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ON THE $K+P$ PROBLEM FOR A THREE-LEVEL QUANTUM SYSTEM: OPTIMALITY IMPLIES RESONANCE

U. BOSCAIN, T. CHAMBRION, and J.-P. GAUTHIER

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".

1. Introduction

1.1. Physical context. In the recent years, people started to approach the control of the Schrödinger equation, using techniques of geometric control theory (see, e.g., [5], [6], [12], [20], [23]). 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 $\hbar = 1$):

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

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

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

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Here $*$ denotes 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 with the physical parameters by $\Omega_j(t) = \mu_j \mathcal{F}_j(t)/2$, $j = 1, 2$, with the external pulsed field $\mathcal{F}_j$ and the couplings μ_j (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, and 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) $... > E_3 > E_2 > E_1$. 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, and E_3 is completely decoupled and is described by 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 what follows):

$$J = \int_0^T \left(|\Omega_1(t)|^2 + |\Omega_2(t)|^2\right) dt. \tag{3}$$

In [9], this problem was studied assuming that the controls Ω_j are "in resonance":

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

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

In [9], the real-resonant problem was treated as follows:

- first, using a time dependent change of coordinates that preserves 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 sequel) 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 preserves invariant both the source and 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 $K^{\mathbb{R}}$ and $K^{\mathbb{C}}$ ($K^{\mathbb{R}} \approx O(2), K^{\mathbb{C}} \approx U(2)$) such that, denoting by $\mathbf{k}^{\mathbb{R}}$ and $\mathbf{k}^{\mathbb{C}}$ the Lie algebras of $K^{\mathbb{R}}$ and $K^{\mathbb{C}}$, respectively:

  a. the Lie algebras $\mathbf{L}, \mathbf{k}$ of the pair (G, K) have associated Cartan decomposition $\mathbf{L} = \mathbf{k} \oplus \mathbf{p}$, with the usual commutation relations;
  b. the right-invariant distribution is determined by the $\mathbf{p}$-subspace of $\mathbf{L}$;
  c. the right invariant subriemannian metric is determined by a scalar multiple of $\mathrm{Kil}\big|_p$, where $\mathrm{Kil}\big|_p$ is the Killing form restricted to $\mathbf{p}$;
  d. the source S and the target T of the optimal control problem are $S = K_{g_0} = g_0 K {g_0}^{-1}$, the conjugation of K by g_0, and $T = g_0 S$, respectively;
- subriemannian problems on semisimple Lie groups in which the distribution is determined by the $\mathbf{p}$ subspace of a Cartan decomposition and the metric is proportional to $\mathrm{Kil}\big|_p$ (called in the sequel ($\mathbf{k} \oplus \mathbf{p}$)-*problems*) have two important features:
  - abnormal extremals (if they exist) 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 developped by Jurdjevic in [17, 18]. In particular, he proved that the Hamiltonian system given by PMP is completely integrable and he gave explicit expressions for geodesics. For the sake of completeness, the Jurdjevic's technique is summarized in Appendix B;

- as 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 [18], the connection between the geodesics for the $\mathbf{k} \oplus \mathbf{p}$ 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 verify, it is possible to project on the symmetric space G/K_{g_0}, but this problem is not invariant with respect to the action of G on G/K_{g_0}. In fact, we obtain a *singular Riemannian* problem over G/K_{g_0} (as we have shown in the paper [9], for the real-resonant case).

With this methods, for the real-resonant problem we get in a more natural way the result of [9], and we give much simpler expressions for geodesics and optimal controls. In the general-complex problem, in addition to finding explicitly the expression for optimal trajectories and controls we prove our main result.

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

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

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

This fact was pointed out as an open question in [9]. In other words, *optimal trajectories for the real-resonant problem are optimal also for the general-complex one.*

Remark 3. The fact that the optimality implies resonance was also proved in [9] for the two-level case, reducing the problem to an isoperimetric one. 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 the optimality implies resonance is nothing but the (trivial) solution of the classical isoperimetric problem (or Dido problem) on the Riemannian sphere. We refer to [9] for details.

Remark 4. In addition to physical applications, the three-level problem is interesting, in particular, since it has a nontrivial geometric structure, but it is completely computable. On the other hand, 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 obtains a problem in which the control distribution is determined by a strict subspace of $\mathbf{p}$ only. In this case, the Jurdjevic formula fails to be true, and the integrability of PMP is an open problem. See Remarks 12 and 14 (the last in Appendix B). In this case the Hamiltonian has the form

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

Remark 5. For questions related to invariance under time reparametrization of our optimal trajectories, we refer to [9].

