Selective and Robust Time Optimal SO(3)-Transformations

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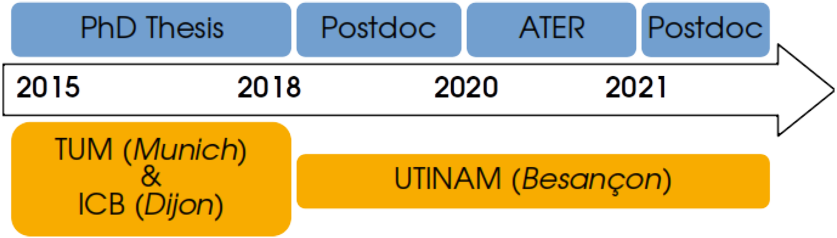
Self introduction

Career :



PhD Thesis : Steffen Glaser & Dominique Sugny.

Postdocs / ATER : Bruno Bellomo, Dominique Sugny, David Viennot, José Lages, Dima Shepelyansky, Alexei Chepelianskii.

Fields of research

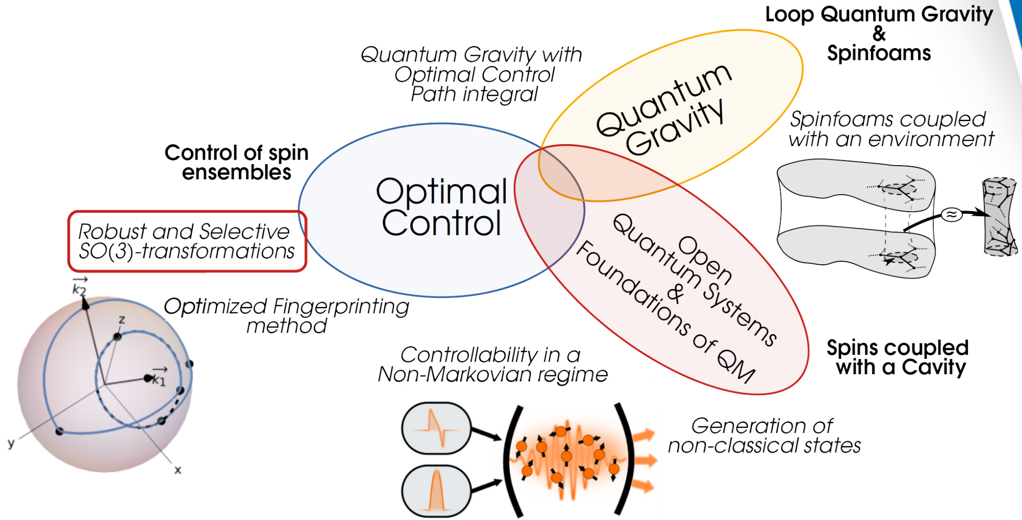


Table of Contents

Optimal Control of Spin-1/2 Particles: Motivations

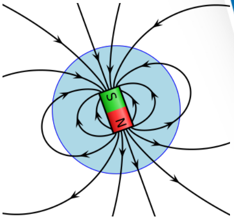
Spin-1/2 particles and magnetization vector

Spin-1/2 particle

A spin-1/2 particle can be considered as an "elementary magnetic dipole" (source of the magnetic field), which can be described (at least in our case study), by its magnetization vector $\vec{M} = (M_x, M_y, M_z) \in \mathbb{R}^3$.

Dynamics of a *single* spin-1/2 can be modeled using the Bloch equation (without relaxation):

