overrightarrow{H}$ with the Hamiltonian

$$H = H_0 + (H_1^2 + H_2^2)^{1/2},$$

while for the energy minimization problem, the corresponding Hamiltonian (in the normal case) is given by:

$$H = H_0 + \frac{1}{2}(H_1^2 + H_2^2).$$

Despite similar Hamiltonians, the analysis of this article for the energy-minimization problem compared with the one of the time-minimal control problem will show significant different results. Moreover for the energy minimization case, the geometric framework is neat and completed by numerical simulations using codes developed for this kind of problem, it will allow to get a global analysis of the optimal control problem and robustness properties of the solutions with respect to the dissipative parameters. Two principal reasons can be mentioned to explain this discrepancy. In both cases, the problem is similar for a specific value of the parameters: for $\gamma_- = 0$ and $\gamma_+ = \Gamma$, the optimal control problem amounts to analyze a *quasi-Riemannian* problem on the two-sphere of revolution given by the *Grushin metric*: $g = d\phi^2 + \tan^2 \phi d\theta^2$ where ϕ is the angle along a meridian, while θ is the angle of revolution along the $z-$ axis. If $\gamma_- = 0$, both Hamiltonian flows are *Liouville integrable*, but only in the energy minimization problem the extremal curves solutions of the Hamiltonian vector field $\overrightarrow{H}$ can be obtained by integrating in spherical coordinates a *mechanical system*: $\frac{1}{2}\dot{\phi}^2 + V(\phi) = h$ on the level set $H = h$, where V is a potential and the qualitative properties of the flow can be deduced from the graph of V only. The second reason is rather technical. For the time-minimal control problem, the Hamiltonian vector field $\overrightarrow{H}$ is not smooth on the surface

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Σ and leads to complicated asymptotic behaviors for the extremal solutions. For the energy minimization problem, it remains smooth on the whole space and asymptotic behaviors are related to those of smooth Hamiltonian vector fields.

This article is organized in two sections. In the first section, we present the geometric analysis of the extremal flow. Using spherical coordinates, the Hamiltonian takes the form:

$$H = p_\rho(\gamma_- \cos\phi - \rho(\delta\cos^2\phi + \Gamma)) + p_\phi(-\frac{\gamma_-}{\rho}\sin\phi + \delta\sin\phi\cos\phi) + \frac{1}{2}(p_\phi^2 + p_\theta^2\cot^2\phi),$$

where $\delta = \gamma_+ - \Gamma$. It is interpreted as a deformation of the Grushin case which occurs for $\gamma_- = 0$ and $\delta = 0$. In this case, the extremal curves are the geodesics of the Grushin metric: $g = d\phi^2 + \tan^2\phi d\theta^2$ on the two-sphere of revolution. For such a metric, the analysis of [4] allows to describe the *conjugate and cut loci*, hence solving the optimal control problem. In order to analyze the deformation of this model, the problem in the general case is related to a mechanical system of the form: $\frac{1}{2}\dot\phi^2 + V(\phi) = 0$ where V is a potential, and for which the analysis splits into two parts. If $\gamma_- = 0$, the corresponding system restricted to the two-sphere is conservative and the extremal flow is integrable. Making a δ-deformation of the Grushin case for which there exists only one type of extremal curves, we observe if $\gamma_- = 0$, two types of extremal curves: *short* periodic curves not crossing the equator and *long* periodic curves crossing the equator, which are deformations of the extremal curves of the Grushin model. In the general case $\gamma_- \neq 0$, the analysis is less complete, but the asymptotic behavior of the solutions when $t \to +\infty$ can be described using general methods of Hamiltonian dynamics. The final section is devoted to the numerical simulations based on our geometric discussion to conclude the analysis.

II. Geometric analysis of the extremal curves

A. Maximum principle

First of all, we recall some standard results concerning the maximum principle needed in our computations, see [2] for the details.

Preliminaries: Consider the energy minimization problem: $\min_{u(\cdot)} \int_0^T \sum_{i=1}^m u_i^2(t)dt$ where the transfer time T is fixed for a smooth system of the form: $\dot q = F_0(q) + \sum_{i=1}^m u_i F_i(q)$ on a smooth manifold M and where the set of admissible controls $\mathcal{U}$ is the set of bounded measurable mapping $u : [0,T] \to \mathbb{R}^m$ such that the corresponding trajectory $q(\cdot, u, q_0)$, initiating from q_0 is defined on the whole interval.

