Two applications of geometric optimal control to the dynamics of spin particle

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Summary. The purpose of this article is to present the application of methods from geometric optimal control to two problems in the dynamics of spin particles. First, we consider the saturation problem for a single spin system and second, the control of a linear chain of spin particles with Ising couplings. For both problems the minimizers are parameterized using Pontryagin Maximum Principle and the optimal solution is found by a careful analysis of the corresponding equations.

1 Introduction

The past few years have witnessed an intense recent research activity on the optimal control of the dynamics of spin systems controlled by a radio frequency magnetic field (RF-magnetic field) with application to Nuclear Magnetic Resonance (NMR) spectroscopy and Medical Resonance Imaging (MRI). A pioneer application of geometric optimal control was the contribution to the saturation problem of a single spin system [**?**], where the authors replaced the standard inversion recovery sequence by the time minimal solution formed by a sequence of bang RF-pulses with maximal amplitude and pulses with intermediate amplitude corresponding to singular trajectories in optimal control [**?**]. This result is a consequence of the Pontryagin Maximum Principle [**?**] after performing a reduction to a two dimensional system which allows a complete analysis of the problem.

The first objective of this article is to present in details the geometric tools to analyze this saturation problem as well as some extensions of it in relation with the contrast problem in MRI [**?**, **?**]. The second objective of this article is to discuss the time optimal control of a linear chain of spin particles with Ising couplings [?] in relation with quantum computing. Restricting to the case of three spins we introduce the geometric framework to analyze the problem and we improve the preliminary results contained in [?, ?]. As for the single spin system, the minimizers are parameterized using the Maximum Principle and the optimal solution is computed using the framework of recent developments of invariant sub-Riemannian geometry (SR-geometry) on SO(3) [?].

2 Preliminary: The Pontryagin Maximum Principle

In this section, we recall the necessary optimality conditions [?] which allows us to parameterize the optimal solutions. For our purpose it is sufficient to formulate them in the time minimum case.

2.1 Necessary optimality conditions

Consider the minimum time problem for a smooth control system:

$$\frac{dx}{dt}(t) = f(x(t), u(t)), \tag{1}$$

where $x(t) \in M$, with M a $n-$dimensional manifold, the control domain U is a subset of R^m and the state variable satisfies the boundary conditions $x(0) \in M_0$ and $x(t_f) \in M_1$, with M_0, M_1 being smooth submanifolds of M.

We introduce the pseudo-Hamiltonian:

$$H(x, p, u) = \langle p, f(x, u) \rangle, \tag{2}$$

where $\langle , \rangle$ is the scalar product and $p \in T^*M$ denotes the adjoint vector. The Maximum Principle states that if the trajectory $t \to x(t)$, $t \in [0, t_f]$ associated to the admissible control $u : [0, t_f] \to U$ is optimal, then there exists $p : [0, t_f] \to T^*M$ non zero and absolutely continuous such that the following equations are satisfied almost everywhere on $[0, t_f]$:

$$\frac{dx}{dt}(t) = \frac{\partial H}{\partial p}(x(t), p(t), u(t)) \tag{3}$$

$$\frac{dp}{dt}(t) = -\frac{\partial H}{\partial x}(x(t), p(t), u(t)), \tag{4}$$

as well as the maximum condition:

$$M(x(t), p(t)) = \max_{v \in U} H(x(t), p(t), v) \tag{5}$$

where $H(x(t), p(t), u(t)) = M(x(t), p(t))$. Moreover $M(x(t), p(t))$ is constant along the trajectory and the following boundary conditions are satisfied:

$$x(0) \in M_0,\ x(t_f) \in M_1, \tag{6}$$

$$p(0) \perp T_{x(0)}M_0,\ p(t_f) \perp T_{x(t_f)}M_1 (\text{Transversality conditions}). \tag{7}$$

3 The Saturation Problem

In this section, we recall prior results on the single spin system and introduce the model for multiple spins.

