

On the $K + P$ Problem for a Three-level Quantum System: Optimality Implies Resonance

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Abstract We apply techniques of subriemannian geometry on Lie groups to laser-induced population transfer in a three-level quantum system. The aim is to induce transitions by two laser pulses, of arbitrary shape and frequency, minimizing the pulse energy. We prove that the Hamiltonian system given by the Pontryagin Maximum Principle is completely integrable, since this problem can be stated as a “ $\mathbf{k} \oplus \mathbf{p}$ problem” on a simple Lie group. Optimal trajectories and controls are exhausted. The main result is that optimal controls correspond to lasers that are “in resonance”.

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1 Introduction

1.1 Physical context

In the recent past years, people started to approach the control of the Schrödinger equation, using techniques of geometric control theory (see for instance [5, 11, 19, 22]). In this paper we apply techniques of subriemannian geometry on Lie groups to the population transfer problem in a three-level quantum system driven by two external fields (in the rotating wave approximation) of arbitrary shape and frequency. The aim is to induce complete population transfer by minimizing the pulse energy. The dynamics is governed by the time dependent Schrödinger equation (in a system of units such that $\hbar = 1$):

$$i \frac{d\psi(t)}{dt} = H\psi(t), \quad (1)$$

where $\psi(\cdot) : \mathbb{R} \rightarrow \mathbb{C}^3$ and:

$$H = \begin{pmatrix} E_1 & \Omega_1 & 0 \\ \Omega_1^* & E_2 & \Omega_2 \\ 0 & \Omega_2^* & E_3 \end{pmatrix}. \quad (2)$$

Here (*) indicates the complex conjugation involution. The controls $\Omega_1(\cdot), \Omega_2(\cdot)$, that we assume to be different from zero only in a fixed interval $[0, T]$, are connected to the physical parameters by $\Omega_j(t) = \mu_j \mathcal{F}_j(t)/2$, $j = 1, 2$, with \mathcal{F}_j the external pulsed field and μ_j the couplings (intrinsic to the quantum system) that we have restricted to couple only levels j and $j + 1$ by pairs.

Remark 1 This finite-dimensional problem can be thought as the reduction of an infinite-dimensional problem in the following way. We start with a Hamiltonian which is the sum of a “drift-term” H_0 , plus a time dependent potential $V(t)$ (the control term, i.e. the lasers). The drift term is assumed to be diagonal, with eigenvalues (energy levels) $\dots > E_3 > E_2 > E_1$. Then in this spectral resolution of H_0 , we assume the control term $V(t)$ to couple only the energy levels E_1, E_2 and E_2, E_3 . The projected problem in the eigenspaces corresponding to E_1, E_2, E_3 is completely decoupled and is described by the Hamiltonian (2).

The problem is the following:

Problem. Assume that for time $t \leq 0$ the state of the system lies in the eigenspace corresponding to the ground eigenvalue E_1 . We want to determine suitable controls $\Omega_i(\cdot)$, $i = 1, 2$, such that for time $t \geq T$, the system reaches the eigenspace corresponding to E_3 , requiring that these controls minimize the cost (energy in the following):

$$J = \int_0^T (|\Omega_1(t)|^2 + |\Omega_2(t)|^2) dt. \quad (3)$$

In [8] this problem was studied assuming that the controls Ω_j are “in resonance”:

$$\begin{aligned} \Omega_j(t) &= u_j(t) e^{i(\omega_j t + \alpha_j)}, \quad \omega_j = E_{j+1} - E_j, \\ u_j(\cdot) : \mathbb{R} &\rightarrow \mathbb{R}, \quad \alpha_j \in [-\pi, \pi], \quad j = 1, 2. \end{aligned} \quad (4)$$

In the sequel we call this second problem (of minimizing the cost (3), which in this case reduces to $\int_0^T ((u_1(t))^2 + u_2(t)^2) dt$), the “real-resonant” problem. The first problem (with arbitrary complex controls) will be called the “general-complex” problem.

In [8], the real-resonant problem was treated as follows:

- first, using a time dependent change of coordinates that leaves invariant the source (eigenstate 1) and the target (eigenstate 3), it was possible to eliminate the drift term and hence to reduce the problem to a singular-Riemannian problem over the real sphere S^2 ;
- second, the Hamiltonian system obtained from the Pontryagin Maximum Principle (PMP in the following) was Liouville integrable and explicit expressions for geodesics were found (although not so simple expressions).

In this paper, we address both problems in a more abstract setting:

- in both cases, first, we eliminate the drift. For the general-complex case, we use a time dependent change of coordinates plus a gauge transformation. Again, this change of coordinates leaves invariant both the source and the target;
- second, in both cases, we lift the problem into a right-invariant subriemannian control problem on a real simple Lie group G , ($G = G^{\mathbb{R}} = SO(3)$ for the real-resonant problem and $G = G^{\mathbb{C}} = SU(3)$ for the general-complex one). This subriemannian problem has very special features: There is an element g_0 of $G^{\mathbb{R}} \subset G^{\mathbb{C}}$, and subgroups $K^{\mathbb{R}}, K^{\mathbb{C}}$, ($K^{\mathbb{R}} \approx O(2), K^{\mathbb{C}} \approx U(2)$) such that, denoting by $\mathfrak{k}^{\mathbb{R}}, \mathfrak{k}^{\mathbb{C}}$ the Lie algebras of $K^{\mathbb{R}}, K^{\mathbb{C}}$ respectively:
 - a. The Lie algebras $\mathfrak{L}, \mathfrak{k}$ of the pair (G, K) have associated Cartan decomposition $\mathfrak{L} = \mathfrak{k} \oplus \mathfrak{p}$, with the usual commutation relations,
 - b. The right-invariant distribution is determined by the \mathfrak{p} subspace of \mathfrak{L} ,
 - c. The right invariant subriemannian metric is determined by a scalar multiple of $Kil|_p$, where $Kil|_p$ is

the Killing form restricted to \mathfrak{p} ,

d. The source S and the target T of the optimal control problem are respectively $S = K_{g_0} = g_0 K g_0^{-1}$, the conjugation of K by g_0 , and $T = g_0 S$;

- subriemannian problems on semi-simple Lie groups in which the distribution is determined by the \mathfrak{p} subspace of a Cartan decomposition and the metric is proportional to $Kil|_{\mathfrak{p}}$ (called in the following $(\mathfrak{k} \oplus \mathfrak{p})$ -problems) have two important features:
 - abnormal extremals (if any) are never optimal since the so called *Goh condition* (which is a necessary condition for optimality of abnormal extremals, see [4]) is never satisfied (see Appendix C);
 - normal extremals can be computed with a very powerful technique developed by Jurdjevic in [16, 17]. In particular he proved that the Hamiltonian system given by the PMP is completely integrable and he gave explicit expressions for geodesics. For sake of completeness, the Jurdjevic's technique is summarized in Appendix B;
- as the PMP requires, we apply suitable transversality conditions, corresponding to the source and the target. These conditions allow to restrict the set of admissible extremals.
- we prove that all the geodesics satisfying the transversality conditions have the same length. Optimality follows.

Remark 2 In the paper [17], the connection between the geodesics for the $\mathfrak{k} \oplus \mathfrak{p}$ problem and the geodesics of the Riemannian symmetric space G/K is made. But in our case:

- (a) we are not on the Riemannian symmetric space G/K , but on some other homogeneous space G/\tilde{K} , $\tilde{K} \subset K$, $\tilde{K} \neq K$;
- (b) as the reader can check, it is possible to project on the symmetric space G/K_{g_0} , but this problem is not invariant by the action of G on G/K_{g_0} . In fact, we get a *singular Riemannian* problem over G/K_{g_0} (as we have shown in the paper [8]).

With this methods, for the real-resonant problem we get in a more natural way the result of [8], and we give much simpler expressions for geodesics and optimal controls. In the general-complex problem, besides finding explicitly expression for optimal trajectories and controls we prove our main result:

Theorem 1 (Main Result) *For the three-level problem with complex controls, optimality implies resonance. More precisely, controls $\Omega_1(\cdot), \Omega_2(\cdot)$ are optimal if and only if they have the following form:*

$$\begin{cases} \Omega_1(t) = \cos(t/\sqrt{3})e^{i[(E_2 - E_1)t + \varphi_1]}, \\ \Omega_2(t) = \sin(t/\sqrt{3})e^{i[(E_3 - E_2)t + \varphi_2]}. \end{cases} \quad (5)$$

where φ_1, φ_2 are two arbitrary phases. Here the final time T is fixed in such a way subriemannian geodesics are parameterized by arclength, and it is given by $T = \frac{\sqrt{3}}{2}\pi$.