According to the maximum principle, the optimal solutions are a subset of a set of *extremal curves* solutions of the equations:

$$\frac{dq}{dt} = \frac{\partial \tilde H}{\partial p},\ \frac{dp}{dt} = -\frac{\partial \tilde H}{\partial q} \quad (2)$$

where $\tilde H(q,p,u)$ is the *pseudo-Hamiltonian* $H_0 + \sum_{u=1}^m u_i H_i + p_0 \sum_{i=1}^m u_i^2$, H_i being defined as $H_i = \langle p, F_i(q)\rangle$, $i = 0, 1, \cdots, m$. Moreover an extremal control has to satisfy the maximization condition:

$$\tilde H(q,p,u) = \max_{v\in\mathbb{R}^m} \tilde H(q,p,v), \quad (3)$$

and p_0 is constant and non positive. In this situation, one immediately deduces that the maximization condition leads to solve the equation: $\frac{\partial \tilde H}{\partial u} = 0$ and one must distinguish two cases:

1) *Normal case*: If $p_0 < 0$, it can be normalized to $p_0 = -1/2$ and solving $\frac{\partial \tilde H}{\partial u} = 0$ leads to $u_i = H_i$, $i = 1, \cdots, m$. Plugging such u_i into $\tilde H$ defines a *true Hamiltonian*: $H_n = H_0 + \frac{1}{2}\sum_{i=1}^m H_i^2$ whose (smooth) solutions correspond to *normal extremal curves* $z(\cdot) = (q(\cdot), p(\cdot))$ while normal extremal controls are given by $u_i = H_i(z)$, $i = 1, \cdots, m$.
2) *Abnormal case*: It is the case where $p_0 = 0$ and hence such extremals have to satisfy the constraints: $H_i = 0$, $i = 1, \cdots, m$. Such extremals do not depend on the cost and correspond to the so-called *singular trajectories* of the system [2].

B. Geometric computations of the extremals

We shall complete the computation in our case by introducing adapted geometric coordinates. If $q = (x, y, z)$ are the cartesian coordinates for the state q restricted to the Bloch ball: $|q| \le 1$, using spherical coordinates:

$$x = \rho\sin\phi\cos\theta,\ y = \rho\sin\phi\sin\theta,\ z = \rho\cos\phi,$$

the system becomes

$$\begin{aligned} \dot\rho &= \gamma_-\cos\phi - \rho(\delta\cos^2\phi + \Gamma) \\ \dot\phi &= -\frac{\gamma_-\sin\phi}{\rho} + \delta\sin\phi\cos\phi + v_2 \\ \dot\theta &= -\cot\phi v_1 \end{aligned} \quad (4)$$

where $\delta = \gamma_+ - \Gamma$ and the new control $v = v_1 + iv_2$ is given by: $v = e^{-i\theta}u$. Note in particular that the cost is invariant:

$$\int_0^T (v_1^2 + v_2^2)dt = \int_0^T (u_1^2 + u_2^2)dt.$$

We also deduce the Hamiltonian H_n associated to normal extremals which is given in spherical coordinates by:

$$H_n = p_\rho(\gamma_-\cos\phi - \rho(\delta\cos^2\phi + \Gamma)) + p_\phi(-\frac{\gamma_-}{\rho}\sin\phi + \delta\sin\phi\cos\phi) + \frac{1}{2}(p_\phi^2 + p_\theta^2\cot^2\phi).$$

In the abnormal case, we have $H_1 = H_2 = 0$ and using spherical coordinates, this gives

$$p_\phi = 0,\ p_\theta\cot\phi = 0.$$

Such extremals correspond to singular trajectories of the system and have been already analyzed in the time-minimal control problem [3]. Differentiating with respect to time $H_1 = H_2 = 0$, one gets:

$$\begin{aligned} \{H_1, H_0\} + v_2\{H_1, H_2\} &= 0 \\ \{H_2, H_0\} - v_1\{H_1, H_2\} &= 0 \end{aligned} \quad (5)$$

We have two cases: $p_\phi = p_\theta = 0$, $\phi \neq \pi/2$ or $p_\phi = 0$ and $\phi = \pi/2$.