$$\frac{d\vec{M}}{dt} = -\gamma \vec{B}(\vec{q}, t) \wedge \vec{M}(t).$$

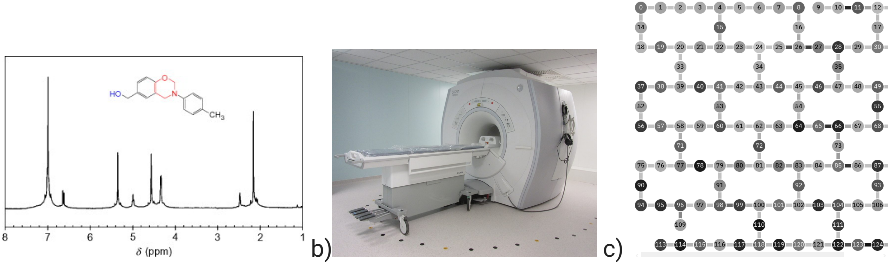


With $\vec{B}(\vec{q}, t) \in \mathbb{R}^3$ a position and time dependent magnetic field, $\gamma \in \mathbb{R}_+$ is the gyromagnetic ratio, and $\wedge$ denotes the vector cross product.

Spin-1/2 and applications

Behaviors of spin-1/2 systems (or 2 level quantum systems) are at the core of many technologies. For examples:

- **Magnetic Resonance Spectroscopy**
- **Magnetic Resonance Imaging**
- **Quantum Computing**



a) b) c)

Figure 1: a) NMR spectrum b) a MRI scanner and c) Structure of IBM's 127-qubits processor.

Control of Spin-1/2 particles

Global idea:

Input (E.M. field)	$\rightarrow$	Ensemble of spins $(N_s \geq 1)$ $\uparrow$ Environement	$\rightarrow$	Output (back-reaction of the ensemble to the E.M. field)

Environment:

- decoherence
- Inhomogeneity of the physical parameters : resonance frequency, interaction strength,...

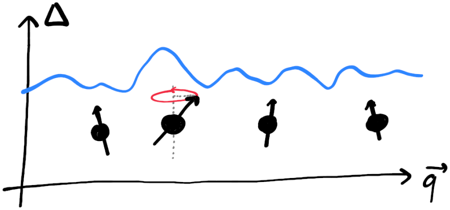
Usually, the environment reduces the fidelity of the output with respect to the expected/idealized result.

An example of inhomogeneity effect

In a given rotating frame, we can rewrite the Bloch equation into:

$$\frac{d\vec{M}}{dt} = -\begin{pmatrix} \omega_x(t,\vec{q}) \\ \omega_y(t,\vec{q}) \\ \Delta(\vec{q}) \end{pmatrix} \wedge \vec{M}(t).$$

with Δ the offset from a given frequency ω_z of reference. ω_x and ω_y are two control fields.



An example of inhomogeneity effect

- Bloch's equation:

$$\frac{d\vec{M}}{dt} = -\begin{pmatrix} \omega_x(t,\vec{q}) \\ \omega_y(t,\vec{q}) \\ \Delta(\vec{q}) \end{pmatrix} \wedge \vec{M}(t).$$

- We can perform simple rotations of the Bloch vector using ω_x and ω_y constant over a time interval.
- **Example:** for $\Delta = 0$, $\vec{M}(0) = (0,0,1)$, and using $\omega_x T = \pi/2$, $\omega_y = 0$, we have $\vec{M}(T) = (0,1,0)$. The solution is not robust against modifications of Δ.
- Square pulse
- Optimal pulse

Introduction to Optimal Control Theory

General statement

- Let us consider a system whose physical configuration (at time t) is modeled by a vector $x(t) = \{x^a(t)\}_{a=1..n} \in \mathbb{R}^n$, and is controlled by a control field $u(t) \in \mathbb{R}^m$.
- System dynamics are governed by the differential equation:

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

- The goal is to transform the initial state $x(0) = x_0$ into a target state x_{target} at $t = t_f \geq 0$, by using only the control field u, while minimizing one or several quantities, called *cost function* (or *figure of merit*).

General statement

Cost functions can be decomposed into two different categories:

Terminal cost
A function $h(x(t_f), t_f)$ that depends only on the final state.

Dynamical cost
A functional:

$$\int_0^{t_f} f_0(x(t), u(t), t)dt.$$

It can depend on the entire trajectory of x and u.

A general cost function is:

$$F = h(x(t_f), t_f) + \int_0^{t_f} f_0(x(t), u(t), t)dt. \quad (2)$$

General statement

Problem

How can we determine: $u^\star = \min_u F$, such that $\frac{dx^a}{dt} = f^a(x, u, t)$?