3.1 The case of a single spin and its extensions to systems of spins

The single spin system is modeled by the Bloch equation written in a moving frame and adapted coordinates:

$$\frac{dx}{dt}(t) = -\Gamma x(t) - u_2(t)z(t) \tag{8}$$

$$\frac{dy}{dt}(t) = -\Gamma y(t) + u_1(t)z(t) \tag{9}$$

$$\frac{dz}{dt}(t) = \gamma(1-z(t)) - u_1(t)y(t) + u_2(t)x(t), \tag{10}$$

where $q=(x,y,z)$ represents the magnetization vector restricted to the Bloch ball: $\mid q \mid \leq 1$, (Γ,γ) are the physical parameters which are the signature of the chemical species and satisfies $2\Gamma \geq \gamma > 0$, and $u=(u_1,u_2)$ is the bounded RF-applied magnetic field $\mid u \mid \leq m$.

The objective of the saturation problem is to bring the magnetization vector q from the north pole : $N=(0,0,1)$ (which is the equilibrium point of the free system) to the center $O=(0,0,0)$ of the Bloch ball. The physical interpretation is related to the fact that in MRI, the amplitude $\mid q \mid$ corresponds to a grey level, with $\mid q \mid = 1$ corresponding to white and $\mid q \mid = 0$ to black. A direct generalization of the statement above is to bring the system from a forced equilibrium position (associated to a nonzero fixed constant control) to the center O.

Equations (**??**)-(**??**) can be written in a compact form as an affine control system

$$\frac{dq}{dt}(t) = F(q(t)) + u_1(t)G_1(q(t)) + u_2(t)G_2(q(t)) \tag{11}$$

where F represents the dissipation of the system and the G_i's the controlled vector fields:

$$F(q(t)) = \begin{pmatrix} -\Gamma x(t) \\ -\Gamma y(t) \\ \gamma(1-z(t)) \end{pmatrix}, \quad G_1(q(t)) = \begin{pmatrix} 0 \\ z(t) \\ -y(t) \end{pmatrix}, \quad G_2(q(t)) = \begin{pmatrix} -z(t) \\ 0 \\ x(t) \end{pmatrix}. \tag{12}$$

An extension with application to MRI is to consider an ensemble of N spin systems, associated to the same chemical species (i.e. with the same physical parameters Γ and γ). We denote by $q_s(t), s=1,\ldots,N$, the solutions of the system:

$$\frac{dq_s}{dt}(t) = F(q_s(t)) + (1-\varepsilon_s)\{u_1(t)G_1(q_s(t)) + u_2(t)(G_2(q_s(t))\} \tag{13}$$

where the control $u=(u_1,u_2)$ satisfies $\mid u \mid \leq m$.

The saturation problem for the ensemble of spins is to steer the system from the north pole $N=((0,0,1),\ldots,(0,0,1))$ to the center $O=((0,0,0),\ldots(0,0,0))$ of the products of the Bloch balls. This is equivalent to the saturation problem in MRI, where the amplitude $m(1-\varepsilon_s)$ corresponds to the variation of the applied RF-field induced by the spatial position of the spin s in the image.

3.2 The Saturation problem in minimum time for a single spin

First of all, we observe that due to the symmetry of revolution of the problem with respect to the polarizing $z-$axis we can restrict our analysis to a $2D-$ single-input system:

$$\frac{dy}{dt}(t) = -\Gamma y(t) + u(t)z(t) \tag{14}$$

$$\frac{dz}{dt}(t) = \gamma(1-z(t)) - u(t)y(t), \tag{15}$$

where $\mid u(t) \mid \leq m$. The system can be written as $\frac{dq}{dt} = F(q) + uG(q)$, with $q = (y,z)$.

Applying the Maximum Principle, an optimal solution is found by concatenation of regular and singular arcs defined as follows.

Definition 1. *For a system of the form $\frac{dq}{dt} = F(q) + uG(q)$, the control is said to be:*

- *singular if $\langle p(t), G(q(t))\rangle \equiv 0$, and is determined by differentiating this implicit equation.*
- *regular if $\langle p(t), G(q(t))\rangle \neq 0$, and is given for a.e. t by $u(t) = m\,\mathrm{sign}\langle p(t), G(q(t))\rangle$.*

One denotes by σ_s a singular arc, and by $\sigma_{\pm m}$ bang arcs such that the control is given by $u = \pm m$ and $\sigma_1\sigma_2$ an arc σ_1 followed by an arc σ_2.