For the first case, using the invariance by feedback, the computations amount to consider the system $\dot{q} = F_0' + v_1' F_1' + v_2' F_2$:

$$\dot{\rho} = \gamma_- \cos\phi - \rho(\delta\cos^2\phi + \Gamma),\ \dot{\phi} = v_2',\ \dot{\theta} = v_1'.$$

Since $[F_1', F_2'] = 0$, we deduce from (5) the relations: $\{H_1', H_0'\} = \{H_2', H_0'\} = 0$. We observe that v_1' can be set to 0 and hence the computation amounts to determine the singular control for the 2D-single input system obtained by restricting the dynamics to the evolution of (ρ, ϕ), the control being v_2'. In the second case, we have $\dot{\theta} = 0$ and still the problem is reduced to compute the singular trajectories for the evolution of (ρ, ϕ) controlled by v_2'. Moreover, since $\phi = \pi/2$ we must have $\dot{\phi} = v_2' = 0$.

In both cases, the computation is reduced to the determination of the singular trajectories of the system $\dot{q}' = F_0' + v_2' F_1'$:

$$\begin{aligned} \dot{\rho} &= \gamma_- \cos\phi - \rho(\delta\cos^2\phi + \Gamma) \\ \dot{\phi} &= v_2'. \end{aligned} \tag{6}$$

The singular trajectories are located on the set where $\det(F_1', [F_0', F_1']) = 0$. Computing this gives:

$$\sin\phi(2\rho\delta\cos\phi - \gamma_-) = 0$$

and hence $\phi = 0,\ \pi$ or $2\rho\delta\cos\phi = \gamma_-$. In particular, $\phi = \pi/2$ is solution for $\delta \neq 0$ only if $\gamma_- = 0$. The singular control is computed using:

$$\langle p, [[F_0', F_1'], F_0'] + v_2'[[F_0', F_1'], F_1'] \rangle = 0.$$

We deduce:

Lemma 1: In the case $\delta \neq 0$, a singular extremal has to satisfy $p_\phi = 0$ and can be:

- $\phi = \pi/2$ if $\gamma_- = 0$ and $\theta = \theta_0$ constant.
- $\phi \neq \pi/2$ and corresponds to a singular trajectory of the 2D-system:

$$\dot{y} = -\Gamma y - u_1 z,\ \dot{z} = \gamma_- - \gamma_+ z + u_1 z$$

assuming the control field $u = u_1$ real. It is given in polar coordinates by $\phi = 0$ or $2\rho\delta\cos\phi = \gamma_-$, while $p_\theta = 0$ is the transversality condition meaning that the θ-variable is not taken into account. The angle θ satisfies: $\dot{\theta} = -\cot\phi v_1$ where v_1 is *any control*.

Remark 1: The role of singular extremals in the energy minimization problem will be not discussed in this article. This point is analyzed in [5] for the 2D- system.

C. The analysis in the normal case

The Hamiltonian takes the following form

$$H_n = \gamma_-(p_\rho\cos\phi - \frac{p_\phi}{\rho}\sin\phi) + H$$

where

$$H = -\rho p_\rho(\delta\cos^2\phi + \Gamma) + \frac{1}{2}p_\phi\delta\sin(2\phi) + \frac{1}{2}(p_\phi^2 + p_\theta^2\cot^2\phi).$$

We deduce immediately the following result:

Proposition 1: If $\gamma_- = 0$, the Hamiltonian H_n reduces to H and is completely integrable. Introducing $r = \ln\rho$, it takes the form:

$$H = -p_r(\delta\cos^2\phi + \Gamma) + \frac{1}{2}p_\phi\delta\sin(2\phi) + \frac{1}{2}(p_\phi^2 + p_\theta^2\cot^2\phi)$$

where the set of parameters $\Lambda = (\gamma_+, \Gamma)$ is such that $2\Gamma \geq \gamma_+ \geq 0$. The Hamiltonian is invariant for the central symmetry: $(p_\phi, \phi) \mapsto (-p_\phi, \pi - \phi)$ and moreover a transformation of the form $p \mapsto \lambda p,\ \Lambda \mapsto \lambda\Lambda,\ \lambda > 0$, transforms H into λH.

A key property in our analysis is the fact that we can introduce a mechanical system. We have:

$$\dot{\phi} = \frac{\partial H_n}{\partial p_\phi} = -\frac{\gamma_-}{\rho}\sin\phi + \frac{1}{2}\delta\sin 2\phi + p_\phi$$

and H_n can be written:

$$\begin{aligned} &\frac{1}{2}(p_\phi + \frac{\delta}{2}\sin(2\phi) - \frac{\gamma_-\sin\phi}{\rho})^2 + \gamma_- p_\rho\cos\phi - \\ &\rho p_\rho(\delta\cos^2\phi + \Gamma) + \\ &\frac{1}{2}p_\theta^2\cot^2\phi - \frac{1}{2}(\frac{\delta\sin 2\phi}{2} - \frac{\gamma_-\sin\phi}{\rho})^2. \end{aligned}$$

Hence we have:

Proposition 2: The equation $H_n = h$ can be written:

$$\frac{1}{2}\dot{\phi}^2 + V(\phi) = h$$

where

$$\begin{aligned} V = &\gamma_- p_\rho\cos\phi - \rho p_\rho(\delta\cos^2\phi + \Gamma) - \\ &\frac{1}{2}(\delta\frac{\sin(2\phi)}{2} - \frac{\gamma_-\sin\phi}{\rho})^2 + \frac{1}{2}p_\theta^2\cot^2\phi \end{aligned}$$

is a potential.