This fact was pointed out as an open question in [8]. In other words, *optimal trajectories for the real-resonant problem are optimal also for the general-complex one.*

Remark 3 The fact that optimality implies resonance was also proved in [8] for the two-level case, reducing the problem to an isoperimetric problem. More precisely the two-level problem, which is described by the Hamiltonian:

$$H = \begin{pmatrix} E_1 & \Omega(t) \\ \Omega^*(t) & E_2 \end{pmatrix}.$$

can be reduced to a 3 dimensional contact subriemannian problem, with a special feature: it has a symmetry, transverse to the distribution. It is a standard fact that such a subriemannian problem is an isoperimetric problem (in the sense of the calculus of variations) on the quotient by the symmetry. In this case, the fact that optimality implies resonance is nothing but the (trivial) solution of the classical isoperimetric problem (or Dido problem) on the Riemannian sphere. We refer to [8] for details.

Remark 4 Besides physical applications, the three-level problem is particularly interesting since it has a non-trivial geometric structure, but it is completely computable. On the other side the two-level problem, described in Remark 3 (although it is a $\mathbf{k} \oplus \mathbf{p}$ problem, with a nice geometric description) has a quite trivial solution.

Systems with more than 3 levels appear to be more difficult to treat. The drift can be eliminated in the same way, but one gets a problem in which the control distribution is determined by a strict subspace of \mathbf{p} only. In this case the Jurdjevic's formula fails to be true, and the integrability of the PMP is an open problem. See Remarks 12 and 14 (the last in Appendix B). In this case the Hamiltonian reads:

$$H = \begin{pmatrix} E_1 & \Omega_1(t) & 0 & \cdots & 0 \\ \Omega_1^*(t) & E_2 & \Omega_2(t) & \ddots & \vdots \\ 0 & \Omega_2^*(t) & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & E_{n-1} & \Omega_{n-1}(t) \\ 0 & \cdots & 0 & \Omega_{n-1}^*(t) & E_n \end{pmatrix}. \quad (6)$$

Remark 5 For questions related to invariance under time reparameterization of our optimal trajectories, we refer to [8].

1.2 A crucial fact

At this level, we want to point out an obvious, but important symmetry property. It is important for computations in the following, but also for practical applicability of the result.

The optimal control problem we consider (in \mathbb{C}^3 or in the complex sphere in \mathbb{C}^3) is invariant under multiplication by a constant phase $e^{i\varphi}$. Hence, the problem of minimizing the energy from a fixed point in the ground eigenstate, to the third eigenstate, is the same as minimizing the energy to move from the full ground eigenstate, to the same target: actually, if $(\psi(t), \Omega(t))$ is an optimal pair trajectory-control, from ψ_0 in the ground eigenstate to the third one, $(e^{i\varphi}\psi(t), \Omega(t))$ is an optimal trajectory from $e^{i\varphi}\psi_0$. Moreover, as a consequence, whatever the initial condition ψ_0 in the ground eigenspace, the optimal control is the same. This is very important for applicability. Although it is a time dependent problem, these considerations hold also for the real-resonant problem.

1.3 The problem downstairs and upstairs

The problem of inducing a transition from the first to the third eigenstate, can be formulated, as usual, at the level of the wave function $\psi(t)$ but also at the level of the time evolution operator (the resolvent), denoted here by $g(t)$:

$$\psi(t) = g(t)\psi(0), \quad g(t) \in U(3), \quad g(0) = id. \quad (7)$$

In the following we will call the optimal control problem for $\psi(t)$ and for $g(t)$ respectively *the "problem downstairs"* and *the "problem upstairs"*.

The state-vector $\psi(t)$, solution of the time-dependent Schrödinger equation $i\dot{\psi} = H\psi$, where H is given by formula (2) can be expanded in the canonical basis of \mathbb{C}^3 , formed by elements $\varphi_1 = (1, 0, 0)$, $\varphi_2 = (0, 1, 0)$, $\varphi_3 = (0, 0, 1)$: $\psi(t) = c_1(t)\varphi_1 + c_2(t)\varphi_2 + c_3(t)\varphi_3$, with $|c_1(t)|^2 + |c_2(t)|^2 + |c_3(t)|^2 = 1$. For $t < 0$ and $t > T$, $|c_i(t)|^2$ is the probability of measuring energy E_i . Notice that, since $\Omega_j(t) = 0$, for all $t < 0$, $t > T$, $j = 1, 2$, we have:

$$\frac{d}{dt}|c_i(t)|^2 = 0 \quad \text{for } t < 0 \text{ and } t > T.$$

At the level of the wave function, we formulate the problem in following way. Assuming $|c_1(t)|^2 = 1$ for $t < 0$, we want to determine suitable control functions $\Omega_j(\cdot)$, $j = 1, 2$, such that $|c_3(t)|^2 = 1$ for time $t > T$, requiring that they minimize the cost (3). Thus we have a control problem on the real sphere $S^5 \subset \mathbb{C}^3$ with initial point belonging to the circle \mathcal{S}_C^d defined by $|c_1|^2 = 1$ and target \mathcal{T}_C^d defined by $|c_3|^2 = 1$. Equivalently, as we said in 1.2, the initial point $\psi(0)$ can be considered as free in \mathcal{S}_C^d . In the following the labels $(^d)$ and $(^u)$, indicate

respectively downstairs and upstairs. Sources and targets upstairs (that will be called \mathcal{S}_c^u and \mathcal{T}_c^u) will be computed in Section 4.3 after elimination of the drift. Why we use the subscript (c), will be made clear in Remark 8.

1.4 Contents of the Paper

The paper is organized as follows. In Section 2, we define precisely the $\mathfrak{k} \oplus \mathfrak{p}$ problem and in Section 3, we discuss the elimination of the drift term. In Section 4 we formulate our problems in the $\mathfrak{k} \oplus \mathfrak{p}$ form and we define sources and the targets. In Section 5 we compute optimal trajectories reaching the final target and satisfying transversality conditions. The proof of Theorem 1 follows. In Appendix A we point out an interesting consequence of the Cartan decomposition, while in Appendix B and C respectively, we explain the Jurdjevic's formalism and why abnormal extremals are not optimal in a semi-simple $\mathfrak{k} \oplus \mathfrak{p}$ problem.

2 The $\mathfrak{k} \oplus \mathfrak{p}$ Problem

For sake of simplicity in the exposition, all over the paper, when we deal about Lie groups and Lie algebras, we always consider that they are groups and algebras of matrices.

Let \mathbf{L} be a semi-simple Lie algebra and let us denote the Killing form by $Kil(\cdot, \cdot)$, $Kil(X, Y) = Tr(ad_X \circ ad_Y)$. In the following we recall what we mean by a Cartan decomposition of \mathbf{L} .

Definition 1 *A Cartan decomposition of a semi-simple Lie algebra \mathbf{L} is any decomposition of the form:*

$$\mathbf{L} = \mathfrak{k} \oplus \mathfrak{p}, \text{ where } [\mathfrak{k}, \mathfrak{k}] \subseteq \mathfrak{k}, \quad [\mathfrak{p}, \mathfrak{p}] \subseteq \mathfrak{k}, \quad [\mathfrak{k}, \mathfrak{p}] \subseteq \mathfrak{p}. \quad (8)$$

Remark 6 Since \mathbf{L} is semi-simple then relations (8) implies $[\mathfrak{p}, \mathfrak{p}] = \mathfrak{k}$, $[\mathfrak{k}, \mathfrak{p}] = \mathfrak{p}$ (see Appendix A for the proof). This fact will be crucial for the elimination of abnormal extremals.

Definition 2 *The right-invariant $\mathfrak{k} \oplus \mathfrak{p}$ control problem on a compact semi-simple Lie group G is the subriemannian problem with right-invariant distribution induced by \mathfrak{p} and cost:*

$$\int_0^T \langle \dot{g} g^{-1}, \dot{g} g^{-1} \rangle dt,$$

where $\langle \cdot, \cdot \rangle := -\alpha Kil|_{\mathfrak{p}}(\cdot, \cdot)$, $\alpha > 0$.

The constant α is clearly not relevant. It will be used just to obtain good normalizations.

In the following we will be interested in $\mathfrak{k} \oplus \mathfrak{p}$ problems on $so(3)$ and $su(3)$, for which we have respectively $Tr(ad_X \circ ad_Y) = Tr(X Y)$ and $Tr(ad_X \circ ad_Y) = 5 Tr(X Y)$. Then, in order to get for both Lie algebras the useful relation:

$$\langle X, Y \rangle = -\frac{1}{2} Tr(X Y), \quad X, Y \in \mathfrak{p}, \quad (9)$$

we must set $\alpha = 1/2$ for $so(3)$ and $\alpha = 1/10$ for $su(3)$.