Looks like classical mechanics! $\rightarrow$ calculus of variation...

...but, we have a few differences:

- We have two quantities x and u, which are not treated exactly in the same manner.
- There is no natural canonical momentum $\rightarrow$ *"usual" Lagrangian may not be useful*.

The "optimal control trick"

We consider an extended state of configuration $X = (x, \dot{x}, p, \dot{p}, u, \dot{u})$, where $p \in \mathbb{R}^n$ is called the adjoint sate of x.

We define a Lagrangian $L(X(t))$, and an action S:

$$S = \int_{t_0}^{t_f} L(X)\, dt = \int_{t_0}^{t_f} dt \left[f_0(x, u, t) + p_a \left(\dot{x}^a - f^a(x, u, t) \right) \right] \tag{3}$$

Note:

- Einstein's notation is used.
- p plays the role of Lagrange multipliers.
- By construction of L, we have extremums of S when $\dot{x}^a = f^a$.

> See: *M.Contreras, & al., 'Dynamic Optimization and Its Relation to Classical and Quantum Constrained Systems', Physica A, 479 (2017)*, for a detailed and pedagogical discussion.

Euler-Lagrange equations

Minimization of the action $S \to$ Computation of the first order variations of S from an arbitrary trajectory of reference.

Theorem 1

Let $\mathbf{C}$ be the set of all curves $X : [t_i, t_f] \to \mathbb{R}^n$ of class C^2. Let $\gamma \in \mathbf{C}$ be a *reference* curve with extremities (t_0, x_0), (t_1, x_1). Let $\gamma' \in \mathbf{C}$ be *another* curve with extremities $(t_0 + \delta t_0, x_0 + \delta x_0)$, $(t_1 + \delta t_1, x_1 + \delta x_1)$. We define $h(t) = \gamma'(t) - \gamma(t)$. Then, if we set $\Delta S = S(\gamma') - S(\gamma)$, we have:

$$\Delta S = \int_{t_0}^{t_1} \left(\frac{\partial L}{\partial X^a} - \frac{d}{dt}\frac{\partial L}{\partial \dot{X}^a} \right)_{|\gamma} h^a dt + \left[\frac{\partial L}{\partial \dot{X}^a}_{|\gamma} \delta X^a \right]_{t_0}^{t_1}$$

$$+ \left[\left(L - \frac{\partial L}{\partial \dot{X}^a} \dot{X}^a \right)_{|\gamma} \delta t \right]_{t_0}^{t_1} + o^2(D(\gamma, \gamma'))$$

With $D(\gamma, \gamma')$ a distance between the curves in $\mathbf{C}$.

Euler-Lagrange equations

We consider the case of fixed boundaries (i.e. $\delta X^a = 0$ ans $\delta t = 0$).

Then, extremums of S, given by $\Delta S = 0$, are characterized by the *Euler-Lagrange* equation:

$$\frac{\partial L}{\partial X^a} - \frac{d}{dt}\frac{\partial L}{\partial \dot{X}^a} = 0.$$

Application to the O.C. Lagrangian:

$$\begin{cases} \dfrac{\partial L}{\partial x^a} - \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{x}^a} = 0 \\ \dfrac{\partial L}{\partial p_a} - \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{p}_a} = 0 \\ \dfrac{\partial L}{\partial u^c} - \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{u}_c} = 0 \end{cases} \Rightarrow \begin{cases} \dot{p}_a = \dfrac{\partial}{\partial x^a}(f_0 - f^b \delta^a{}_b) \\ \dot{x}^a = f^a \\ \dfrac{\partial f_0}{\partial u^c} = p_b \dfrac{\partial f^b}{\partial u^c}. \end{cases} \qquad (4)$$

The equation $\frac{\partial f_0}{\partial u^c} = p_b \frac{\partial f^b}{\partial u^c} \longrightarrow$ **allows us to determine** $u(t) = u(x(t), p(t))$.