In particular if $\gamma_- = 0$, the potential reads:

$$V(\phi) = -p_r(\delta\cos^2\phi + \Gamma) - \frac{1}{8}\delta^2\sin^2(2\phi) + \frac{1}{2}p_\theta^2\cot^2\phi.$$

If we set $\psi = \pi/2 - \phi$, one gets:

$$V(\psi) = -p_r(\delta\sin^2\phi + \delta) - \frac{1}{8}\delta^2\sin^2(2\psi) + \frac{1}{2}p_\theta^2\tan^2\psi.$$

Hence $V(-\psi) = V(\psi)$.

Another important property is that $V(\phi) \to +\infty$, when $\phi \to 0,\ \pi$, if $p_\theta \neq 0$.

Also consider the case $p_\theta = 0$. Due to the symmetry of revolution, it is associated to the energy minimization problem for an initial condition located on the z- axis, see [3] for a similar analysis in the time-minimal control problem. It amounts to control the system using a real field and the optimal control problem becomes $\min_{u_1(\cdot)}\int_0^T u_1^2(t)dt$ for the 2D-system:

$$\dot{y} = -\Gamma u - u_1 z,\ \dot{z} = \gamma_- - \gamma_+ z + u_1 y.$$

If $\gamma_- = 0$, a special case occurs when $\delta = \gamma_+ - \Gamma = 0$: the ρ-variable cannot be controlled and the energy minimization problem is equivalent to the length minimization problem for the metric $g = d\phi^2 + \tan^2\phi d\theta^2$. This metric appears also in the time-minimal control problem, since if we parametrize by arc-length, the length corresponds to the time. We introduce:

Definition 1: The quasi-Riemannian metric (with a singularity at the equator) $g = d\phi^2 + \tan^2\phi d\theta^2$ is called the standard Grushin metric on the two-sphere of revolution. Moreover, to summarize our previous analysis, we have:

Proposition 3: If $\gamma_- = 0$, the normal extremals are solutions of a mechanical system on the two-sphere of revolution described by

$$\frac{1}{2}\dot{\phi}^2 + V(\phi) = h,$$

the potential being given by:

$$V(\phi) = -p_r(\delta\cos^2\phi + \Gamma) - \frac{1}{8}\delta^2\sin^2(2\phi) + \frac{1}{2}p_\theta^2\cot^2\phi,$$

where p_r and p_θ are constant. If $\delta = 0$, one can set $p_r = 0$ and the normal extremals are the geodesic curves solutions of the Grushin metric $g = d\phi^2 + \tan^2\phi d\theta^2$. The mechanical system has a singularity at the equator $\phi = \pi/2$ and is reflexionnaly symmetric with respect to this line.

From the above proposition, we deduce that our analysis is an extension of the work of [4] for quasi-Riemannian metrics on a two-sphere of revolution, to a family of mechanical systems. It can be compared to the time-minimal case [7] which extends the Riemann case to Finsler metrics.

We now analyze the mechanical system in the integrable case $\gamma_- = 0$. We consider the case $p_\theta \neq 0$. Fixing the level set to $H = h$, one can reduce the integration to find the solutions of $\dot{\phi}^2/2 + V(\phi) = h$, while the remaining equations are:

$$\dot{\theta} = p_\theta(\frac{1}{\sin^2\phi} - 1),\ \dot{r} = -\delta\sin^2\phi - \gamma_+.$$

To clarify, we introduce in this section the following notations:

$$b = \Gamma - \gamma_+,\ a = \frac{1}{2} + \frac{p_r}{b},\ \overline{h} = h + p_r\gamma_+ + \frac{p_\theta^2}{2}.$$