Let $\{X_j\}$ be an orthonormal (right-invariant) frame for the subspace \mathfrak{p} of \mathbf{L} , with respect to the metric defined in Definition 2. Then the $\mathfrak{k} \oplus \mathfrak{p}$ problem reads:

$$\dot{g} = \left(\sum_j u_j X_j \right) g, \quad \min \int_0^T \sum_j u_j^2 dt, \quad u_j \in \mathbb{R}. \quad (10)$$

From relations (8), one gets that the so called "Goh condition" is never satisfied (see Appendix C). As a consequence:

Proposition 1 *In the problem defined in Definition 2, every strict abnormal extremal (if any) is not optimal.*

Remark 7 The $\mathfrak{k} \oplus \mathfrak{p}$ problem can be also stated in the case where \mathbf{L} is of noncompact type. In this case, to have a positive definite metric, we have to require that \mathfrak{k} is a maximal compact subalgebra of \mathbf{L} , and we must define $\langle \cdot, \cdot \rangle := +\alpha Kil|_{\mathfrak{p}}(\cdot, \cdot)$, $\alpha > 0$.

3 Elimination of the Drift Term

In this section, we show how to eliminate the drift term from a n -level system of the form (6) with general-complex and real-resonant controls. For $\Omega \in \mathbb{C}$, let us denote by $M_j(\Omega)$ and $N_j(\Omega)$ the $n \times n$ matrices:

$$\begin{cases} M_j(\Omega)_{k,l} = \delta_{j,k}\delta_{j+1,l}\Omega + \delta_{j+1,k}\delta_{j,l}\Omega^* \\ N_j(\Omega)_{k,l} = \delta_{j,k}\delta_{j+1,l}\Omega - \delta_{j+1,k}\delta_{j,l}\Omega^* \end{cases}, \quad j = 1, \dots, n-1, \quad (11)$$

where δ is the Kronecker symbol: $\delta_{i,j} = 1$ if $i = j$, $\delta_{i,j} = 0$ if $i \neq j$. Let $\Delta = \text{diag}(E_1, \dots, E_n)$, $\omega_j = E_{j+1} - E_j$, $j = 1, \dots, n-1$. We will consider successively the general complex problem (in dimension n):

$$i\dot{\psi} = H\psi, \quad H = \Delta + \sum_{j=1}^{n-1} M_j(\Omega_j), \quad \text{where } \Omega_j \in \mathbb{C},$$

(this is nothing but another notation for the matrix (6)), and the real-resonant problem:

$$H = \Delta + \sum_{j=1}^{n-1} M_j(e^{i(\omega_j t + \alpha_j)} u_j), \quad u_j, \alpha_j \in \mathbb{R}.$$

In both problems, ψ lies in the complex sphere in \mathbb{C}^n , and we want to connect the source $\mathcal{S}_{\mathbb{C}}^d = \{(e^{i\varphi}, 0, \dots, 0)\}$ to the target $\mathcal{T}_{\mathbb{C}}^d = \{(0, \dots, 0, e^{i\varphi})\}$, by minimizing:

$$J = \int_0^T \sum_{j=1}^{n-1} |\Omega_j|^2 dt, \quad \text{which in the real-resonant case is } J = \int_0^T \sum_{j=1}^{n-1} u_j^2 dt.$$

In both cases, we first make the change of variable $\psi = e^{-i\Delta t} \Lambda$ (interaction representation), to get (here $Ad_\phi B := \phi B \phi^{-1}$):

$$i\dot{\Lambda} = \sum_{j=1}^{n-1} (Ad_{e^{i\Delta t}} M_j(\Omega_j)) \Lambda = \sum_{j=1}^{n-1} M_j(e^{-i\omega_j t} \Omega_j) \Lambda.$$

Let us stress that the source $\mathcal{S}_{\mathbb{C}}^d$ and the target $\mathcal{T}_{\mathbb{C}}^d$ are preserved by this first change of coordinates.

3.1 The general-complex case

In that case, we make the time-dependent *gauge transformation* (i.e. cost preserving change of controls):

$$e^{-i\omega_j t} \Omega_j = i\tilde{\Omega}_j.$$

Hence our problem become (after the change of notation $\Lambda \rightarrow \psi$, $\tilde{\Omega}_j \rightarrow u_j$):

$$\begin{cases} \mathbf{a.} & \min \int_0^T \sum_{j=1}^{n-1} |u_j|^2 dt, \quad x(0) \in \mathcal{S}_{\mathbb{C}}^d, \quad x(T) \in \mathcal{T}_{\mathbb{C}}^d, \\ \mathbf{b.} & \dot{\psi} = \sum_{j=1}^{n-1} N_j(u_j)\psi, \quad u_j(t) \in \mathbb{C}. \end{cases} \quad (12)$$

Notice that the matrices $N_j(1), N_j(i)$ generate $su(3)$ as a Lie algebra. For $n = 3$, the Schrödinger equation (12b) writes, in matrix form:

$$\dot{\psi} = \tilde{H}_{\mathbb{C}} \psi \quad \text{where} \quad \tilde{H}_{\mathbb{C}} := \begin{pmatrix} 0 & u_1(t) & 0 \\ -u_1^*(t) & 0 & u_2(t) \\ 0 & -u_2^*(t) & 0 \end{pmatrix}. \quad (13)$$

The cost and the relation between controls before and after elimination of the drift are:

$$J = \int_0^T (|u_1(t)|^2 + |u_2(t)|^2) dt, \quad (14)$$

$$\begin{cases} \Omega_1(t) = u_1(t) e^{i[(E_2 - E_1)t + \pi/2]}, \\ \Omega_2(t) = u_2(t) e^{i[(E_3 - E_2)t + \pi/2]}, \end{cases} \quad (15)$$

3.2 The real-resonant case

In this case, since $\Omega_j = u_j e^{i(\omega_j t + \alpha_j)}$, we have:

$$i\dot{\Lambda} = \sum_{j=1}^{n-1} M_j(e^{i\alpha_j} u_j) \Lambda, \quad u_j \in \mathbb{R}. \quad (16)$$

We make another diagonal, linear change of coordinates:

$$\Lambda = e^{iL} \phi, \quad L = \text{diag}(\lambda_1, \dots, \lambda_n), \quad \text{for } \lambda_1, \dots, \lambda_n \in \mathbb{R}.$$

This gives:

$$i\dot{\phi} = \sum_{j=1}^{n-1} M_j(e^{i(\alpha_j + \lambda_{j+1} - \lambda_j)} u_j) \phi.$$

Choosing the λ_j 's for $e^{i(\alpha_j + \lambda_{j+1} - \lambda_j)} = i$, we get:

$$\dot{\phi} = \sum_{j=1}^{n-1} N_j(u_j) \phi, \quad u_j(t) \in \mathbb{R}. \quad (17)$$

The source and the target are also preserved by this change of coordinates. Notice that the matrices $N_j(1), j = 1 \dots n-1$ in (17), generate $so(n)$ as a Lie algebra in its presentation by skew-symmetric matrices. This means that the orbit of the system (17) through the points $(\pm 1, 0, \dots, 0)$ is the real sphere S^{n-1} . In other words, the action on \mathbb{C}^n of the subgroup $SO(n) \subset SU(n)$, restricts to the reals. Hence (by multiplication on the right by $e^{i\varphi}$), the orbit through the points $(\pm e^{i\varphi}, 0, \dots, 0)$ is the set $S^{n-1} e^{i\varphi}$. Therefore, (after the change of notation $\phi \rightarrow \psi$) the real-resonant problem reduces to the problem over S^{n-1} (see sections 4.1 for more details):

$$\begin{cases} \min \int_0^T \sum_{j=1}^{n-1} u_j^2 dt, & x(0) \in \{(\pm 1, 0, \dots, 0)\}, \quad x(T) \in \{(0, \dots, 0, \pm 1)\}, \\ \dot{\psi} = \sum_{j=1}^{n-1} N_j(u_j) \psi, & u_j(t) \in \mathbb{R}. \end{cases}$$

For $n = 3$ we get for the Schrödinger equation in matrix form:

$$\dot{\psi} = \tilde{H}_{\mathbb{R}} \psi \quad \text{where} \quad \tilde{H}_{\mathbb{R}} := \begin{pmatrix} 0 & u_1(t) & 0 \\ -u_1(t) & 0 & u_2(t) \\ 0 & -u_2(t) & 0 \end{pmatrix}, \quad (18)$$

The cost is given again by formula (14) and the relation between controls before and after elimination of the drift is:

$$\begin{aligned} \Omega_j(t) &= u_j(t) e^{i(\omega_j t + \alpha_j)}, \quad \omega_j = E_{j+1} - E_j, \\ u_j(\cdot) : \mathbb{R} &\rightarrow \mathbb{R}, \quad \alpha_j \in [-\pi, \pi], \quad j = 1, 2. \end{aligned} \quad (19)$$