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 sequel, but also for practical applicability of the result.

The optimal control problem under consideration (in $\mathbb{C}^3$ or in the complex sphere in $\mathbb{C}^3$) is invariant under the 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 be the initial condition ψ_0 in the ground eigenspace, the optimal control is <u>the same</u>. This is very important for applications. 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 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 $g(t)$:

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

In the sequel, we will call the optimal control problem for $\psi(t)$ and $g(t)$, 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 $\varphi_1 = (1,0,0)$, $\varphi_2 = (0,1,0)$, and $\varphi_3 = (0,0,1)$: $\psi(t) = c_1(t)\varphi_1 + c_2(t)\varphi_2 + c_3(t)\varphi_3$, 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. Note that, since $\Omega_j(t) = 0$, for all $t < 0$, $t > T$, $j = 1, 2$, we have:

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

At the level of the wave function, we formulate the problem in the 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 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 $\mathcal{S}^d_{\mathbb{C}}$ defined by $|c_1|^2 = 1$ and target $\mathcal{T}^d_{\mathbb{C}}$ defined by $|c_3|^2 = 1$. Equivalently, as we have said in 1.2, the initial point $\psi(0)$ can be considered as free in $\mathcal{S}^d_{\mathbb{C}}$. In the sequel, the superscripts d and u denote, respectively, "downstairs" and "upstairs." Sources and targets upstairs (that will be called $\mathcal{S}^u_{\mathbb{C}}$ and $\mathcal{T}^u_{\mathbb{C}}$) will be computed in Sec. 4.3 after elimination of the drift. Why we use the subscript $\mathbb{C}$, will be made clear in Remark 8.

1.4. **Contents of the paper.** The paper is organized as follows. In Sec. 2, we define precisely the $\mathbf{k} \oplus \mathbf{p}$ problem and in Sec. 3, we discuss the elimination of the drift term. In Sec. 4 we formulate our problems in the $\mathbf{k} \oplus \mathbf{p}$ form and define the sources and targets. In Sec. 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 semisimple $\mathbf{k} \oplus \mathbf{p}$ problem.

2. The $\mathbf{k} \oplus \mathbf{p}$ problem

For the sake of simplicity in the exposition, all over the paper, when we deal with Lie groups and Lie algebras, we always assume 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 $\mathrm{Kil}(\cdot,\cdot)$, $\mathrm{Kil}(X,Y) = \mathrm{Tr}(\mathrm{ad}_X \circ \mathrm{ad}_Y)$. In the sequel, we recall what we mean by a Cartan decomposition of $\mathbf{L}$.

Definition 1. A Cartan decomposition of a semisimple Lie algebra $\mathbf{L}$ is any decomposition of the form

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

Remark 6. Since $\mathbf{L}$ is semisimple, relations (8) imply $[\mathbf{p},\mathbf{p}] = \mathbf{k}$, $[\mathbf{k},\mathbf{p}] = \mathbf{p}$ (see Appendix A for the proof). This fact is crucial for the elimination of abnormal extremals.

Definition 2. The right invariant $\mathbf{k} \oplus \mathbf{p}$ control problem on a compact semisimple Lie group G is the subriemannian problem with the right invariant distribution induced by $\mathbf{p}$ and cost:

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

where $\langle\ ,\ \rangle := -\alpha\, \mathrm{Kil}\big|_p(\ ,\ )$, $\alpha > 0$.

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

In the sequel we will be interested in $\mathbf{k}\oplus\mathbf{p}$ problems on so(3) and su(3), for which we have $\mathrm{Tr}(\mathrm{ad}_X \circ \mathrm{ad}_Y) = \mathrm{Tr}(XY)$ and $\mathrm{Tr}(\mathrm{ad}_X \circ \mathrm{ad}_Y) = 6\,\mathrm{Tr}(XY)$, respectively. Then, in order to obtain the useful relation

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

for both Lie algebras, we should set $\alpha = 1/2$ for so(3) and $\alpha = 1/12$ for su(3).

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

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

From relations (8), one obtains that the so-called *"Goh condition"* is never satisfied (see Appendix C). As a consequence, we have the following proposition.