The first step is to compute the singular arcs. They satisfy $\langle p(t), G(q(t)\rangle = 0$, and differentiating this equation with respect to time one gets the relations:

$$\langle p(t), G(q(t))\rangle = \langle p(t), [G,F](q(t))\rangle = 0, \tag{16}$$

$$\langle p(t), [[G,F],F](q(t)) + u(t)[[G,F],G](q(t))\rangle = 0, \tag{17}$$

where $[,]$ denotes the Lie bracket.The singular trajectories are therefore located on the set $S = \{q;\ det(G,[G,F])(q) = 0\}$, which is given in our case by $y(-2\delta z + \gamma) = 0$ with the notation $\delta = \gamma - \Gamma$. It is formed by the $z-$ axis of revolution $y = 0$ and the horizontal direction: $z_0 = \gamma/2\delta$.

The singular control is computed as a feedback using (**??**). We have $u(t) = \langle p(t), [[G,F],F](q(t))/[[G,F],G](q(t))\rangle$ which implies:

- For $y = 0$, the singular control is zero and the corresponding system is $\frac{dz}{dt}(t) = \gamma(1-z(t))$. It relaxes to the equilibrium state.
- For $z_0 = \gamma/2\delta$, the feedback singular control is $u_s = \gamma(2\Gamma - \gamma)/2\delta y$ and the dynamics is given by:

$$\frac{dy}{dt}(t) = -\Gamma y(t) - \frac{\gamma^2(2\Gamma - \gamma)}{4(\gamma - \Gamma)^2 y(t)}, \tag{18}$$

and $u_s \to \infty$ when $y \to 0$. The time to steer $(-1,*)$ to $(0,*)$ is given by the integral $T = \int_0^1 \frac{dy}{\Gamma y + \frac{\gamma^2(2\Gamma-\gamma)}{4(\gamma-\Gamma)^2 y}}$ which can be easily computed.

The interesting case in the saturation problem is when the horizontal line $z_0 = \gamma/2\delta$ is such that $-1 < z_0 < 0$ which imposes the following condition on the physical parameters: $2\Gamma > 3\gamma$, and we shall restrict our analysis to this case.

To complete the analysis, we must determine the optimality status of the singular line. It can be small time maximizing (slow) or minimizing (fast). To distinguish the two cases one uses the generalized Legendre-Clebsch condition [**?**] as follows. Let $D'' = det(G,F) = \gamma z(z-1) + \Gamma y^2$ and $C = \{D'' = 0\}$ be the collinear set. If $\gamma > 0$, this set is not reduced to a point, but forms an oval curve joining the north pole $(0,1)$ to the center $(0,0)$ of the Bloch ball and the intersection with the horizontal singular line is empty. Denoting $D = det(G,[[G,F],G])$, the singular lines are fast displacement directions if $DD'' > 0$ and slow if $DD'' < 0$. From this condition one deduces that the $z-$axis of revolution is fast if $1 > z > z_0$ and slow if $z_0 > z > -1$, while the horizontal singular line is fast.

From this analysis, we deduce that the standard inversion sequence: $u(t) = m$ to steer $(0,1)$ to $(0,-*)$ followed by $u(t) = 0$ to relax the system along the $z-$ axis is not time optimal. It has to be replaced by a policy using the horizontal singular line. The complete analysis is not straightforward since $| u_s | \to \infty$ when $y \to 0$ along the singular horizontal line and the singular control saturates the constraint $| u | \leq m$.

The final result is given in Theorem **??**, see [**?**] for more details.

Theorem 1. *In the time minimal saturation problem, the optimal policy is of the form* $\sigma_m \sigma_s \sigma_m \sigma_s$.

Interpretation

The first bang arc is used to move the system from the equilibrium point $(0,1)$ to the horizontal singular line while the second bang arc σ_m connects the horizontal singular arc to the vertical and this occurs before saturating the singular control.

4 The geometry of a linear three spin system with Ising couplings

4.1 Mathematical model

We restrict ourselves to the optimal control of three coupled spins, but the problem can be generalized to a chain with any number of spins. We follow here the presentation of [**?**, **?**].