Remark 8 In the following, besides to the labels $(^d)$ and $(^u)$ that indicate respectively downstairs and upstairs, we will use the labels (\mathbb{C}) and (\mathbb{R}) to indicate respectively the general-complex problem and the real-resonant one. When these labels are dropped in a formula, we mean that it is valid for both the real-resonant and the general-complex problem. With this notation:

$$\begin{aligned} \mathcal{S}_{\mathbb{C}}^d &= \{(e^{i\varphi}, 0, 0)\}, & \mathcal{T}_{\mathbb{C}}^d &= \{(0, 0, e^{i\varphi})\}, \\ \mathcal{S}_{\mathbb{R}}^d &= \{(\pm 1, 0, 0)\}, & \mathcal{T}_{\mathbb{R}}^d &= \{(0, 0, \pm 1)\}. \end{aligned}$$

4 The $\mathfrak{k} \oplus \mathfrak{p}$ Form of the Problem, Controllability, Sources and Targets

4.1 Controllability

First notice that, after elimination of the drift, the problem upstairs is in $SU(3)$ and not in $U(3)$ (the center of $U(3)$ is eliminated). Moreover, as we already observed, in the real resonant case, starting from $(1, 0, 0)$, we have the standard action of $SO(3)$ on \mathbb{R}^3 . From the fact that the matrices $\tilde{H}_{\mathbb{R}}$ generate $so(3)$ as a Lie algebra, it follows easily that the orbit through $(1, 0, 0)$ is the real sphere S^2 of equation:

$$c_1^2 + c_2^2 + c_3^2 = 1, \quad c_j \in \mathbb{R}, \quad j = 1, 2, 3. \quad (20)$$

It is equivalent to say that the real-resonant problem is not controllable on S^5 . This fact is explained in details in [8]. Moreover in [8] it is proved that on each of these spheres S^2 the control problem reduces to a singular-Riemannian problem. The “relevant locus”, which is the union of all the orbits (translations of S^2) passing through the eigenstate number 1, has an interesting non trivial geometric description. It is the only non orientable sphere-bundle over S^1 .

After elimination of the drift, the real-resonant problem upstairs is on $SO(3)$, and the general-complex problem upstairs is in $SU(3)$. We have:

Proposition 2 *After elimination of the drift, the real resonant problem upstairs is completely controllable on $G_{\mathbb{R}} := SO(3) \subset U(3)$, and the general-complex problem is completely controllable on $G_{\mathbb{C}} := SU(3) \subset U(3)$. As a consequence, by transitivity of the action on the real and complex spheres, the corresponding problems downstairs are controllable on S^2 and S^5 .*

Proof. This is a consequence of the general theorems of controllability of left-invariant control systems on compact groups: the *Lie-rank condition* is necessary and sufficient for controllability (see [18]). ■

Remark 9 In fact, before the elimination of the drift, the general complex problem upstairs is in $U(3)$, due to the nonzero trace of Δ . For the same reason as in Proposition 2, it is completely controllable.

4.2 The problems in the $\mathfrak{k} \oplus \mathfrak{p}$ form

For the lifted problem, from $\dot{\psi} = \tilde{H}\psi$, using (7) one gets:

$$\dot{g} = \tilde{H}g. \quad (21)$$

where $\tilde{H}_{\mathbb{R}}$ generates $so(3)$ and $\tilde{H}_{\mathbb{C}}$ generates $su(3)$ (as Lie algebras, for distinct values of the controls). For both Hamiltonians, the problem of minimizing the cost (14) is a $\mathfrak{k} \oplus \mathfrak{p}$ problem.

In fact in the real-resonant case equation (21) can be written as:

$$\dot{g} = (u_1 X_1 + u_2 X_2)g,$$

where:

$$X_1 = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad X_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}. \quad (22)$$

Setting:

$$X_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \mathfrak{p} := \text{span}(\{X_1, X_2\}), \quad \text{and} \quad \mathfrak{k} = \text{span}(\{X_3\}),$$

one gets relations (8) (with $\mathbf{L} = so(3)$). Moreover the distribution is right-invariant and the frame (22) is orthonormal for the metric (9).

In the case of $su(3)$ we have:

$$\dot{g} = (u_1X_1 + u_2X_2 + u_3Y_1 + u_4Y_2)g, \quad u_j \in \mathbb{R},$$

where X_1 and X_2 are given by formula (22) and Y_1, Y_2 by:

$$Y_1 = \begin{pmatrix} 0 & i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad Y_2 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & i \\ 0 & i & 0 \end{pmatrix}.$$

One can easily check that relations (8) are verified with $\mathbf{p} := \text{span}(\{X_1, X_2, Y_1, Y_2\})$ and $\mathbf{k} := \text{span}(\{Z_1, Z_2, Z_3, Z_4\})$, where:

$$Z_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad Z_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad Z_3 = \begin{pmatrix} i & 0 & 0 \\ 0 & -i & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad Z_4 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & -i \end{pmatrix},$$

are the remaining 4 generators of $su(3)$. Again the distribution is right-invariant and the frame $\{X_1, X_2, Y_1, Y_2\}$ orthonormal for the metric (9).

Remark 10 • (general complex case) \mathbf{k} is a subalgebra of $su(3)$ containing a maximal Abelian subalgebra of $su(3)$, which is generated by Z_3 and Z_4 . From [9] (see also [14]) it follows that \mathbf{k} must be a Borel subalgebra. In this case, it is $u(1) \times su(2) = u(2)$.

Let us denote by $S(U(1) \times U(2))$ (resp. $S(Z_2 \times O(2))$), the groups of matrices of the form:

$$B = \left(\begin{array}{c|c} \epsilon & 0 \\ \hline 0 & U_\epsilon \end{array} \right), \quad \text{where } \det(B) = 1,$$

with $\epsilon \in U(1)$, (resp. $\epsilon \in Z_2 = \{-1, 1\}$), and $U_\epsilon \in U(2)$ (resp. $U_\epsilon \in O(2)$), $S(U(1) \times U(2)) \approx U(2)$, $S(Z_2 \times O(2)) \approx O(2)$.

Set:

$$g_0 := \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \quad (23)$$

$g_0 \in SO(3) \subset SU(3)$, $g_0^2 = g_0^{-1}$. In the real-resonant case, we will denote by $K^{\mathbb{R}}$ the subgroup of $G^{\mathbb{R}} = SO(3)$, conjugate by g_0^{-1} to $S(Z_2 \times O(2)) \approx O(2)$, with Lie algebra $\mathbf{k}^{\mathbb{R}} = \{X_3\}_{LA}$.

In the general-complex case, we denote by $K^{\mathbb{C}}$ the subgroup of $G^{\mathbb{C}} = SU(3)$ conjugate by g_0^{-1} to $S(U(1) \times U(2)) \approx U(2)$ with Lie algebra $\mathbf{k}^{\mathbb{C}} = \{Z_1, Z_2, Z_3, Z_4\}_{LA}$.

- In the general-complex case, the corresponding Riemannian symmetric space G/K is $SU(3)/S(U(2) \times U(1)) \sim \mathbb{C}P^2$ that has rank 1 (see Helgason [13], pp. 518), and the Cartan subalgebra of \mathbf{p} has dimension 1 only, as one can check easily.
- In the real-resonant case, it is $\mathbb{R}P^2$, the 2-dimensional projective space.

Remark 11 Notice that in the real-resonant problem the distribution is a contact distribution. In this case it is a standard fact (see for instance [1, 3, 6, 10, 12]) that there are no abnormal extremals. On the other hand, the distribution of the general complex problem is not a contact distribution and abnormal extremals do exist. Anyway they are not optimal, due to the fact that the "Goh condition" (see Appendix C) fails to hold.

Remark 12 (n-level case) For $n \geq 4$ the Hamiltonian given in formula (12) generates $so(n)$ or $su(n)$ respectively with real or complex controls. Anyway it never gives rise to a $\mathfrak{k} \oplus \mathfrak{p}$ problem since the distribution is only a strict subspace of \mathfrak{p} . As explained in Remark 14 this fact causes the failure of the proof of the integrability of the PMP. No results in this paper about optimal trajectories can be easily generalized to 4 or more levels. For 4 or more levels the integrability of the PMP, and the fact that optimality implies resonance, are open questions.

4.3 Sources and Targets

In this section, we describe sources and targets for the real-resonant and the general-complex problems upstairs.

As we already said, from section 1.2, sources and targets downstairs, for the general-complex problem and the real-resonant one, are respectively the circles $\mathcal{S}_{\mathbb{C}}^d$, $\mathcal{T}_{\mathbb{C}}^d$, and the sets $\mathcal{S}_{\mathbb{R}}^d = \{(\pm 1, 0, 0)\}$, $\mathcal{T}_{\mathbb{R}}^d = \{(0, 0, \pm 1)\}$.