Hamiltonian formalism

Equivalently, we can use the Hamiltonian formalism:

Hamiltonian

$$H_p = P_a \dot{X}^a - L$$
$$= p_a f^a - f_0 + p_{u,c} \dot{u}^c,$$

with $p_{u,c}$ the adjoint state of the control field, that we can set to 0 in our case, because there is no constraint of the form $\dot{u}^c = \ldots$.

Hamilton's equations

$$\frac{\partial H_p}{\partial X^a} = -\dot{P}_a \; ; \; \frac{\partial H_p}{\partial P^a} = \dot{X}^a$$

Hamiltonian formalism

The correspondence between the equations of dynamics is then:

$$\begin{cases} \dfrac{\partial L}{\partial x^a} - \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{x}^a} = 0 \\ \dfrac{\partial L}{\partial p_a} - \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{p}_a} = 0 \\ \dfrac{\partial L}{\partial u^c} - \dfrac{d}{dt}\dfrac{\partial L}{\partial \dot{u}_c} = 0 \end{cases} \Leftrightarrow \begin{cases} \dfrac{\partial H_p}{\partial x^a} = -\dot{p}_a \\ \dfrac{\partial H_p}{\partial p_a} = \dot{x}_a \\ \dfrac{\partial H_p}{\partial u^c} = 0 \end{cases} \Rightarrow \begin{cases} \dot{p}_a = \dfrac{\partial}{\partial x^a}(f_0 - f^b \delta^a{}_b) \\ \dot{x}^a = f^a \\ \dfrac{\partial f_0}{\partial u^c} = p_b \dfrac{\partial f^b}{\partial u^c}. \end{cases}$$

Theorem 2

Weak Pontryagin Minimum (Maximum) Principle (**PMP**) :

$$\frac{\partial H_p}{\partial u^c} = 0.$$

The case of bounded control fields

In the case where the control field is in $U \subset \mathbb{R}^m$

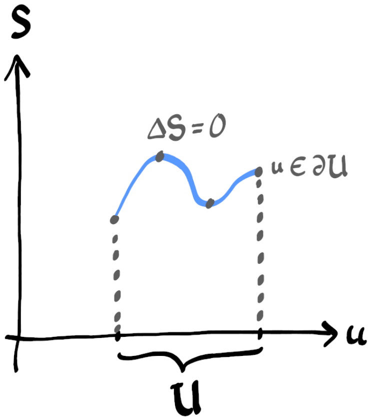
Theorem 3

The general PMP :

$$\frac{\partial H_p}{\partial u^c} = 0$$

or

$$u(t) \in \partial U.$$



Summary

- Control field $\rightarrow$ generalized coordinates.
- Introduce the adjoint state p.
- Extremums of the action $\rightarrow$ equations of dynamics in the extended space of configurations.
- The PMP provides constrains on the control field, which can be expressed as a function of the state x and its adjoint state p.

Optimization problem $\rightarrow$ analysis of trajectories of a classical dynamical system.

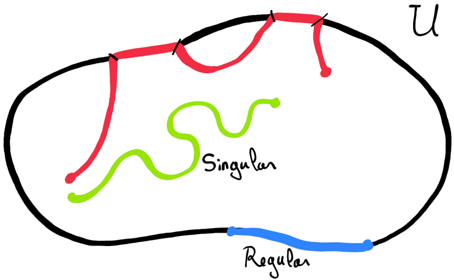
Classification of trajectories

Singular trajectory

The trajectory of the extended system X is said singular on $I = [t_1, t_2]$ if $\frac{\partial H_p}{\partial u^c} = 0 \; \forall t \in I$.

Regular trajectory

The trajectory of the extended system X is said regular on $I = [t_1, t_2]$ if $u(t) \in \partial U \; \forall t \in I$.