We introduce the spin 1/2 matrices σ_α, where α represents the number of the particle carrying spin, related to the Pauli matrices by a 1/2 factor. Such matrices satisfy:

$$[\sigma_x, \sigma_y] = i\sigma_z, \;\; \sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1/4. \tag{19}$$

The Hilbert space of the system consists of a dimensional space formed by the tensorial product of the three two dimensional spin 1/2 Hilbert spaces. The Hamiltonian of the system can be written as follows:

$$H = H_C + H_F, \tag{20}$$

where H_C the Hamiltonian of the free system and H_F the Hamiltonian corresponding to the RF-magnetic field are given by

$$H_C = 2J_{12}\sigma_{1z}\sigma_{2z} + 2J_{23}\sigma_{2z}\sigma_{3z} \tag{21}$$

$$H_F = u(t)\sigma_{2y}, \tag{22}$$

with the coefficients J_{ij} representing the coupling constants between the spins i and j.

We consider the time evolution of the vector $X = (x_1, x_2, x_3, x_4)$ where $x_1 = \langle \sigma_{1x} \rangle, x_2 = \langle 2\sigma_{1y}\sigma_{2z} \rangle, x_3 = \langle 2\sigma_{1y}\sigma_{2x} \rangle, x_4 = \langle 4\sigma_{1y}\sigma_{2y}\sigma_{3z} \rangle$ where $\langle \; \rangle$ denotes here the expectation value. To compute the dynamics, we introduce the density matrix ρ, a 8×8-matrix which satisfies :

$$\frac{d\rho}{dt} = -i[H, \rho]. \tag{23}$$

Using the definition of the expectation value of a given operator:

$$\langle O \rangle = Tr(O\rho), \tag{24}$$

one gets:

$$\frac{d}{dt}\langle \sigma_{1x} \rangle = Tr(\sigma_{1x}\frac{d\rho}{dt}) = -iTr(\sigma_{1x}[H,\rho]) = -iTr([\sigma_{1x},H]\rho). \tag{25}$$

Hence we deduce that:

$$\frac{dx_1}{dt} = -J_{12}Tr(2\sigma_{1y}\sigma_{2z}\rho). \tag{26}$$

By rescaling the time by the factor J_{12}, we obtain:

$$\frac{dx_1}{dt} = -x_2. \tag{27}$$

Similar computations lead to the evolution of X given by:

$$\frac{dX}{dt} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & -u & 0 \\ 0 & u & 0 & -k \\ 0 & 0 & k & 0 \end{pmatrix} X, \;\; k = J_{23}/J_{12}. \tag{28}$$

The optimal control problem is to transfer in minimum time the initial position $(1,0,0,0)$ to the position $(0,0,0,1)$ as an intermediate step to realize the transfer in minimum time from σ_{1x} to σ_{3x}. Indeed it connects the first spin to the third one by controlling the second spin.

Introducing the coordinates

$$r_1 = x_1, r_2 = \sqrt{x_2^2 + x_3^2}, r_3 = x_4, \tag{29}$$

and

$$\tan\alpha = x_3/x_2, \tag{30}$$

we obtain the system:

$$\frac{d}{dt}\begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix} = \begin{bmatrix} 0 & -\cos\alpha & 0 \\ \cos\alpha & 0 & -k\sin\alpha \\ 0 & k\sin\alpha & 0 \end{bmatrix} \begin{bmatrix} r_1 \\ r_2 \\ r_3 \end{bmatrix}, \tag{31}$$

where $r = (r_1, r_2, r_3) \in S^2$ (the two dimensional sphere), and $u_1 = -k\sin\alpha$, $u_3 = -\cos\alpha$.

In those coordinates the minimum time problem is equivalent to find the fastest transfer on the sphere from $(1,0,0)$ to $(0,0,1)$. It can be written:

$$\frac{dr_1}{dt} = u_3 r_2, \;\; \frac{dr_2}{dt} = -u_3 r_1 + u_1 r_3, \;\; \frac{dr_3}{dt} = -u_1 r_2, \tag{32}$$

$$\min_{u(.)} \int_0^T (I_1 u_1^2 + I_3 u_3^2) dt, \;\; k^2 = I_1/I_3. \tag{33}$$