In both cases, we decide that the canonical projection $\pi : G \rightarrow G/\tilde{K}$ maps \tilde{K} to the point $(1, 0, 0)$ in the complex and real sphere in \mathbb{C}^3 (resp. \mathbb{R}^3). Here $\tilde{K}_{\mathbb{C}} = SU(2)$ (general complex case) and $\tilde{K}_{\mathbb{R}} = SO(2)$ (real resonant case). Let $\mathcal{S}^u = \pi^{-1}(\mathcal{S}^d)$. Then $\mathcal{S}_{\mathbb{C}}^u = S(U(1) \times U(2))$, $\mathcal{S}_{\mathbb{R}}^u = S(Z_2 \times O(2))$.

The element $g_0 \in SO(3)$ defined in the previous section maps $\mathcal{S}_{\mathbb{C}}^d$ to $\mathcal{T}_{\mathbb{C}}^d$. Then $\mathcal{T}^u := \pi^{-1}(\mathcal{T}^d) = g_0 \mathcal{S}^u$ in both cases as it is easy to check.

It is clear that a trajectory $g(t)$ of the system upstairs:

$$\dot{g} = \tilde{H}g, \quad t \in [0, T]$$

such that $g(0) \in \mathcal{S}^u$, $g(T) \in \mathcal{T}^u$, maps into a trajectory $g(t)\tilde{K}$ of the system on the sphere,

$$\dot{g}\tilde{K} = \tilde{H}g\tilde{K} \quad g(0)\tilde{K} \in \mathcal{S}^d, \quad g(T)\tilde{K} \in \mathcal{T}^d$$

with the same control, hence the same cost. Conversely, if $x(t)$, $t \in [0, T]$, is a trajectory on the sphere, of the system $\dot{x} = \tilde{H}x$, that maps the point $(\varepsilon, 0, 0)$, $|\varepsilon| = 1$ to the point $(0, 0, \varepsilon')$, $|\varepsilon'| = 1$. Then, the corresponding fundamental matrix solution $g(t)$ satisfies, for all $s \in \mathcal{S}^u$, $g(0)s = s \in \mathcal{S}^u$:

$$g(T).s.(\varepsilon, 0, 0) = (0, 0, \varepsilon') = g_0.(\varepsilon', 0, 0)$$

Therefore, $g_0^{-1}g(T).s.(\varepsilon, 0, 0) = (\varepsilon', 0, 0)$ and $g_0^{-1}.g(T).s \in \mathcal{S}^u$, $g(T) \in g_0 \mathcal{S}^u = \mathcal{T}^u$. This shows that, for all $s \in \mathcal{S}^u$, the lifted solution upstairs satisfies $g(0).s \in \mathcal{S}^u$, $g(T).s \in \mathcal{T}^u$.

Hence we get the following table:

PROBLEM	SOURCE	TARGET
real-resonant	$\mathcal{S}_{\mathbb{R}}^u := \left\{ \left(\begin{array}{c c} Z_2 & 0 \\ \hline 0 & O(2) \end{array} \right) \in SO(3) \right\} = S(Z_2 \times O(2))$	$\mathcal{T}_{\mathbb{R}}^u := g_0 \mathcal{S}_{\mathbb{R}}^u = g_0 S(Z_2 \times O(2))$
general-complex	$\mathcal{S}_{\mathbb{C}}^u := \left\{ \left(\begin{array}{c c} U(1) & 0 \\ \hline 0 & U(2) \end{array} \right) \in SU(3) \right\} = S(U(1) \times U(2))$	$\mathcal{T}_{\mathbb{C}}^u := g_0 \mathcal{S}_{\mathbb{C}}^u = g_0 S(U(1) \times U(2))$

5 Expression for Geodesics, Controls and Transversality Conditions

5.1 Preliminaries

As explained in Appendices B and C, candidates optimal trajectories for the $\mathfrak{k} \oplus \mathfrak{p}$ problem are only “normal geodesics” and are given by the following formula:

$$g(t) = e^{-A_k t} e^{(A_k + A_p)t} g(0), \quad (24)$$

where $g(0)$ is the starting point belonging to the source. Set $M(0) = M_p(0) + M_k(0) = A = A_k + A_p \in \mathbf{L}$ for the initial value of the covector $P(0) = d_{R_g}^* p_{g(0)} = \langle M(0), \cdot \rangle$, where $\langle \cdot, \cdot \rangle$ is given in (9), and with the notations of Appendix B. Here, $A_p = M_p(0)$, $A_k = M_k(0)$ are the orthogonal projections of $M(0) = A$ on \mathbf{p} and \mathbf{k} respectively. Geodesics are parametrized by arclength iff:

$$\langle A_p, A_p \rangle = 1 \quad (25)$$

5.2 Transversality conditions

In both cases, our source is $K_{g_0} = g_0 K g_0^{-1}$ where g_0 has been defined in formula (23) and $K_{g_0}^{\mathbb{C}} = S(U(1) \times U(2))$, $K_{g_0}^{\mathbb{R}} = S(Z(2) \times O(2))$. Let us notice the two following facts:

Facts:

1. Transversality conditions at the source may be required at the identity only.
2. Transversality conditions at the source imply transversality conditions at the target.

Proof : Point 1 comes from right-invariance and the fact that the source is a subgroup. Point 2 comes from the following lemma 1. ■

Let $(g(t), \Omega(t))$, $t \in [0, T]$ be a normal extremal corresponding to the covector $p_{g(t)}$, such that $g(0) = Id$.

Lemma 1 $p_{Id}(Ad_{g_0} \mathbf{k}) = 0$ implies $p_{g(t)}(dL_{g(t)} Ad_{g_0} \mathbf{k}) = 0$, $\forall t \in [0, T]$.

Proof : (with the notations of Appendix B). Set $I = p_{g(t)}(dL_{g(t)} Ad_{g_0} \mathbf{k}) = dR_{g(t)}^* P(t)(dL_{g(t)} Ad_{g_0} \mathbf{k})$. Then $I = P(t)(Ad_{g(t)g_0} \mathbf{k}) = \langle M(t), Ad_{g(t)g_0} \mathbf{k} \rangle$. But:

$$\begin{aligned} M(t) &= M_p(t) + M_k(t) = M_p(t) + M_k(0), \\ M(t) &= e^{-M_k(0)t} M_p(0) e^{M_k(0)t} + M_k(0) = e^{-M_k(0)t} (M_p(0) + M_k(0)) e^{M_k(0)t} = Ad_{e^{-M_k(0)t}} M(0), \end{aligned}$$

and $g(t) = e^{-M_k(0)t} e^{M(0)t}$. Then:

$$I = \langle Ad_{e^{-M_k(0)t}} M(0), Ad_{e^{-M_k(0)t}} Ad_{e^{M(0)t}} Ad_{g_0} \mathbf{k} \rangle,$$

and since the killing form is Ad_G invariant, $I = \langle M(0), Ad_{e^{M(0)t}} Ad_{g_0} \mathbf{k} \rangle$. Hence, for the same reason:

$$I = \langle Ad_{e^{-M(0)t}} M(0), Ad_{g_0} \mathbf{k} \rangle = \langle M(0), Ad_{g_0} \mathbf{k} \rangle = P(0)(Ad_{g_0} \mathbf{k}) = p_{Id}(Ad_{g_0} \mathbf{k}) = 0. \quad \blacksquare$$

Similarly to N_1, N_2 , (cfr. formula (11)) let us define $N_{1,3}$ by:

$$N_{1,3}(a_3 e^{i\theta_3}) = \begin{pmatrix} 0 & 0 & a_3 e^{i\theta_3} \\ 0 & 0 & 0 \\ -a_3 e^{-i\theta_3} & 0 & 0 \end{pmatrix}. \quad (26)$$

Let us set, in the real-resonant case $A_p = a_1 N_1(1) + a_2 N_2(1)$ and $A_k = a_3 N_{1,3}(1)$. In the general complex case, set $A_p = N_1(a_1 e^{i\theta_1}) + N_2(a_2 e^{i\theta_2})$, $A_k = a_4 Z_3 + a_5 Z_4 + N_{1,3}(a_3 e^{i\theta_3})$. Here, $a_i \in \mathbb{R}$ and $\theta_i \in [-\pi, \pi]$.

5.3 The real-resonant case ($\mathbf{G}=\mathbf{SO}(3)$)

Proposition 3 For the real-resonant problem, the transversality conditions $Kil(A, T_{id} \mathcal{S}_{\mathbb{R}}^u) = 0$ implies $a_2 = 0$.