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

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

3. Elimination of the drift term

In this section, we show how to eliminate the drift term from n-level system of 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:

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

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

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

(this is nothing but another notation for 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 $\mathcal{S}_{\mathbb{C}}^d = \{(e^{i\varphi}, 0, ..., 0)\}$ with the target $\mathcal{T}_{\mathbb{C}}^d = \{(0, ..., 0, e^{i\varphi})\}$, by minimizing the functional

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

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

$$i\dot{\Lambda} = \sum_{j=1}^{n-1} \left(\mathrm{Ad}_{e^{i\Delta t}} M_j(\Omega_j)\right)\Lambda = \sum_{j=1}^{n-1} M_j\left(e^{-i\omega_j t}\Omega_j\right)\Lambda.$$

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

3.1. **The general-complex case.** In this 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 becomes (after the change of notation $\Lambda \to \psi$, $\tilde{\Omega}_j \to u_j$):

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

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

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

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

$$J = \int_0^T \left(|u_1(t)|^2 + |u_2(t)|^2\right) dt, \tag{14}$$

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

3.2. **The real-resonant case.** In this case, since $\Omega_j = u_j e^{i(\omega_j t+\alpha_j)}$, we have:

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

We make another diagonal linear change of coordinates:

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

This gives:

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

Choosing λ_j for $e^{i(\alpha_j+\lambda_{j+1}-\lambda_j)} = i$, we obtain

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

The source and target are also preserved by this change of coordinates. Note 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 system (17) through the points $(\pm 1, 0, \dots, 0)$ is the real sphere S^{n-1}. In other words, the action of the subgroup $\mathrm{SO}(n) \subset \mathrm{SU}(n)$ on $\mathbb{C}^n$, can be restricted 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 the notation $\phi \to \psi$) the real-resonant problem reduces to the problem over S^{n-1} (see Sec. 4.1 for more details):

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

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

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

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

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

Remark 8. In the sequel, in addition to the superscripts d and s that denote "downstairs" and "upstairs," respectively, we will use the subscripts $\mathbb{C}$ and $\mathbb{R}$ to indicate the general-complex problem and the real-resonant one, respectively. When these labels are omitted in a formula, we mean that it is valid for both the real-resonant and general-complex problem. With this notation,

$$\begin{gathered} \mathcal{S}^d_{\mathbb{C}} = \{(e^{i\varphi}, 0, 0)\}, \quad \mathcal{T}^d_{\mathbb{C}} = \{(0, 0, e^{i\varphi})\}, \\ \mathcal{S}^d_{\mathbb{R}} = \{(\pm 1, 0, 0)\}, \quad \mathcal{T}^d_{\mathbb{R}} = \{(0, 0, \pm 1)\}. \end{gathered}$$

4. The $\mathbf{k} \oplus \mathbf{p}$ form of the problem, controllability, sources, and targets

4.1. **Controllability.** We note first 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 easily follows that the orbit through $(1,0,0)$ is the real sphere S^2 of the equation

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

In other words, the real-resonant problem is not controllable on S^5. This fact is explained in detail in [9]. Moreover, in [9] 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 orbits (translations of S^2) passing through the eigenstate number 1, has an interesting nontrivial geometric description. It is the only nonorientable 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 on SU(3). We have the following proposition.

Proposition 2. *After elimination of the drift, the real resonant problem upstairs is completely controllable on $G_{\mathbb{R}} := \mathrm{SO}(3) \subset U(3)$, and the general-complex problem is completely controllable on $G_{\mathbb{C}} := \mathrm{SU}(3) \subset U(3)$. As a consequence, by the 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 [19]). □

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 $\mathbf{k} \oplus \mathbf{p}$ form.** For the lifted problem, from $\dot{\psi} = \tilde{H}\psi$, using (7) one obtains:

$$\dot{g} = \tilde{H} g, \tag{21}$$

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 cost (14) is a $\mathbf{k} \oplus \mathbf{p}$ problem. In fact, in the real-resonant case, Eq. (21) can be written as

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

where

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

Setting

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

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

In the case of su(3) we have:

$$\dot{g} = (u_1 X_1 + u_2 X_2 + u_3 Y_1 + u_4 Y_2)g, \quad u_j \in \mathbb{R},$$

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

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

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

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

$$Z_4 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & -i \end{pmatrix}$$

are the remaining 4 generators of su(3). Again, the distribution is right invariant and the frame $\{X_1, X_2, Y_1, Y_2\}$ is orthonormal for 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 [10] (see also [15]) it follows that $\mathbf{k}$ must be a Borel subalgebra. In this case, it is $u(1) \times \mathrm{su}(2) = u(2)$.