This problem is equivalent to a Riemannian problem on the sphere S^2, with a singularity at the equator $r_2 = 0$, the metric being

$$g = \frac{dr_1^2 + k^2 dr_3^2}{r_2^2}. \tag{34}$$

Introducing the spherical coordinates

$$r_2 = \cos\varphi, \qquad r_1 = \sin\varphi\cos\theta, \qquad r_3 = \sin\varphi\sin\theta, \tag{35}$$

where $\varphi = \pi/2$ is the equator, the metric g takes the form

$$g = (\cos^2\theta + k^2\sin^2\theta)d\varphi^2 + 2(k^2-1)\tan\varphi\sin\theta\cos\theta d\varphi d\theta \\ + \tan^2\varphi(\sin^2\theta + k^2\cos^2\theta)d\theta^2,$$

with the associated Hamiltonian

$$H = \frac{1}{4k^2}\{p_\varphi^2(\sin^2\theta + k^2\cos^2\theta) + p_\theta^2\text{cotan}^2\varphi(\cos^2\theta + k^2\sin^2\theta) \\ -2(k^2-1)p_\varphi p_\theta \text{cotan}\varphi\sin\theta cos\theta\}.$$

If $k = 1$, the Hamiltonian takes the form $H = \frac{1}{4}(p_\varphi^2 + p_\theta^2\text{cotan}^2\varphi)$ and describes the standard Grushin metric on S^2.

4.2 Connection with invariant metrics on SO(3) and integration

A first approach consists in lifting the problem on SO(3). We introduce the matrix $R(t) = (r_{ij}(t))$ of SO(3) where $r_1 = r_{11}, r_2 = r_{12}, r_3 = r_{13}$ are the components of the first row and we consider the right-invariant control system:

$$\frac{d}{dt}R^t = \begin{bmatrix} 0 & u_3 & 0 \\ -u_3 & 0 & u_1 \\ 0 & -u_1 & 0 \end{bmatrix} R^t. \tag{36}$$

The first column equation corresponds to our problem. Hence our optimal control problem becomes:

$$\min_{u(.)} \int_0^T (I_1u_1^2 + I_3u_3^2)dt \tag{37}$$

for the right invariant control system with the following boundary conditions:

$$R^t(0) = \begin{bmatrix} 1 & * & * \\ 0 & * & * \\ 0 & * & * \end{bmatrix}, \; R^t(T) = \begin{bmatrix} 0 & * & * \\ 0 & * & * \\ 1 & * & * \end{bmatrix}, \tag{38}$$

and we want to steer the first axis of the frame R^t from e_1 to e_3 , where e_i denotes the canonical basis.

Equivalently, it is transformed into a left-invariant control problem to use the computations in [**?**]:

$$\frac{dR}{dt} = R\begin{bmatrix} 0 & -u_3 & 0 \\ u_3 & 0 & -u_1 \\ 0 & u_1 & 0 \end{bmatrix}, \; \min_{u(.)} \int_0^T (I_1u_1^2 + I_3u_3^2)dt \tag{39}$$

with the corresponding boundary conditions. This defines a left-invariant SR-problem on SO(3) depending on the parameter $k^2 = I_1/I_3$. Upon an appropriated limit process $I_2 \to +\infty$, it is related to the Euler-Poinsot rigid body motion [**?**]:

$$\frac{dR}{dt} = R\begin{bmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{bmatrix}, \; \min_{u(.)} \int_0^T (I_1u_1^2 + I_2u_2^2 + I_3u_3^2)dt \tag{40}$$

which is well-known model for invariant metrics on SO(3) depending on 2 parameters, the ratio I_2/I_1 and I_3/I_1. There are two special cases:

1. The bi-invariant case $I_1 = I_2 = I_3$ where the geodesics solutions are the rotations of SO(3).
2. The case of revolution where $I_1 = I_2$.

The optimal solutions can be parameterized by the Pontryagin maximum principle and thanks to the explicit formula given in [**?**], the solutions can be computed in both the Riemannian and the sub-Riemannian cases using the elliptic functions. See [**?**] for the details of the computations. We here only sketch the main points.