If we denote $x = \sin^2\phi$, we obtain

$$V(\phi) = \tilde{V}(x) = \frac{b^2}{2x}(x^3 - 2ax^2 + \frac{p_\theta}{b^2}) - p_r\gamma_+ - \frac{p_\theta^2}{2}.$$

and introducing

$$W(x) = \frac{b^2}{2x}(x^3 - 2ax^2 + \frac{p_\theta^2}{b^2}),$$

one deduces that ϕ satisfies the equation

$$\dot{\phi} = \pm\sqrt{2(\overline{h} - W(x(\phi)))}.$$

Since $x = \sin^2\phi$, $x \in [0, 1]$ but we extend the domain to the whole $\mathbb{R}$. First of all we observe that

$$\lim_{x\to\pm 0} W(x) = \pm\infty,\quad \lim_{x\to\pm\infty} W(x) = +\infty,$$

and

$$W(1) = -bp_r + \frac{p_\theta^2}{2}.$$

Further, we have

$$W'_x = \frac{b^2}{x^2}(x^3 - ax^2 - \frac{p_\theta^2}{2b^2}).$$

Hence $\lim_{x\to 0} W'_x = \infty$ and the critical points of W are defined by the roots of the cubic polynomial

$$P_1(x) = x^3 - ax^2 - \frac{p_\theta^2}{2b^2}.$$

Since $P_1(0) = -\frac{p_\theta^2}{2b^2} \leq 0$ and $P'_1(0) = 0$, if $p_\theta \neq 0$ the polynomial $P_1(x)$ has one positive real root x_*, and the other possible real roots of P_1 (at most two) are negative. In particular it follows that $W(x)$ can have at most one critical point on $]0, 1[$. This is explained below.

Characterization of the critical point x_*

By construction, the critical point x_* is a positive zero of the function W', and thus it solves the following equation

$$b^2x - ab^2 = \frac{p_\theta^2}{2x^2}.$$

It is then easy to see that in the domain $x \geq 0$, the graph of the linear function $f_1 = b^2x - ab^2$ intersects the graph of $f_2 = -\frac{1}{2}p_\theta^2x^{-2}$ only once, and the intersection point $x_* < 1$ if and only if $f_1(1) > f_2(1)$. This yields the following condition

$$a < 1 - \frac{p_\theta^2}{2b^2},$$

or, equivalently,

$$2p_r\delta < \delta^2 - p_\theta^2.$$

Phase portraits

Now consider the potential $\tilde{W}(\phi) = W(x(\phi))$. We have

$$\tilde{W}'(\phi) = 2W'(x(\phi))\sin\phi\cos\phi,$$

hence $\tilde{W}'(\frac{\pi}{2}) = 0$. Taking into account the symmetry of the function $\tilde{W}$ with respect to the equator $\phi = \frac{\pi}{2}$, we finally obtain two cases accordingly to the values of the dissipative parameters Γ, γ_+ and the first integrals p_r and p_θ:

Type I: $a < 1 - \frac{p_\theta^2}{2b^2}$, then $x_* < 1$. The motion of the system takes place in the region $\overline{h} \geq W(x_*)$. There are three equilibrium states

$$\phi_{*0} = \frac{\pi}{2},$$

corresponding to a local maximum of the potential and

$$\phi_{*1} = \arcsin\sqrt{x_*},\ \phi_{*2} = \pi - \arcsin\sqrt{x_*},$$

corresponding to a local minimum of the potential. They belong respectively to the energy levels $W(1)$ and $W(x_*)$. There are two types of periodical trajectories: to each value $W(x_*) < \overline{h} < W(1)$ corresponds two periodic orbits in each hemisphere which are symmetric with respect to the equator, and for $\overline{h} > W(1)$ there exists a unique periodic orbit crossing the equatorial plane $\phi = \frac{\pi}{2}$ and the two pieces are symmetric with respect to the equator. The transition between the two cases gives a limit case which is non periodic and corresponds to a separatrix which exists on the energy level $\overline{h} = W(1)$.

Type II: $a \geq 1 - \frac{p_\theta^2}{2b^2}$**.** In this case the motion of the system takes place in the region $h \geq W(1)$ and there exists a unique equilibrium state $\phi_{*0} = \frac{\pi}{2}$. The only type of periodic orbits cross the equatorial plane and corresponds to the energy levels $\overline{h} > W(1)$. Those orbits can be identified with the analogous orbits of the Case I. This leads to the following definition.

Definition 2: For the generic motion of the mechanical system $\frac{\dot{\phi}^2}{2} + V(\phi) = h$, we have two types of periodic orbits: orbits located in one hemisphere, called short orbits and orbits crossing the equators called long orbits.