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

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

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

We set:

$$g_0 := \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \tag{23}$$

$g_0 \in \mathrm{SO}(3) \subset \mathrm{SU}(3)$, ${g_0}^2 = {g_0}^{-1}$. In the real-resonant case, we will denote by $K^{\mathbb{R}}$ the subgroup of $G^{\mathbb{R}} = \mathrm{SO}(3)$, conjugate by ${g_0}^{-1}$ to $S(Z_2 \times O(2)) \approx O(2)$, with the 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 the 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 $SU(3)/S(U(2) \times U(1)) \sim \mathbb{CP}^2$ that has rank 1 (see Helgason [14], p. 518), and the Cartan subalgebra of $\mathbf{p}$ has dimension 1 only, as one can easily verify.
- In the real-resonant case, it is $\mathbb{RP}^2$, the 2-dimensional projective space.

Remark 11. Note that in the real-resonant problem the distribution is a contact distribution. In this case it is a standard fact (see, e.g., [1], [3], [7], [11], and [13]) 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 $\mathbf{k} \oplus \mathbf{p}$ problem since the distribution is only a strict subspace of $\mathbf{p}$. As explained in Remark 14, this fact causes the failure of the proof of the integrability of PMP. No results of this paper about optimal trajectories can be easily generalized to 4 or more levels. For 4 or more levels the integrability of PMP, and the fact that the optimality implies resonance, are open questions.

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

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

In both cases, we decide that the canonical projection $\pi : G \to G/\tilde{K}$ maps $\tilde{K}$ to the point $(1, 0, 0)$ in the complex and real sphere in $\mathbb{C}^3$ (resp. $\mathbb{R}^3$). Here $\tilde{K}_{\mathbb{C}} = \mathrm{SU}(2)$ (general complex case) and $\tilde{K}_{\mathbb{R}} = \mathrm{SO}(2)$ (real resonant case). Let $\mathcal{S}^u = \pi^{-1}(\mathcal{S}^d)$. Then $\mathcal{S}^u_{\mathbb{C}} = S(U(1) \times U(2))$, $\mathcal{S}^u_{\mathbb{R}} = S(Z_2 \times O(2))$. The element $g_0 \in \mathrm{SO}(3)$ defined in the previous section maps $\mathcal{S}^d_{\mathbb{C}}$ to $\mathcal{T}^d_{\mathbb{C}}$. Then $\mathcal{T}^u := \pi^{-1}(\mathcal{T}^d) = g_0 \mathcal{S}^u$ in both cases as it is easy to verify.

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 $s \in \mathcal{S}^u$, $g(0)s = s \in \mathcal{S}^u$:

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

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

Hence we obtain the following table:

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

5. Expression for geodesics, controls, and transversality conditions

5.1. **Preliminaries.** As explained in Appendices B and C, candidates for optimal trajectories for the $\mathbf{k} \oplus \mathbf{p}$ problem are only "normal geodesics" and are given by the following formula:

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

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 by (9), and with the notations of Appendix B. Here, $A_p = M_p(0)$ and $A_k = M_k(0)$ are the orthogonal projections of $M(0) = A$ on $\mathbf{p}$ and $\mathbf{k}$ respectively. Geodesics are parametrized by the arclength iff

$$\langle A_p, A_p \rangle = 1. \tag{25}$$

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 $K^{\mathbb{C}}_{g_0} = S(U(1)\times U(2))$, $K^{\mathbb{R}}_{g_0} = S(Z(2)\times O(2))$. Let us note the two following facts.

Facts.

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

Proof. Item 1 comes from right invariance and the fact that the source is a subgroup. Item 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 $g(0) = \mathrm{Id}$.