We introduce the following matrices:

$$A_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \ A_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \ A_3 = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{41}$$

with the Lie brackets relations:

$$[A_1, A_2] = -A_3, \ [A_1, A_3] = A_2, \ [A_2, A_3] = -A_1. \tag{42}$$

The optimal control problem is then stated as:

$$\frac{dR}{dt} = \sum_{i=1}^{3} u_i R A_i, \ \min_{u(.)} \int_0^T \sum_{i=1}^{3} I_i u_i^2 dt. \tag{43}$$

Applying the Maximum Principle and denoting by H_i the symplectic lifts of the vector fields RA_i leads to introduce the pseudo-Hamiltonian:

$$H = \sum_{i=1}^{3} u_i H_i - \frac{1}{2} \sum_{i=1}^{3} I_i u_i^2. \tag{44}$$

From the maximization condition $\frac{\partial H}{\partial u} = 0$ we deduce that $u_i = H_i / I_i$, $i = 1, 2, 3$. Plugging back this expression for the controls u_i in the Hamiltonian H defines the true Hamiltonian:

$$H_n = \frac{1}{2}\left(\frac{H_1^2}{I_1} + \frac{H_2^2}{I_2} + \frac{H_3^2}{I_3}\right). \tag{45}$$

Then we derive the Euler equation:

$$\frac{dH_i}{dt} = \{H_i, H_n\}, \tag{46}$$

where $\{,\}$ is the Poisson bracket. Using Lie brackets computations, one obtains:

$$\frac{dH_1}{dt} = H_2 H_3 \left(\frac{1}{I_3} - \frac{1}{I_2}\right), \tag{47}$$

$$\frac{dH_2}{dt} = H_1 H_3 \left(\frac{1}{I_1} - \frac{1}{I_3}\right), \tag{48}$$

$$\frac{dH_3}{dt} = H_1 H_2 \left(\frac{1}{I_2} - \frac{1}{I_1}\right). \tag{49}$$

The SR-case can be derived formally by setting $u_2 = \varepsilon v_2, \varepsilon \to 0$ to obtain a bi-input system. Since $u_i = H_i / I_i$, this is equivalent to $I_2 \to +\infty$. The Hamiltonian reduces to:

$$H_n = \frac{1}{2}\left(\frac{H_1^2}{I_1} + \frac{H_3^2}{I_3}\right), \tag{50}$$

with the corresponding Euler equation where the parameter $k^2 = I_1 / I_3$ is the invariant classifying the SR-metrics.

To get an uniform integration procedure we use the following result from [**?**].

Proposition 1. *For each invariant Hamiltonian on SO(3) (the Riemannian and the SR-case) the system is integrable by quadrature using the four first integrals: the Hamiltonian H_n and the Hamiltonian lifts of the right invariant vector fields $A_i R$.*

Integration

The general algorithm consists in integrating the Euler equation, while the remaining quadrature is deduced using the Euler angles Φ_i defined by taking the following decomposition of a matrix R in SO(3):

$$R = (\exp \Phi_1 \mathrm{A}_3) \circ (\exp \Phi_2 \mathrm{A}_2) \circ (\exp \Phi_3 \mathrm{A}_3) \tag{51}$$

while the angles Φ_2, Φ_3 can be found from the relations:

$$H_1 = - \mid H \mid \sin \Phi_2 \cos \Phi_3,\ \ H_2 = \mid H \mid \sin \Phi_2 \sin \Phi_3,\ \ H_3 = \mid H \mid \cos \Phi_2 \tag{52}$$

and the angle Φ_1 is computed by integrating the differential equation

$$\frac{d\Phi_1}{dt} = \frac{\mid H \mid}{(H_2 \sin \Phi_3 - H_1 \cos \Phi_3)} (\sin \Phi_3 \frac{\partial H_n}{\partial H_2} - \cos \Phi_3 \frac{\partial H_n}{\partial H_1}). \tag{53}$$

In the SR-case, the Euler equation is integrated as follows. We fix the level set of the true Hamiltonian to 1/2: $H_n = 1/2$, and we introduce α such that $\cos\alpha = H_1/\sqrt{I_1}$ and $\sin\alpha = H_3/\sqrt{I_3}$. We obtain the pendulum equation:

$$\frac{d^2\alpha}{dt^2} = \frac{k^2-1}{2I_1} \sin 2\alpha,\ \ k^2 = I_1/I_3. \tag{54}$$

Details of the parameterizations of the solutions are given in [**?**]. The computations in the Riemannian case are standard [**?**, **?**].

In conclusion, in the spin time optimal problem the optimal solutions can be found among extremals solutions of the Maximum Principle.