D. Symmetries and optimality

Using the discrete symmetric group on the set of extremals, we can determine obvious symmetrical properties.

1) The integrable case: Consider the case $\gamma_- = 0$ and $p_\theta \neq 0$. The relation $H_n = h$ gives

$$\frac{1}{2}\dot{\phi}^2 + V(\phi) = h$$

where the potential is

$$V(\phi) = -p_r(\delta\cos^2\phi + \Gamma) - \frac{1}{8}\delta^2\sin^2(2\phi) + \frac{1}{2}p_\theta^2\cot^2\phi.$$

We fix p_θ and p_r and for each initial condition $\phi(0)$, we have two extremal curves on the level set h, starting respectively from $\dot{\phi}(0)$ and $-\dot{\phi}(0)$. They are distinct and periodic if and only if $\dot{\phi}(0) \neq 0$ and the level set is without equilibrium point (for the fixed values of p_r and p_θ). If T is the corresponding period, we immediately deduce:

Proposition 4: For fixed p_r and p_θ, the two periodic extremal curves starting from $\phi(0)$, $\dot{\phi}(0) \neq 0$ and with the same $\theta(0)$, $r(0)$ intersect at the same point, with the same cost, after one period T.

Moreover, we have:

Proposition 5: If the corresponding curves of the above proposition are long periodic extremals, then they intersect after an half-period $T/2$.

Proof: For long periodic extremals, one can use the property that the system and the cost are reflexionnally symmetric with respect to the equator. Hence, both curves starting from $\dot{\phi}(0)$ and $-\dot{\phi}(0)$ intersect on the antipodal parallel $\pi - \phi(0)$ at the time $T/2$ and with the same cost. It is also true for the θ and r components. ∎

2) The general case: In the general case, the extremal curves are reflexionnally symmetric with respect to meridian planes. Fixing $q(0) = (\phi(0), \theta(0), r(0))$, $(p_\phi(0), p_r(0))$ and considering the two extremal curves with p_θ and $-p_\theta$, one deduces that they are symmetric with respect to the reflexion $(\phi, \theta) \mapsto (\phi, -\theta)$. Hence, we have:

Proposition 6: If we consider the two extremal curves starting from $q(0)$, $(p_\phi(0), p_r(0), \pm p_\theta)$ then they intersect at the same point and with the same cost on the opposite half meridian.

III. Geometric algorithms and numerical simulations

A modern and pragmatic treatment of such an optimal control problem needs the development of appropriate geometric algorithms and appropriate codes which are used to make the numerical simulations. Such codes based on the techniques of geometric control theory are an important work mainly developed in a parallel research project in orbital transfer, where low propulsion technique was used. We shall make a short presentation of one of these codes, the Cotcot code [10], prior to the presentation of the numerical results.

A. The Cotcot code

The role of this code is to compute extremals and conjugate points in the case where the Hamiltonian describing the extremal field is smooth. Noting H_n this Hamiltonian and fixing the extremities $q_0,\ q_1$ of the problem, the extremals are solutions of:

$$\dot{z}(t) = \overrightarrow{H}_n(z(t))$$

and if the boundary conditions are given by q_0 and q_1, one must find the zeros of the *shooting equation*:

$$E : (T, p_0) \mapsto \Pi(\exp T\overrightarrow{H}_n(q_0, p_0)) - q_1$$

where T is the transfer time.

In order to compute the conjugate points, one must compute in parallel the Jacobi fields solutions of the variational equation:

$$\delta\dot{z}(t) = d\overrightarrow{H}_n(z(t))\delta z(t)$$

along the given extremal.

The aim of the code COTCOT (Conditions of Order Two, COnjugate Times [10]) is to provide the numerical tools:

1) to integrate the smooth Hamiltonian vector field $\overrightarrow{H}_n$
2) to solve the associated shooting equation
3) to compute the corresponding Jacobi fields along the extremals
4) to evaluate the resulting conjugate points.

The code is written in Fortran language, while automatic differentiation is used to generate the Hamiltonian differential equation and the variational one. For the users, the advanced language is Matlab, see [1] for a precise description of the COTCOT code with the underlying algorithms: ODE integrators, Newton method solver. The conjugate point test consists in checking a rank condition, which is based on two methods: evaluating zeros of a determinant or a SVD (singular value decomposition).

B. Extremals and conjugate points

Using a direct integration of the Hamiltonian system we detail in this section the behavior of the extremals in the integrable ($\gamma_- = 0$) and non-integrable cases ($\gamma_- \neq 0$).