Selective and Robust Time Optimal SO(3) Transformations

SO(3) transformations

Due to the cross product in the Bloch equation, we have $\vec{M}(t) = \hat{U}(t)\vec{M}(0)$ and $\hat{U}(t) \in SO(3)$.
$\hat{U}(t)$ is the solution of the differential equation:

$$
\begin{aligned}
\frac{d\hat{U}(\Delta,t)}{dt} &= \begin{pmatrix} 0 & \Delta & -\omega_y(t) \\ -\Delta & 0 & \omega_x(t) \\ \omega_y(t) & -\omega_x(t) & 0 \end{pmatrix} \hat{U}(\Delta,t) \\
&= \left(\omega_x(t)\hat{\epsilon}_x + \omega_y(t)\hat{\epsilon}_y + \Delta\hat{\epsilon}_z\right)\hat{U}(\Delta,t), \\
\hat{U}(\Delta,0) &= \hat{\mathbb{I}},
\end{aligned} \tag{5}
$$

- $\Delta \in \mathbb{R}$ is the frequency offset (resonance at $\Delta = 0$).
- $\omega_x(t) \in \mathbb{R}$ and $\omega_y(t) \in \mathbb{R}$ are two control fields such that $\omega_x(t)^2 + \omega_y(t)^2 \leq \omega_0^2$.
- $\hat{\epsilon}_x$, $\hat{\epsilon}_y$ and $\hat{\epsilon}_z$ are generators of the $\mathfrak{so}(3)$ algebra.
- $\hat{\mathbb{I}}$ is the identity matrix.

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The control problem

$$\frac{d\hat{U}(\Delta,t)}{dt} = (\omega_x(t)\hat{\epsilon}_x + \omega_y(t)\hat{\epsilon}_y + \Delta\hat{\epsilon}_z)\,\hat{U}(\Delta,t), \qquad (6)$$
$$\hat{U}(\Delta,0) = \hat{\mathbb{I}},$$

- At resonance ($\Delta = 0$) we would like to produce a transformation of the form $\hat{U}_{target}(0) = e^{\phi\hat{\epsilon}_x}$ at the final time T.
- For $\Delta \neq 0$, we have in general $\hat{U}(\Delta,T) \neq e^{\phi\hat{\epsilon}_x}$.

To quantify the selectivity or robustness of a control field, we introduce the following fidelity function:

$$F(\Delta) = \|\hat{U}(\Delta,T,\omega_x,\omega_y) - \hat{U}_{target}(\Delta = 0)\|^2, \qquad (7)$$

where $\|\cdot\|$ is the Frobenius norm.

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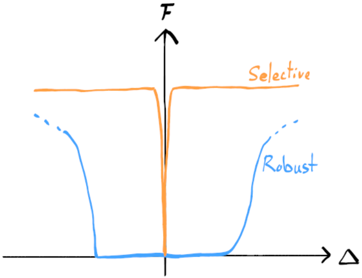
The control problem

Robust transformation

A transformation is said "robust" on the interval $I = [\Delta_a, \Delta_b]$ if for all $\Delta \in I$, $F(\Delta) \leq \varepsilon$, with ε quantifying the maximum permissible error.

Selective transformation

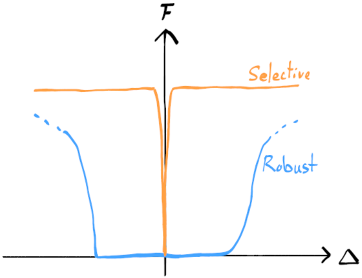
A transformation is said "selective" if it produces the desired $\hat{U}_{target}$ at $\Delta = 0$, and leaves the system unchanged for $\Delta \neq 0$, i.e. $\hat{U}(\Delta, T) \approx \hat{\mathbb{I}}$ for $\Delta \neq 0$.