4.3 Direct integration on the sphere

We identify S^2 as the homogenous space SO(3)/SO(2) . In this interpretation, the Hamiltonian $\mid H \mid^2 = H_1^2 + H_2^2 + H_3^2$ corresponds to the bi-invariant case and represents the Casimir function which commutes with the Hamiltonian associated to every invariant Riemannian and sub-Riemannian metrics.

On the homogeneous space this defines the round sphere with constant curvature $+1$, whose metric in spherical coordinates is given by :

$$g = d\varphi^2 + \sin^2\varphi d\theta^2 \tag{55}$$

and with Hamiltonian

$$F = p_\varphi^2 + \frac{p_\theta^2}{\sin^2\varphi}. \tag{56}$$

We have the following result.

Lemma 1. *Consider the standard Grushin metric on S^2 with Hamiltonian $H_0 = p_\varphi^2 + p_\theta^2 \mathrm{cotan}^2\varphi$. Then $\{H_0, F\} = 0$ where F is the Hamiltonian of the round metric on S^2, $F = p_\varphi^2 + \frac{p_\theta^2}{\sin^2\varphi}$.*

Proof. Using the symmetry of revolution of the Grushin metric, we have that p_θ is a constant (Clairaut relation). Hence p_θ^2 is a constant. Therefore $p_\varphi^2 + \frac{\cos^2\varphi}{sin^2\varphi} p_\theta^2 + p_\theta^2$ is a constant, which means that F is a first integral .

Up to a constant renormalization the Hamiltonian becomes:

$$H = H_0 + k^* H', \;\; k^* = k^2 - 1, \tag{57}$$

where

$$H' = G^2, \;\; G = p_\varphi \cos\theta - p_\theta \text{cotan}\varphi \sin\theta. \tag{58}$$

We have the following.

Proposition 2. *The following relations are satisfied:*

$$\{H_0, F\} = \{G, F\} = 0. \tag{59}$$

Therefore, $\{H, F\} = 0$ *for each* k^*.

Integration

To integrate the geodesic flow we use the standard Birkhoff method, see [**?**, **?**] for the details. The Hamiltonian H admits a first integral F which is quadratic in p and corresponds to a Liouville metric on S^2. The metric is written in the isothermal form:

$$g = \lambda(x,y)(dx^2 + dy^2) \tag{60}$$

outside the equator using a rescaling of r_3.

Any diffeomorphism

$$x = \varphi(u,v), \;\; y = \psi(u,v) \tag{61}$$

which is preserving the isothermal form and the orientation satisfies the Cauchy-Riemann relation:

$$\varphi_u = \psi_v, \;\; \varphi_v = -\psi_u. \tag{62}$$

In the isothermal coordinates, the first integral becomes:

$$F(x,y) = b_1(x,y)p_x^2 + 2b_2(x,y)p_x p_y + b_3(x,y)p_y^2. \tag{63}$$

We introduce:

$$R = (b_1 - b_3) + 2ib_2 \tag{64}$$

which is an holomorphic function of $z = x + iy$ using Birkhoff's relations [**?**]. Let us denote

$$w = u + iv, \tag{65}$$

and let us introduce the holomorphic change of variables

$$\Phi : w \to z. \tag{66}$$

We obtain

$$p_x = D(p_u \psi_v - p_v \psi_u), \;\; p_y = D(-p_u \varphi_v + p_v \varphi_u), \tag{67}$$

with

$$D = (\varphi_u \psi_v - \psi_u \varphi_v)^{-1}. \tag{68}$$

Expressing F in the (u,v) coordinates we have:

$$F(u,v) = p_u^2 b_1'(u,v) + 2p_u p_v b_2'(u,v) + p_v^2 b_3'(u,v). \tag{69}$$

An easy computation shows that:

$$S = (b_1' - b_3' + 2ib_2') = D^2(\varphi_u - i\psi_u)^2(b_1 - b_3 + 2ib_2) \tag{70}$$
$$= (\varphi_u + i\psi_u)^{-2}(b_1 - b_3 + 2ib_2). \tag{71}$$

We choose the change of coordinates such that we have the following normalization: $S = 1$. Hence, we must solve the equation

$$(\varphi_u + i\psi_u) = \sqrt{R(z)}. \tag{72}$$

In the new coordinates the metric takes the Liouville normal form:

$$g(u,v) = (f(u) + g(v))(du^2 + dv^2), \tag{73}$$

and the integration is standard see for instance [**?**].