In the integrable case, we illustrate the different analytical results that we have determined. We consider the case of Figure 1 where both short and long periodic orbits exist. In this example, we only modify the value of $p_\phi(0)$ to change the energy h of the system. We respectively obtain short and long orbits for $h < 6$ and $h > 6$. For p_ρ and p_θ fixed, there exist two trajectories starting from $(r(0), \phi(0), \theta(0))$ which intersect with the same cost on the antipodal parallel ($\phi = \pi - \phi(0)$) for long periodic orbits and on the initial parallel ($\phi = \phi(0)$) for short periodic orbits. These two extremals

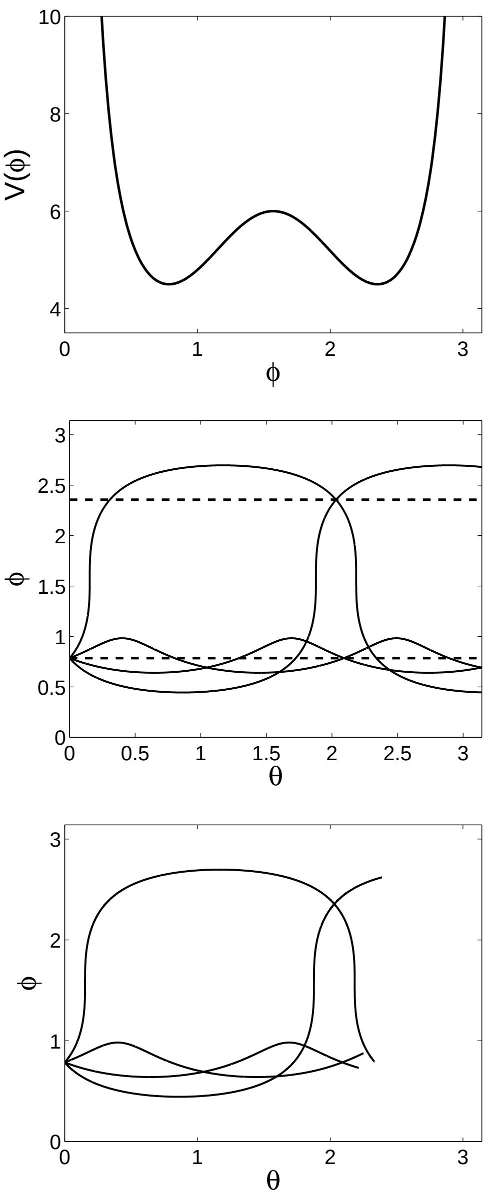

Fig. 1. (top): Plot of the potential V as a function of ϕ. (middle): plot of four extremals corresponding to $p_\phi(0) = -1,\ 0,\ 1$ and 2. (bottom) Same as (middle) but up to the first conjugate point. Other numerical values are taken to be $\Gamma = 3$, $\gamma_+ = 2$, $\phi = \pi/4$, $p_\rho = -2$ and $p_\theta = 1$. The extremals associated to $p_\phi(0) = 0$ and 1 are short periodic orbits with an energy equal to 5.5, while extremals with initial adjoint states $p_\phi(0) = -1$ and 2 are long periodic orbits with an energy equal to 6.5. The horizontal dashed lines indicate the positions of the parallel of equation $\phi = \pi/4$ and the antipodal one of equation $\phi = 3\pi/4$ where short and long periodic orbits respectively intersect with the same time.

are defined by the two values of $p_\phi(0)$ for which the energy is the same. Such trajectories are displayed in Figure 1 both for long and short periodic orbits. We have also determined by using the CotCot code the position of the first conjugate points for these extremals.

In the non-integrable case, the asymptotic behavior when $t \to +\infty$ is described for any values of Γ and γ_+ by the following conjecture, which is based on numerical computations.

Conjecture 1: The asymptotic stationary points $(\rho_f, \phi_f, \theta_f)$ are characterized by $\rho_f = |\gamma_-|/\gamma_+$, and $\phi_f = 0$ if $\gamma_- > 0$ or $\phi_f = \pi$ if $\gamma_- < 0$.
Using the Hamiltonian equations, it is straightforward to show that $(\rho_f, \phi_f, \theta_f)$ satisfy