Proof. We have:

$$Ad_{g_0} \mathbf{k}^{\mathbb{R}} = T_{id} \mathcal{S}_{\mathbb{R}}^u := \left\{ \left(\begin{array}{c|cc} 0 & 0 & 0 \\ 0 & 0 & -\beta \\ 0 & \beta & 0 \end{array} \right), \quad \beta \in \mathbb{R} \right\}.$$

Then equation $Kil(A, T_{id} \mathcal{S}_{\mathbb{R}}^u) = 0$ is satisfied for every $\beta \in \mathbb{R}$ if and only if $a_2 = 0$. ■

From Proposition 3, and condition (25), one gets the covectors to be used in formula (24):

$$A^{\pm} = \begin{pmatrix} 0 & \pm 1 & a_3 \\ \mp 1 & 0 & 0 \\ -a_3 & 0 & 0 \end{pmatrix}, \quad (27)$$

Proposition 4 *The geodesics (24), for which $g(0) = Id$, with A given by formula (27), reach the target $T_{\mathbb{R}}^u$ for the smallest time (arclength) $|t|$, if and only if $a_3 = \pm 1/\sqrt{3}$. Moreover, the 4 geodesics (corresponding A^{\pm} and to the signs \pm in a_3) have the same length and reach the target at time:*

$$T = \frac{\sqrt{3}}{2} \pi.$$

Proof. Computing $g(t) = e^{-A_k t} e^{(A_k + A_p)t}$, with A given by formula (27), and recalling that:

$$\psi(t) = g(t)\psi(0) = g(t) \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},$$

one gets for the square of the third component of the wave function:

$$(c_3(t))^2 = \frac{(\cos(t a_3) \sin(t \sqrt{1+a_3^2}) a_3 \sqrt{1+a_3^2} - \cos(t \sqrt{1+a_3^2}) \sin(t a_3) (1+a_3^2))^2}{(1+a_3^2)^2} \quad (28)$$

By lemma (2) in Appendix D, we get the result. ■

Explicit expressions for the wave function and for optimal controls

Let us fix for instance the sign $-$ in (27) and $a_3 = +1/\sqrt{3}$. The expressions of the three components of the wave function are:

$$\begin{cases} c_1(t) = \cos\left(\frac{t}{\sqrt{3}}\right)^3 \\ c_2(t) = \frac{\sqrt{3}}{2} \sin\left(\frac{2t}{\sqrt{3}}\right) \\ c_3(t) = -\sin\left(\frac{t}{\sqrt{3}}\right)^3 \end{cases} \quad (29)$$

Let us stress that this curve is not a circle on S^2 .

Controls can be obtained with the following expressions:

$$u_1 = (\dot{g}g^{-1})_{1,2}, \quad u_2 = (\dot{g}g^{-1})_{2,3} \quad (30)$$

We get:

$$\begin{cases} u_1(t) = -\cos\left(\frac{t}{\sqrt{3}}\right) \\ u_2(t) = \sin\left(\frac{t}{\sqrt{3}}\right) \end{cases} \quad (31)$$

The situation is depicted on Figure 1.

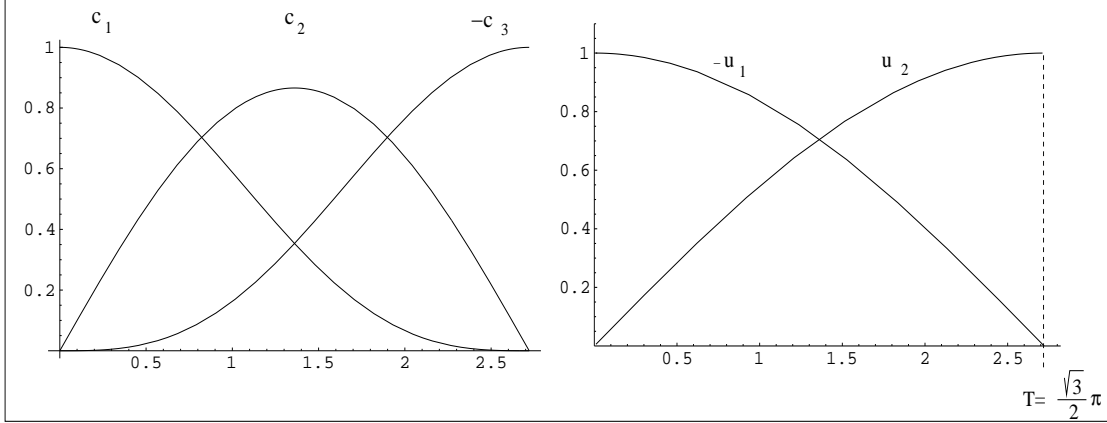


Figure 1

The result given by formulas (29) and (31) is the same result as the one of [8], but it has a simpler form. Using expression (19) (resonance hypothesis), we get for the external fields:

$$\begin{cases} \Omega_1(t) = -\cos(t/\sqrt{3})e^{i(\omega_1 t + \alpha_1)}, \\ \Omega_2(t) = \sin(t/\sqrt{3})e^{i(\omega_2 t + \alpha_2)}. \end{cases} \quad (32)$$

Notice that the phases α_1, α_2 are arbitrary.

5.4 The general-complex case: $G = \text{SU}(3)$

Proposition 5 For the general-complex problem, the transversality conditions $Kil(A, T_{id}\mathcal{S}_{\mathbb{C}}^u) = 0$ implies $a_2 = a_4 = a_5 = 0$.

Proof. We have:

$$Ad_{g_0}\mathbf{k}^{\mathbb{C}} = T_{id}\mathcal{S}_{\mathbb{C}}^u := \left\{ \left(\begin{array}{c|cc} i\alpha_1 & 0 & 0 \\ \hline 0 & i(\alpha_2 - \alpha_1) & \beta_1 + i\beta_2 \\ 0 & -\beta_1 + i\beta_2 & -i\alpha_2 \end{array} \right), \quad \alpha_1, \alpha_2, \beta_1, \beta_2 \in \mathbb{R} \right\}$$

Then equation $Kil(A, T_{id}\mathcal{S}_{\mathbb{C}}^u) = 0$, is satisfied for every $\alpha_1, \alpha_2, \beta_1, \beta_2 \in \mathbb{R}$ if and only if $a_2 = a_4 = a_5 = 0$. \blacksquare

The covector to be used in formula (24) is then:

$$A^{(\theta_1, \theta_3)} = \begin{pmatrix} 0 & e^{i\theta_1} & a_3 e^{i\theta_3} \\ -e^{-i\theta_1} & 0 & 0 \\ -a_3 e^{-i\theta_3} & 0 & 0 \end{pmatrix}. \quad (33)$$

Proposition 6 The geodesics (24), with A given by formula (33) (for which $g(0) = Id$), reach the target $\mathcal{T}_{\mathbb{C}}^u$ for the smallest time (arclength) $|t|$, if and only if $a_3 = \pm 1/\sqrt{3}$. Moreover all the geodesics of the two parameter family corresponding to $\theta_1, \theta_3 \in [-\pi, \pi]$, have the same length:

$$T = \frac{\sqrt{3}}{2}\pi.$$

Proof. The explicit expression for $|c_3|^2$ is given by the right-hand side of formula (28). The conclusion follows as in the proof of Proposition (4).

Explicit expressions for the wave function and for optimal controls

The expressions of the three components of the wave function and of optimal controls are:

$$\begin{cases} c_1(t) = \cos\left(\frac{t}{\sqrt{3}}\right)^3 \\ c_2(t) = -\frac{\sqrt{3}}{2} \sin\left(\frac{2t}{\sqrt{3}}\right)e^{-i\theta_1} \\ c_3(t) = -\sin\left(\frac{t}{\sqrt{3}}\right)^3 e^{-i\theta_3}, \end{cases} \quad (34)$$

$$\begin{cases} u_1(t) = \cos(t/\sqrt{3})e^{i\theta_1} \\ u_2(t) = -\sin(t/\sqrt{3})e^{i(\theta_3-\theta_1)}, \end{cases} \quad (35)$$

Remark 13 Again, notice that none of these trajectories is a circle on the corresponding (translation of) sphere S^2 . Notice that all the geodesics of the family described by Proposition (6) have the same length as the 4 geodesics described by Proposition 4. This proves that the use of the complex Hamiltonian (13) (instead of the real one (18)) does not allow to reduce the cost (14), and this proves Theorem 1 in the introduction.

Formulas (29), (31) can be obtained from formulas (34), (35) setting $\theta_1 = \pi$, $\theta_3 = 0$.

For the general-complex problem, using expressions (35) in (15) one gets for the external fields:

$$\begin{cases} \Omega_1(t) = \cos(t/\sqrt{3})e^{i(\omega_1 t + \theta_1 + \frac{\pi}{2})}, \\ \Omega_2(t) = -\sin(t/\sqrt{3})e^{i(\omega_2 t + \theta_3 - \theta_1 + \frac{\pi}{2})}, \end{cases} \quad (36)$$

where $\omega_1 = E_2 - E_1$, $\omega_2 = E_3 - E_2$.

Formula (36) coincides with formula (5) setting $\varphi_1 := \theta_1 + \pi/2$, $\varphi_2 := \theta_3 - \theta_1 - \pi/2$.