State-of-the-art approach

1. Discretize the Δ axis, specify a target state $\hat{U}_{target}(\Delta)$ at each discretization point, and solve the optimal control problem simultaneously for all the points. *This requires (in general) a lot of points.*

2. Taylor expand F, and cancel the first-order derivatives around a specific value of Δ, i.e. $\frac{\partial^n F}{\partial \Delta^n}|_{\Delta=\Delta'} = 0, n = 1, 2, ..., n_{max}$. *Works well for robust controls, less for selective ones.*



A novel approach

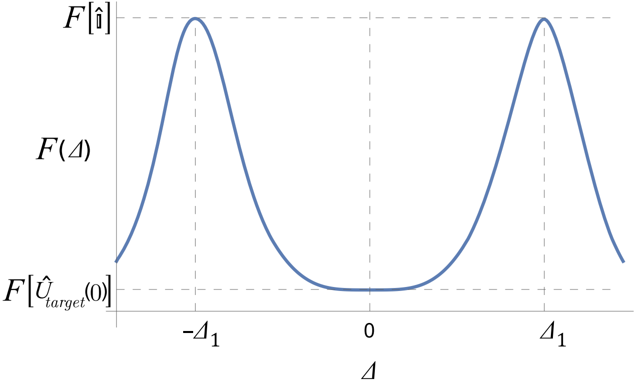
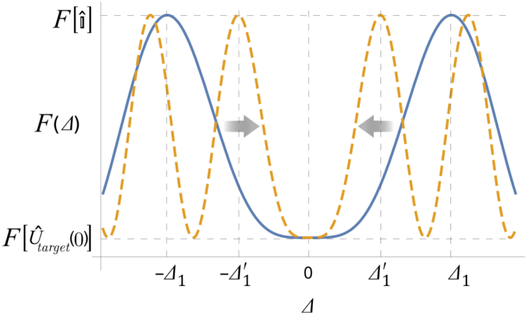


Figure 2: Example of fidelity function

$$F(\Delta) = \|\hat{U}(\Delta, T, \omega_x, \omega_y) - \hat{U}_{target}(\Delta = 0)\|^2 \quad (8)$$

A novel approach



As a first approximation, we can focus on **only two offsets**: $\Delta = 0$, and $\Delta = \Delta_1$.
The target states are:

$$\hat{U}_{target}(0) = e^{\phi \hat{\epsilon}_x} \quad ; \quad \hat{U}_{target}(\Delta_1) = \hat{\mathbb{I}}. \tag{9}$$

The position of Δ_1 sets the level of robustness/selectivity of the control sequence.

Definition of OC quantities

The terminal cost function is $C = \frac{1}{6}\sum_{n=1}^{2} \|\hat{U}_n(T,\omega_x) - \hat{U}_{n,target}\|^2$.
The dynamical cost function is: $\int_0^T dt = T$.
The Hamiltonian is:

$$H_p = \sum_{n=1}^{2} \langle \hat{P}_n | \omega_x \hat{\epsilon}_x + \Delta_{(n)} \hat{\epsilon}_z | \hat{U}_n \rangle.$$

- $\hat{P}_n$ is a 3×3 matrix, which is the adjoint state of $\hat{U}_n$.
- $\langle A|B \rangle = \mathrm{Tr}[A^\intercal B]$ is the matrix scalar product.
- **For symmetry reasons, we can set $\omega_y = 0$, and keep only a single control ω_x.**

Structure of trajectories

Proposition 1
Singular trajectories S are given by constant controls of amplitude $|\omega_S| < \omega_0$.

Proposition 2
Regular trajectories are given by piecewise constant control fields of amplitude $\pm\omega_0$, with switchings when $l_x = \sum_{n=1}^{2} \langle \hat{P}_n | \hat{\epsilon}_x | \hat{U}_n \rangle = 0$.

A constant part of a regular trajectory is called "a bang" B.

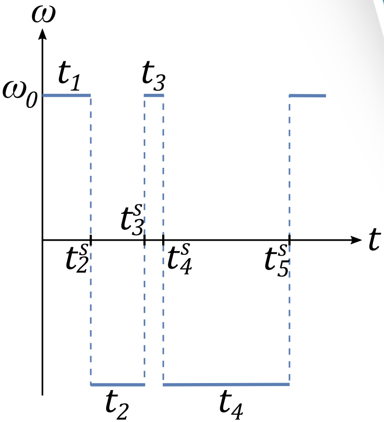


Figure 3: Structure of a regular control field with several switchings.