$$\gamma_- \cos\phi_f = \rho_f(\gamma_+ \cos^2\phi_f + \Gamma \sin^2\phi_f),$$

from which one deduces the conjecture 1. The different behaviors of the extremals are represented in Fig. 2 for $\gamma_- < 0$. After a complicated transient oscillatory structure, every extremal has the same asymptotic limit given by the conjecture 1. This conjecture also illustrates the robustness of the control with respect to parameters uncertainties since the asymptotic behavior of the extremals only depends on the sign of γ_- and not on γ_+ or Γ. This point could be important in view of possible experimental applications in NMR of these optimal control laws. Note also the unbounded and oscillatory behaviors of the two control fields v_1 and v_2. Finally, we have used the COTCOT code to evaluate the position of the conjugate points. As can be checked in Fig. 3, we observe that every extremal possesses a conjugate point, which was not the case in the time-minimal control of the same system [3]. Numerical simulations show that the first conjugate point occurs after the first oscillation of the extremal.

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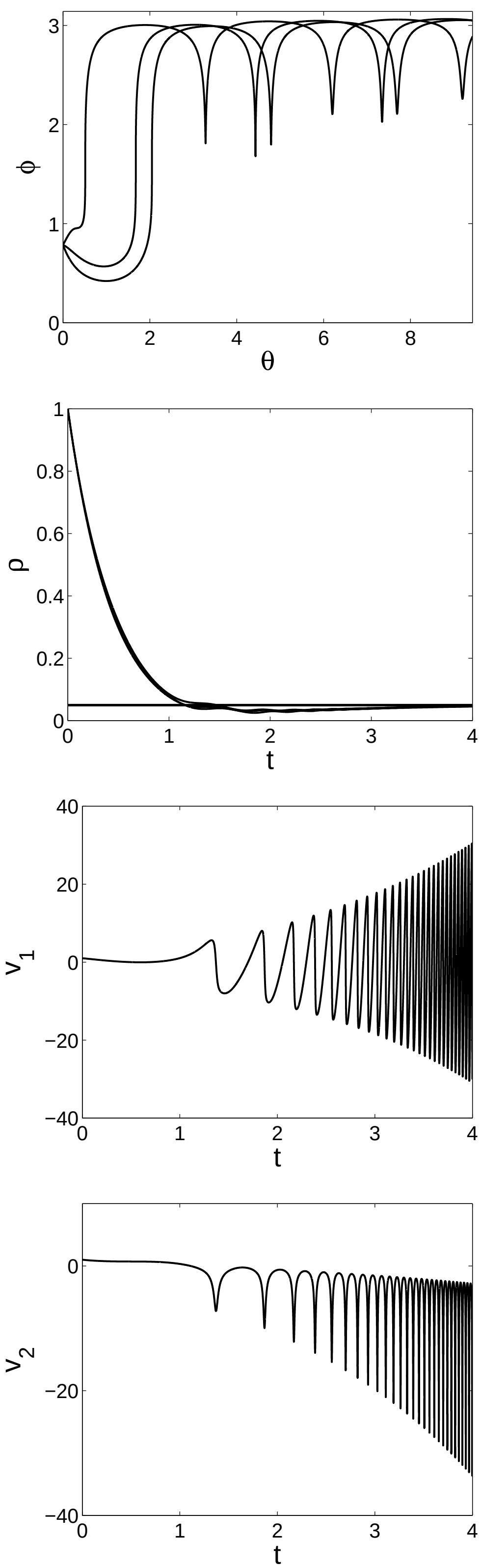

Fig. 2. (top): Evolution of the angle ϕ as a function of the angle θ for $\Gamma = 2.5$, $\gamma_+ = 2$ and $\gamma_- = -0.1$. Initial values are taken to be $\phi(0) = \pi/4$, $p_\rho(0) = -10$, $p_\theta = 1$ and $p_\phi(0) = -1,\ 0$ and 1. (middle) Evolution of the radial coordinate ρ as a function of time. (bottom) Plot of the two optimal control fields v_1 and v_2 as a function of time for $p_\phi(0) = 1$.

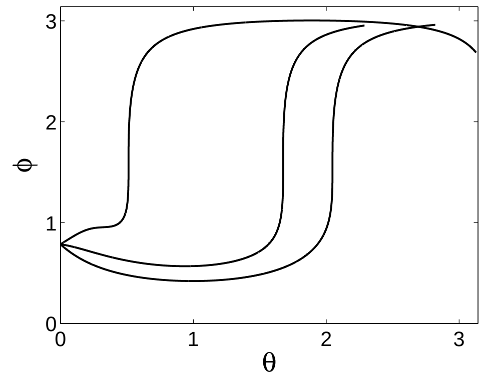

Fig. 3. Same as Fig. 2 but the extremals are plotted up to the first conjugate point.

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