We recall that in previous papers for the real-resonant problem, (see [8] for more details), optimality was set as an assumption while here, it is obtained as a consequence of the PMP.

Moreover we get that the optimal cost and the probabilities $|c_j(t)|^2$, $j = 1, 2, 3$, are independent from $\theta_1, \theta_3 \in [-\pi, \pi]$.

Appendix A: An interesting consequence of the Cartan Decomposition

Theorem 2 *Let \mathbf{L} be a semi-simple Lie algebra and $\mathbf{L} = \mathbf{k} \oplus \mathbf{p}$ a Cartan decomposition (i.e. it holds $[\mathbf{k}, \mathbf{k}] \subseteq \mathbf{k}$, $[\mathbf{p}, \mathbf{p}] \subseteq \mathbf{k}$, $[\mathbf{k}, \mathbf{p}] \subseteq \mathbf{p}$). Then $[\mathbf{k}, \mathbf{p}] = \mathbf{p}$, $[\mathbf{p}, \mathbf{p}] = \mathbf{k}$.*

Proof. We can restrict ourself to the case in which \mathbf{L} is simple, since a semi-simple Lie algebra is a direct sum of simple ideals.

Claim 1: $\mathbf{p} + [\mathbf{p}, \mathbf{p}]$ is an ideal in \mathbf{L}

Proof of Claim 1:

- $[\mathbf{p}, \mathbf{p} + [\mathbf{p}, \mathbf{p}]] = [\mathbf{p}, \mathbf{p}] + [\mathbf{p}, [\mathbf{p}, \mathbf{p}]]$. Using the Cartan relations it follows that the second term is contained in \mathbf{p} . Hence $[\mathbf{p}, \mathbf{p} + [\mathbf{p}, \mathbf{p}]] \subseteq \mathbf{p} + [\mathbf{p}, \mathbf{p}]$.
- $[\mathbf{k}, \mathbf{p} + [\mathbf{p}, \mathbf{p}]] = [\mathbf{k}, \mathbf{p}] + [\mathbf{k}, [\mathbf{p}, \mathbf{p}]]$. Now, using the Cartan relations we have: $[\mathbf{k}, \mathbf{p}] \subseteq \mathbf{p}$ while $[\mathbf{k}, [\mathbf{p}, \mathbf{p}]] = -[\mathbf{p}, [\mathbf{k}, \mathbf{p}]] - [\mathbf{p}, [\mathbf{p}, \mathbf{k}]] \subseteq [\mathbf{p}, \mathbf{p}]$, where we have used the Jacobi identity. Therefore $[\mathbf{k}, \mathbf{p} + [\mathbf{p}, \mathbf{p}]] \subseteq \mathbf{p} + [\mathbf{p}, \mathbf{p}]$.

Claim 2: $\mathbf{k} + [\mathbf{k}, \mathbf{p}]$ is an ideal in \mathbf{L}

Proof of Claim 2:

- $[\mathbf{p}, \mathbf{k} + [\mathbf{k}, \mathbf{p}]] = [\mathbf{p}, \mathbf{k}] + [\mathbf{p}, [\mathbf{k}, \mathbf{p}]] \subseteq [\mathbf{k}, \mathbf{p}] + \mathbf{k}$.

- $[\mathbf{k}, \mathbf{k} + [\mathbf{k}, \mathbf{p}]] = [\mathbf{k}, \mathbf{k}] + [\mathbf{k}, [\mathbf{k}, \mathbf{p}]] \subseteq \mathbf{k} + [\mathbf{k}, \mathbf{p}]$.

From the fact that \mathbf{L} is simple (the only ideals are 0 and \mathbf{L}) it follows $\mathbf{p} + [\mathbf{p}, \mathbf{p}] = \mathbf{L} \Rightarrow [\mathbf{p}, \mathbf{p}] = \mathbf{k}$, $\mathbf{k} + [\mathbf{k}, \mathbf{p}] = \mathbf{L} \Rightarrow [\mathbf{k}, \mathbf{p}] = \mathbf{p}$. ■

Notice that in general is false that $[\mathbf{k}, \mathbf{k}] = \mathbf{k}$. In particular it is false for the Cartan decomposition of $SU(3)$ we used in this paper (\mathbf{k} has a center). Theorem 2 is crucial to prove that, in our case, abnormal extremals are never optimal (see Appendix C).

Appendix B: The $K + P$ Problem

Here following [15] and [16], we recall how to write the PMP for a right-invariant control system on a Lie group G . We do it for a group of matrices only.

Let \mathbf{L} and \mathbf{L}^* be respectively the tangent and cotangent planes at the identity of G . Consider the right-invariant system:

$$\dot{g} = X(u)g, \quad (37)$$

where $X(u) \in \mathbf{L}$ and u belongs to the set of values of controls U . To have a right-invariant optimal control problem, we must also assume a right-invariant cost (that is a cost that does not depend on g , the coordinate on the group):

$$\int_0^T f(u(t)) dt, \quad \text{where } f : U \rightarrow \mathbb{R} \text{ is a smooth function.} \quad (38)$$

Moreover we assume that the initial and final points belong to two given smooth manifolds:

$$g(0) \in M_{in}, \quad g(T) \in M_{fin}. \quad (39)$$

For each $\lambda \in \mathbb{R}$ and $u \in U$ define the Hamiltonian :

$$H_u(\cdot) : \mathbf{L}^* \rightarrow \mathbb{R}, \quad H_u(P) := P(X(u)) + \lambda f(u).$$

We have $dH_u(P) \in (\mathbf{L}^*)^*$, ($P \in \mathbf{L}^*$) and since \mathbf{L} has finite dimension, we can identify $(\mathbf{L}^*)^* \sim \mathbf{L}$ and consider $dH_u(P) \in \mathbf{L}$. Let $B \in \mathbf{L}$ and denote with $ad_B^*(\cdot)$ the operator from $\mathbf{L}^* \rightarrow \mathbf{L}^*$ defined by:

$$[ad_B^*(P)](A) := P(ad_B(A)) = P([B, A]), \quad \forall A \in \mathbf{L}.$$

The PMP (see [21]) is a necessary condition for optimality. For right-invariant control systems it reads (see [15, 16]):

Theorem 3 (PMP for right-invariant control systems) *Consider a couple $(u(\cdot), g(\cdot)) : [0, T] \rightarrow U \times G$ subjected to the dynamics (37) and to the constraints (39). If it minimizes the cost (38), then there exists a constant $\lambda \leq 0$ and a never vanishing absolutely continuous function $P(\cdot) : t \in [0, T] \mapsto P(t) \in \mathbf{L}^*$ such that:*

$$\frac{dg(t)}{dt} = dH_{u(t)}(P(t))g(t) \quad (40)$$

$$\frac{dP(t)}{dt} = -ad_{dH_{u(t)}(P(t))}^*(P(t)). \quad (41)$$

Moreover:

$$H_u(t)(P(t)) = \mathcal{H}(P(t)) \quad \text{where} \quad \mathcal{H}(P(t)) := \max_{v \in U} H_v(P(t)). \quad (42)$$

$$P(0)(T_{g(0)}M_{in} \cdot g^{-1}(0)) = 0, \quad P(t)(T_{g(t)}M_{fin} \cdot g^{-1}(T)) = 0 \quad (\text{transversality conditions}) \quad (43)$$

Here $g(t) \in G$ and $P(t) \in \mathbf{L}^*$ is the covector translated back to the identity. $P(t)$ is related to the usual covector $p_{g(t)} \in T_{g(t)}^*G$ by: $P(t) = dR_{g(t)}^* p_{g(t)}$ or $p_{g(t)} = dR_{g(t)^{-1}}^* P(t)$

The couples $(u(\cdot), g(\cdot))$ satisfying conditions (40), (41) and (42) with $\lambda = 0$ are called *abnormal extremals*. Couples $(u(\cdot), g(\cdot))$ corresponding to $\lambda \neq 0$ (in this case we can normalize $\lambda = -1/2$) are called *normal extremals*.

In the following we show that for normal extremals this Hamiltonian system becomes completely integrable if the problem is $\mathbf{k} \oplus \mathbf{p}$. Abnormal extremals may exist in general, but they are never optimal as explained in Appendix C.

Consider the right-invariant $\mathbf{k} \oplus \mathbf{p}$ problem defined in Definitions 1, 2. Here $\mathbf{L} = \mathbf{k} \oplus \mathbf{p}$ can also be noncompact (in that case \mathbf{k} must be the maximal compact subalgebra of \mathbf{L} , cfr. Remark 7).