General expression of $\hat{U}$

Because the control field is piecewise constant, we have:

$$\hat{U}(T) = \prod_{j=1}^{N_p} e^{(\omega_j \hat{\epsilon}_x + \Delta \hat{\epsilon}_z) t_j}, \quad \omega_j \in [-\omega_0, \omega_0]\ ,\ t_j > 0. \tag{10}$$

In the case of a single singular trajectory, we have:

$$\hat{U}(\Delta, T_S) = e^{T_S(\omega_S \hat{\epsilon}_x + \Delta \hat{\epsilon}_z)}, \tag{11}$$

and the target states are reached if:

$$\begin{cases} T_S \omega_S = \phi \\ T_S \sqrt{\omega_S^2 + \Delta_1^2} = 2k\pi,\ k \in \mathbb{N}. \end{cases} \tag{12}$$

We define Δ_0, the smallest solution of (12), such that $\omega_S = \omega_0$. And we denote by T_0 the corresponding control duration.

Selective Time Optimal Transformations

Selective Time Optimal transformations

Due to the specific structures of the trajectories, **we define selective controls such that:** $\Delta_1 \leq \Delta_0$. At the opposite $\Delta_1 \geq \Delta_0$ is used for robust controls.

Proposition 3

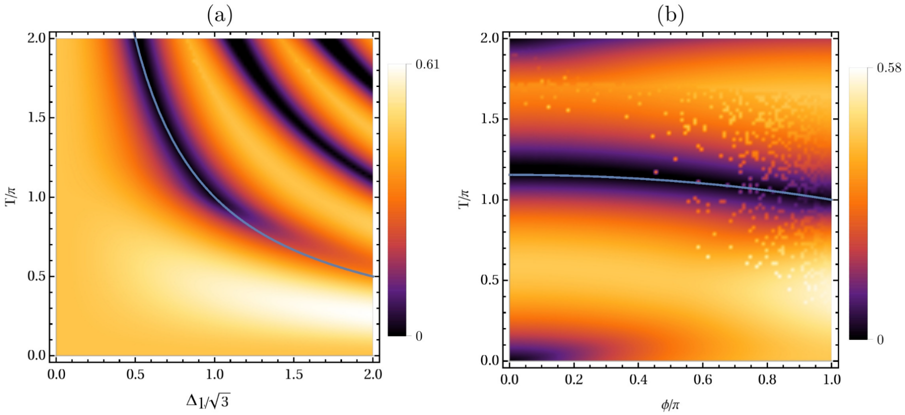
In the selective case, the following trajectories are not time-optimal:

- $B - B$
- $B - B - B$
- $B - B - B - B$
- $S - B$
- $B - S - B$
- $B - ... - B - S - ...$

Conjecture 1

Time-optimal **selective** transformations are given by **singular** trajectories S of Pontryagin's Hamiltonians.

Selective Time Optimal transformations



(a): C as a function T and Δ_1, for a selective rotation of angle $\phi = \pi$ and $\omega_0 = 1$. (b): C as a function of T and ϕ. We set $\omega_0 = 1$ and $\Delta_1 = \sqrt{3}$. In the two cases, each point of the contour plot corresponds to a numerical optimization. Blue solid lines are defined by the equation $\Delta_1 = \sqrt{4\pi^2 - \phi^2}/T_S$.

Robust Time Optimal Transformations

Robust Time optimal transformations

We consider $\Delta_1 > \Delta_0$

Time-optimal robust transformations

Time optimal **robust** transformations are given by **regular** trajectories.

For a regular control, the general form of $\hat{U}$ is:

$$\hat{U}(T) = \prod_{j=1}^{N_p} e^{(\omega_j \hat{\epsilon}_x + \Delta \hat{\epsilon}_z) t_j}, \quad \omega_j = \pm \omega_0 \ , \ t_j > 0.$$

Calculations can be performed for a small number of switchings (i.e., $Np = 2, 3$).