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

Proof. (With the notations of Appendix B.) Set $I = p_{g(t)}(dL_{g(t)}Ad_{g_0}\mathbf{k}) = dR^*_{g(t)^{-1}}P(t)(dL_{g(t)}\mathrm{Ad}_{g_0}\mathbf{k})$. Then $I = P(t)(\mathrm{Ad}_{g(t)g_0}\mathbf{k}) = \langle M(t), \mathrm{Ad}_{g(t)g_0}\mathbf{k}\rangle$. But:

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

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

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

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

$$\begin{aligned}
I &= \langle \mathrm{Ad}_{e^{-M(0)t}}M(0), \mathrm{Ad}_{g_0}\mathbf{k}\rangle = \langle M(0), \mathrm{Ad}_{g_0}\mathbf{k}\rangle = P(0)(\mathrm{Ad}_{g_0}\mathbf{k}) =\\
&= p_{\mathrm{Id}}(\mathrm{Ad}_{g_0}\mathbf{k}) = 0. \qquad \square
\end{aligned}$$

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

$$N_{1,3}(a_3e^{i\theta_3}) = \begin{pmatrix} 0 & 0 & a_3e^{i\theta_3}\\ 0 & 0 & 0\\ -a_3e^{-i\theta_3} & 0 & 0 \end{pmatrix}. \tag{26}$$

Let us set, in the real-resonant case, $A_p = a_1N_1(1) + a_2N_2(1)$ and $A_k = a_3N_{1,3}(1)$. In the general complex case, we set $A_p = N_1(a_1e^{i\theta_1}) + N_2(a_2e^{i\theta_2})$ and $A_k = a_4Z_3 + a_5Z_4 + N_{1,3}(a_3e^{i\theta_3})$. Here $a_i \in \mathbb{R}$ and $\theta_i \in [-\pi,\pi]$.

5.3. **The real-resonant case (G=SO(3)).**

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

Proof. We have:

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

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

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

$$A^{\pm} = \begin{pmatrix} 0 & \pm 1 & a_3 \\ \mp 1 & 0 & 0 \\ -a_3 & 0 & 0 \end{pmatrix}. \tag{27}$$

Proposition 4. *Geodesics* (24), *for which* $g(0) = \mathrm{Id}$, *with* A *given by formula* (27), *reach the target* $\mathcal{T}^u_{\mathbb{R}}$ *for the smallest time* (*arclength*) $|t|$, *if and only if* $a_3 = \pm 1/\sqrt{3}$. *Moreover, the* 4 *geodesics* (*corresponding to* $A^{\pm}$ *and to the signs* $\pm$ *in* a_3) *have the same length and reach the target at the 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 obtains for the square of the third component of the wave function:

$$\begin{aligned}\big(c_3(t)\big)^2 = {} & (\cos(t a_3)\sin(t\sqrt{1 + {a_3}^2})\, a_3\, \sqrt{1 + {a_3}^2} - \\ & - \cos(t\,\sqrt{1 + {a_3}^2})\,\sin(t\, a_3)(1 + {a_3}^2))^2/(1 + {a_3}^2)^2.\end{aligned} \tag{28}$$

By Lemma 2 in Appendix D, we obtain the result. □

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

$$\begin{cases} c_1(t) = \cos\Big(\dfrac{t}{\sqrt{3}}\Big)^3, \\ c_2(t) = \dfrac{\sqrt{3}}{2}\,\sin\Big(\dfrac{2\,t}{\sqrt{3}}\Big), \\ c_3(t) = -\sin\Big(\frac{t}{\sqrt{3}}\Big)^3. \end{cases} \tag{29}$$

Let us stress that this curve is not a circle on S^2. Controls can be obtained with the following expressions:

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

We obtain

$$\begin{cases} u_1(t) = -\cos\left(\dfrac{t}{\sqrt{3}}\right), \\ u_2(t) = \sin\left(\dfrac{t}{\sqrt{3}}\right). \end{cases} \tag{31}$$

The situation is depicted in Fig. 1.

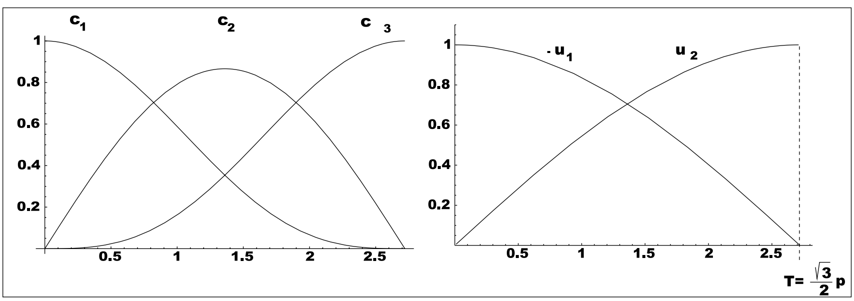

Fig. 1

The result given by formulas (29) and (31) is the same as that of [9], but it has a simpler form. Using expression (19) (resonance hypothesis), we obtain for the external fields:

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

Note that the phases α_1 and α_2 are arbitrary.