Grushin Singularity

The family of metrics g is defined as a metric on the distibution $\Delta = \text{Span}\{F_1, F_3\}$ where F_1, F_3 are respectively the vector fields corresponding to rotations with axis e_1 and e_3. By construction such a metric has a Grushin singularity [**?**] at the equator E where rankΔ is one and the distribution is transverse to the equator. The local normal form near a point of the equator is described in the aforementioned article. Hence our family of metrics defines an almost-Riemannian metric on the sphere with Grushin singularity at the equator.

4.4 The optimality problem

We discuss briefly in this section the optimality problem which can be handled using the technical framework developed in [**?**] combining geometric analysis and numerical techniques.

We use the following concepts. On the almost-Riemannian manifold (S^2, g), the cut point along a geodesic curve γ, projection of an extremal curve solution of the Maximum Principle, emanating from $q_0 \in S^2$ is the first point where it ceases to be minimizing and we denote $C_{cut}(q_0)$ the set of such points forming the cut locus. The first conjugate point is the point where it ceases to be minimizing among the geodesics C^1- close from γ and we denote $C(q_0)$ the set of such points, forming the conjugate locus.

Our optimality problem amounts to transfer with minimum length the point $q_0 = (1,0,0)$ given by $\varphi_0 = \pi/2, \theta_0 = 0$ in spherical coordinates to the point $q_1 = (0,0,1)$ defined by $\varphi_1 = \pi/2, \theta_1 = \pi/2$. In particular the problem is solved by computing the cut locus $C(q_0)$ of the equatorial point.

First, we have the following lemma.

Lemma 2. *The family of metrics g depending upon the parameter k have a discrete symmetry group defined by the two reflexions : $H(\varphi, p_\varphi) = H(\pi - \varphi, -p_\varphi)$ (reflexion with respect to the equator) and $H(\theta, p_\theta) = H(-\theta, -p_\theta)$ (reflexion with respect to the meridian $\theta = 0$).*

The next step is to use the Grushin singularity resolution described in [**?**] and the previous symmetries.

Proposition 3. *Near q_0 identified to* 0, *the conjugate and cut loci for the metric restricted to a neighborhood of* 0 *can be computed using the local model* $dx^2 + \frac{dy^2}{x^2}$. *The cut locus is a segment* $[-\varepsilon, +\varepsilon]$ *minus* 0 *while the conjugate locus is formed by four symmetric curves of the form* $x = cy^2$ *minus* 0 *and tangential to the meridian* $\theta_0 = 0$ *(although the Gaussian curvature is strictly negative and tends to* $-\infty$ *at the equator).*

In [**?**] the cut and conjugate loci in the Grushin case $k = 1$ on S^2 of an equatorial point are completely described making an homotopy $g_\lambda = d\varphi^2 + G_\lambda(\varphi)d\theta^2$, $G_\lambda(\varphi) = \frac{\sin^2\varphi}{(1-\lambda\sin^2\varphi)}$, $\lambda \in [0,1]$ from the round metric to the Grushin case which explains in particular the curvature concentration at the equator in the Grushin case. We get the following result.

Proposition 4. *In the Grushin case* $k = 1$, *the cut locus of the equatorial point* $\varphi_0 = \pi/2, \theta_0 = 0$ *is the whole equator minus this point while the conjugate locus has a double heart shape, with four meridional singularities, two at the origin described previously and two cusps on the opposite meridian.*

The general case is studied in [**?**] using a continuation method on the conjugate locus starting from a Grushin case (observe also that the cut locus is decribed in [**?**] using the equatorial symmetry). From the geometric point of view the neat framework is given by recent works to describe the conjugate and cut loci on Liouville surfaces generalizing the ellipsoid case [**?**, **?**].

Note the following result that can be easily proved .

Proposition 5. *For every* k^*, *the cut locus of the equatorial point is the equator minus the point.*

Proof. A simple computation shows that the Gaussian curvature in each hemisphere is strictly negative. Hence there is no conjugate point for a geodesic starting form the equatorial point before returning to the equator. Due to the reflectional symmetry with respect to the equator, two geodesics starting from the equatorial point intersects with same length when returning to the equator. This proves the result.

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