The Killing form defines a non-degenerate pseudo scalar product on \mathbf{L} . This permits to identify \mathbf{L} with \mathbf{L}^* by:

$$P \in \mathbf{L}^* \longleftrightarrow M \in \mathbf{L} \iff P(C) = Kil(M, C), \quad \forall C \in \mathbf{L}. \quad (44)$$

Let us “translate” equation (41) for $M \in \mathbf{L}$. For each $C \in \mathbf{L}$ we have:

$$\begin{aligned} Kil\left(\frac{dM}{dt}, C\right) &= \frac{dP}{dt}(C) = -[ad_{dH(P(t))}^*(P(t))](C) = -P(t) ([dH(P(t)), C]) \\ &= -Kil(M(t), [dH(P(t)), C]) = +Kil([dH(P(t)), M], C), \end{aligned}$$

where we have used the invariance of the Killing form under Lie Brackets: $Kil([A, B], C) = Kil(A, [B, C])$, that can be easily checked. The equation for $M(t)$ is then in the famous Lax-Poincaré form:

$$\frac{dM(t)}{dt} = [dH(P(t)), M(t)], \quad M(t), dH(P(t)) \in \mathbf{L}. \quad (45)$$

Let $\{X_j\}$ be an orthonormal (right-invariant) frame for the \mathbf{p} part of \mathbf{L} , with respect to the metric defined in Definition 2. We have then $X(u) = \sum_j u_j X_j$ and $f(u) = u_1^2 + \dots + u_{n_p}^2$ (here $u = (u_1, u_2, \dots, u_{n_p})$ and n_p is the dimension of the \mathbf{p} subspace). Moreover decompose $M = M_p + M_k$, where $M_p \in \mathbf{p}$ and $M_k \in \mathbf{k}$.

Proposition 7 *We have $dH(P(t)) = X(u(t)) = M_p(t)$.*

Proof. The first equality can be obtained comparing equation $\dot{g}(t) = X(u(t))g(t)$ with equation (40) and using the fact that the differential of the right translation is a linear isomorphism. Let us consider the second one. From the maximum condition (42) with $\lambda = -1/2$ and $f(u) = u_1^2 + \dots + u_{n_p}^2$, we get:

$$u_i(t) = p_{g(t)}(t)(X_i g(t)) = P(t)(X_i) = Kil(M(t), X_i) = Kil(M_p(t), X_i) \text{ because } X_i = X_i(e) \in \mathbf{p}.$$

In the last equality we used the fact that M_p and M_k are orthogonal subspaces for the Killing form. Therefore $M_p(t) = \sum_j Kil(M_p(t), X_j) X_j = \sum_j u_j(t) X_j = X(u(t))$. ■

With Proposition 7, the equation for M become:

$$\frac{dM_p}{dt} + \frac{dM_k}{dt} = [M_p(t), M_p(t) + M_k(t)] = [M_p(t), M_k(t)]. \quad (46)$$

Using the Cartan commutations relations (8), we have $[M_p(t), M_k(t)] \subset \mathbf{p}$ and equation (46) splits into:

$$\begin{aligned} \frac{dM_k}{dt} &= 0 \Rightarrow M_k(t) = M_k(0), \\ \frac{dM_p}{dt} &= [M_p(t), M_k(0)]. \end{aligned}$$

Hence all the \mathbf{k} -components of the covector are constants of the motion. Integrating the equation for M_p , and setting $A_p := M_p(0)$, $A_k := M_k(0)$, we get:

$$M_p(t) = e^{-A_k t} A_p e^{A_k t} = e^{-ad_{A_k} t} A_p.$$

From equation (40), with $dH(P(t)) = M_p(t)$, we have:

$$\frac{dg(t)}{dt} = (e^{-A_k t} A_p e^{A_k t}) g(t)$$

and the solution is equation (24):

$$g(t) = e^{-A_k t} e^{(A_k + A_p)t} g(0) \quad (47)$$

Setting $A := A_p + A_k$, the transversality conditions (43) reads in \mathbf{L} :

$$Kil(A, T_{g(0)} M_{in} \cdot g^{-1}(0)) = 0, \quad (48)$$

$$Kil(M(t), T_{g(t)} M_{fin} \cdot g^{-1}(t)) = 0. \quad (49)$$

Remark 14 (n-level case) In the case in which the distribution is only a strict subspace of \mathbf{p} , as in the n -level case ($n \geq 4$), $dH(P(t)) = X(u(t))$, but it is not equal to $M_p(t)$ in general. Then equation (46) become:

$$\frac{dM_p}{dt} + \frac{dM_k}{dt} = [X(u(t)), M_p(t) + M_k(t)],$$

where now the right-hand side is not completely contained in \mathbf{p} . This means that not all the \mathbf{k} -components of the covector are constants of the motion, and the proof of the integrability of the Hamiltonian system given above fails.

Appendix C: The Goh Condition

Let us consider any subriemannian metric over a manifold M , defined by its orthonormal frame $\{X_i, i = 1, \dots, p\}$, completely nonintegrable. Then a necessary condition for a strictly abnormal extremal (i.e. an abnormal extremal which is not normal at the same time) to be optimal is that it satisfies the *Goh condition*.

Definition-Theorem (Goh-condition) *Let $(p(t), x(t))$, $t \in [0, T]$ be the Hamiltonian lift of the abnormal extremal $x(t)$ (see Theorem 3). Then:*

$$(p(t)(X_i(x(t))) \equiv 0, \quad p(t) \neq 0, \quad t \in [0, T], \quad (50)$$

and a necessary condition for optimality of $x(\cdot)$ is $\{p(t)(X_i), p(t)(X_j)\}(x(t)) \equiv 0, \quad t \in [0, T]$, or:

$$p(t)([X_i, X_j](x(t))) \equiv 0, \quad t \in [0, T]. \quad (51)$$

This Theorem is a consequence of a (highly non trivial) generalized Maslov index theory developed in [4]. For our right-invariant problem, the relations (50), (51) give:

$$p(0)(X_i(id)) = 0, \quad p(0)([X_i, X_j](id)) = 0,$$

they imply with Theorem 2 of Appendix A, that $p(0)(\mathbf{L}) = 0$. Then $p(0) = 0$. This is a contradiction since $p(t)$ has to be nonzero, for all t .

Hence, strictly abnormal trajectories are never optimal in our $\mathbf{k} \oplus \mathbf{p}$ problem.

Appendix D: A technical computation

Lemma 2 Set $f_a = \cos(ta) \sin(t\sqrt{1+a^2}) \frac{a}{\sqrt{1+a^2}} - \cos(t\sqrt{1+a^2}) \sin(ta)$, then $|f_a| \leq 1$.

Moreover, $|f_a| = 1$ iff $\frac{|a|}{\sqrt{1+a^2}} = \left| \frac{1}{2k} + \frac{k'}{k} \right| < 1$; $k \neq 0$ and $t = \frac{k\pi}{\sqrt{1+a^2}}$.

In particular, the smallest $|t|$ is obtained for $k = \pm 1$, $a = \pm \frac{1}{\sqrt{3}}$, $t = \frac{\pm\pi\sqrt{3}}{2}$.

Proof. Set $\lambda = \frac{a}{\sqrt{1+a^2}}$, $\theta = t\sqrt{1+a^2}$, then

$$\begin{aligned} f_a(t) &= \lambda \cos(\lambda\theta) \sin(\theta) - \cos(\theta) \sin(\lambda\theta) \\ &= \langle (\lambda \cos(\lambda\theta), \sin(\lambda\theta)), (\sin(\theta), -\cos(\theta)) \rangle \\ &= \langle v_1, v_2 \rangle. \end{aligned}$$

Both v_1, v_2 have norm ≤ 1 and $|f_a| \leq 1$. Hence, for $|f_a| = 1$, we must have $\|v_1\| = \|v_2\| = 1$, $v_1 = \pm v_2$. It follows that $\cos(\lambda\theta) = 0$ and $\cos(\theta) = \pm 1$. Hence $\theta = k\pi$, $\lambda\theta = \frac{\pi}{2} + k'\pi$, $\lambda = \frac{1}{2k} + \frac{k'}{k}$. Therefore, $\left| \frac{1}{2k} + \frac{k'}{k} \right| = \lambda < 1$.

Conversely, choose k, k' meeting this condition, and $\theta = k\pi$. Then $\cos(\theta) = \pm 1$, $\sin(\lambda\theta) = \pm 1$, $f_a(t) = \pm 1$.

Now, $|t| = \frac{k\pi}{\sqrt{1+a^2}}$, and the smallest $|t|$ is obtained for $k = \pm 1$ (if $k = 0$, $\theta = 0$ and $f_a(t) = 0$). Moreover,

$\left| \frac{1}{2k} + \frac{k'}{k} \right| < 1$ is possible only for $(k, k') = (1, 0)$ or $(1, -1)$ or $(-1, 0)$ or $(-1, -1)$.

In all cases, $|\lambda| = \frac{1}{2}$, $a = \pm \frac{1}{\sqrt{3}}$, and $t = \pm \frac{\pi\sqrt{3}}{2}$. ■

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