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

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

Proof. We have

$$\mathrm{Ad}_{g_0}\mathbf{k}^{\mathbb{C}} = T_{\mathrm{id}}\mathcal{S}^u_{\mathbb{C}} :=$$

$$:= \left\{ \left(\begin{array}{c|cc} i\alpha_1 & 0 & 0 \\ \hline 0 & i(\alpha_2 - \alpha_1) & \beta_1 + i\beta_2 \\ 0 & -\beta_1 + i\beta_2 & -i\alpha_2 \end{array} \right), \alpha_1, \alpha_2, \beta_1, \beta_2 \in \mathbb{R} \right\}.$$

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

Then the covector to be used in formula (24) is as follows:

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

Proposition 6. *Geodesics* (24), *with A given by formula* (33) (*for which* $g(0) = \mathrm{Id}$), *reach the target* $\mathcal{T}^u_{\mathbb{C}}$ *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 optimal controls. The expressions of the three components of the wave function and optimal controls are:

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

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

Remark 13. Again, note that none of these trajectories is a circle on the corresponding (translation of) the sphere S^2. Note 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 cost (14), and this proves Theorem 1 from Introduction.

Formulas (29) and (31) can be obtained from formulas (34) and (36) for $\theta_1 = \pi$ and $\theta_3 = 0$. For the general-complex problem, using expressions (36) in (15), one obtains for the external fields:

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

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

Formula (35) 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 [9] for more details), optimality was set as an assumption while here, it is obtained as a consequence of PMP.

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

6. Appendix A: An interesting consequence of the Cartan decomposition

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

Proof. We can restrict ourselves 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 $\mathbf{p} + [\mathbf{p},\mathbf{p}] = \mathbf{L} \Rightarrow [\mathbf{p},\mathbf{p}] = \mathbf{k}$, $\mathbf{k} + [\mathbf{k},\mathbf{p}] = \mathbf{L} \Rightarrow [\mathbf{k},\mathbf{p}] = \mathbf{p}$. ☐

Note that in general, $[\mathbf{k}, \mathbf{k}] = \mathbf{k}$ is false. In particular, it is false for the Cartan decomposition of su(3) 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 [16] and [17], we recall how to write PMP for a right invariant control system on a Lie group G. We do this for a group of matrices only.

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

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

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 (i.e., a cost that does not depend on g, the coordinate on the group):

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

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

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

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

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

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

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

PMP (see [22]) is a necessary condition for optimality. For right-invariant control systems it has the following form (see [16], [17]).

Theorem 3 (PMP for right invariant control systems)**.** *Consider a couple* $(u(\cdot), g(\cdot)) : [0, T] \to U \times G$ *subjected to dynamics* (37) *and to constraints* (39)*. If it minimizes 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*:

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

$$\frac{dP(t)}{dt} = -ad^*_{dH_{u(t)}(P(t))}(P(t)). \tag{41}$$

Moreover,

$$H_u(t)(P(t)) = \mathcal{H}(P(t)), \quad \textit{where} \;\; \mathcal{H}(P(t)) := \max_{v\in U} H_v(P(t)), \tag{42}$$

$$\begin{aligned} &P(0)(T_{g(0)}M_{\text{in}} \cdot g^{-1}(0)) = 0, \\ &P(t)(T_{g(T)}M_{\text{fin}} \cdot g^{-1}(T)) = 0 \quad (\textit{transversality conditions}). \end{aligned} \tag{43}$$

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 $p_{g(t)} \in T^*_{g(t)}G$ as $P(t) = dR^*_{g(t)}p_{g(t)}$ or $p_{g(t)} = dR^*_{g(t)^{-1}}P_{g(t)}$.

The couples $(u(\cdot), g(\cdot))$ satisfying conditions (40), (41) and (42) with $\lambda = 0$ are called *abnormal extremals*. The 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 sequel 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 and 2. Here $\mathbf{L} = \mathbf{k}\oplus\mathbf{p}$ can also be noncompact (in this case $\mathbf{k}$ must be the maximal compact subalgebra of $\mathbf{L}$, cf. Remark 7).

The Killing form defines a nondegenerate pseudoscalar product on $\mathbf{L}$. This permits to identify $\mathbf{L}$ with $\mathbf{L}^*$ by

$$P \in \mathbf{L}^* \longleftrightarrow M \in \mathbf{L} \Longleftrightarrow P(C) = \text{Kil}(M, C) \;\; \forall C \in \mathbf{L}. \tag{44}$$

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

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

where we have used the invariance of the Killing form under the Lie brackets: $\text{Kil}([A,B],C) = \text{Kil}(A,[B,C])$ that can be easily verified. The equation for $M(t)$ is then in the famous Lax–Poincaré form:

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

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 $f(u) = u_1^2 + \ldots + u_{n_p}^2$ (here $u = (u_1, u_2, \ldots, u_{n_p})$ 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 Eq. (40) and using the fact that the differential of the right translation is a linear isomorphism. Let us consider the second equality. From the maximum condition (42) with $\lambda = -1/2$ and $f(u) = u_1^2 + \ldots + u_{n_p}^2$, we obtain

$$\begin{aligned} u_i(t) = p_{g(t)}(t)(X_i g(t)) = P(t)(X_i) = \mathrm{Kil}(M(t), X_i) = \\ = \mathrm{Kil}(M_p(t), X_i), \quad \text{since} \quad X_i = X_i(e) \in \mathbf{p}. \end{aligned}$$

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

With Proposition 7, the equation for M becomes

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

Using the Cartan commutation relations (8), we have $[M_p(t), M_k(t)] \subset \mathbf{p}$ Eq. (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 $A_p := M_p(0)$ and $A_k := M_k(0)$, we obtain

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

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

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

and the solution is given by (24):

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

Setting $A := A_p + A_k$, we have that the transversality conditions (43) in $\mathbf{L}$ are as follows:

$$\mathrm{Kil}(A, T_{g(0)}M_{in}.g^{-1}(0)) = 0, \tag{48}$$

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

Remark 14 (n-level case). In the case where 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 Eq. (46) becomes

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

where the right-hand side is now 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 satisfy the *Goh condition.*

Definition-Theorem (Goh-condition) 1. *Let* $(p(t), x(t))$, $t \in [0, T]$ *be the Hamiltonian lift of the abnormal extremal* $x(t)$ (*see Theorem* 3). *Then*

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

and a necessary condition for the optimality of $x(\cdot)$ *is*

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

or

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

This theorem is a consequence of a (highly nontrivial) generalized Maslov index theory developed in [4]. For our right invariant problem, relations (50) and (51) give:

$$p(0)(X_i(\mathrm{id})) = 0, \quad p(0)\big([X_i, X_j])(\mathrm{id})\big) = 0,$$

which implies 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. *We 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* $t = \dfrac{k\pi}{\sqrt{1+a^2}}$. *In particular, the smallest* $|t|$ *is obtained for* $k = \pm 1$, $a = \pm\dfrac{1}{\sqrt{3}}$, $t = \dfrac{\pm\pi\sqrt{3}}{2}$.

Proof. We set $\lambda = \dfrac{a}{\sqrt{1+a^2}}$, $\theta = t\sqrt{1+a^2}$; 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 norms ≤ 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 $\theta = k\pi$, $\lambda\theta = \dfrac{\pi}{2} + k'\pi$, $\lambda = \dfrac{1}{2k} + \dfrac{k'}{k}$. Therefore, $\left|\dfrac{1}{2k} + \dfrac{k'}{k}\right| = \lambda < 1$. Conversely, choose k and k' satisfying this condition and $\theta = k\pi$. Then $\cos(\theta) = \pm 1$, $\sin(\lambda\theta) = \pm 1$, $f_a(t) = \pm 1$.

Now, $|t| = \dfrac{k\pi}{\sqrt{1+a^2}}$, and the smallest $|t|$ is obtained for $k = \pm 1$ (if $k = 0$, $\theta = 0$, and $f_a(t) = 0$). Moreover, $\left|\dfrac{1}{2k} + \dfrac{k'}{k}\right| < 1$ is possible only for $(k, k') = (1, 0)$, or $(1, -1)$, or $(-1, 0)$, or $(-1, -1)$.

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

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Authors' addresses:

U. Boscain
E-mail: ugo.boscain@u-bourgogne.fr

T. Chambrion
E-mail: thomas.chambrion@u-bourgogne.fr

J.-P. Gauthier
E-mail: gauthier@u-bourgogne.fr
Département de Mathématiques, Analyse Appliquée et Optimisation, Université de Bourgogne, 9, Avenue Alain Savary B.P. 47870-21078 Dijon Cedex, France