1-switching regular controls

- Using the the fact that $\hat{U}_{target}(0) = e^{\phi \hat{\epsilon}_x}$ and $\hat{U}_{target}(\Delta_1) = \hat{\mathbb{I}}$, we can determine the durations t_1 and t_2 of each bang:

$$t_1 = t_2 + \frac{\phi}{\omega_0} \; ; \; t_2 = \frac{\phi}{2\omega_0}\left(\frac{n}{k} - 1\right)$$

- The pulses are then parameterized by two integers: n and k.

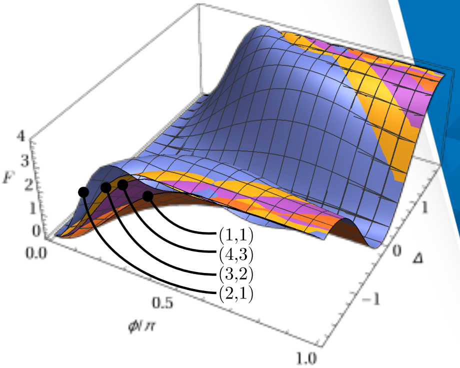


Figure 4: Fidelity of 1-switching controls for different (n, k).

2-switchings regular controls

- Similarly, we can determine the duration t_1, t_2 and t_3 of each bang:

$$t_1 + t_3 = \frac{\phi}{\omega_0}\left(\frac{n}{k} - 1\right)\ ;\ t_1 = \alpha t_3\ ;$$

$$t_2 = (t_1 + t_3) + \phi/\omega_0$$

- The pulses are then parameterized by two integers: n and k, and one real parameter α.
- Using $\frac{\partial^2 F}{\partial \Delta^2}(0) = 0$, we can find the optimal α. For $\phi = \pi$, $\alpha = 1$.

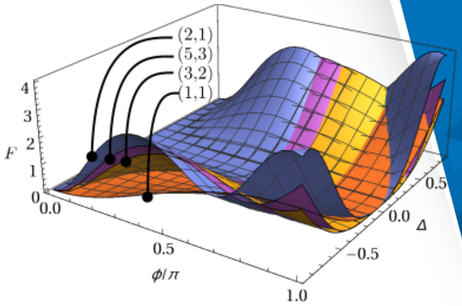


Figure 5: Fidelity of 2-switching controls for different (n, k), and $\alpha = 1$.

2-switchings regular controls

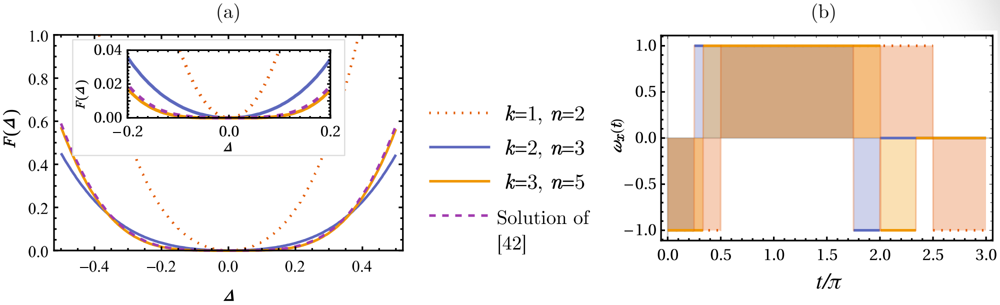


Figure 6: (a) Fidelity function F for a π-pulse for different values of (n, k), and for the solution of [42] (obtained with a numerical optimization). The inset shows F near $\Delta = 0$. (b) Control field associated with each solution. Control times are respectively: 3π, 2π , 2.34π, 2.34π (top to bottom in the legend).

[42] L. Van Damme, & al, Phys. Rev. A, 95:063403, Jun 2017.

Conclusion

Conclusion

- Design of selective and robust $SO(3)$-transformations.
- Computations are based on a model of two matrices of rotation, associated with two different offsets.
- Time optimal selective transformations are given by constant control fields of amplitude $|\omega_S| < \omega_0$.
- Robust transformations are given by regular "bang-bang" control fields parameterized by a few parameters. It is then easy to find a "good solution".

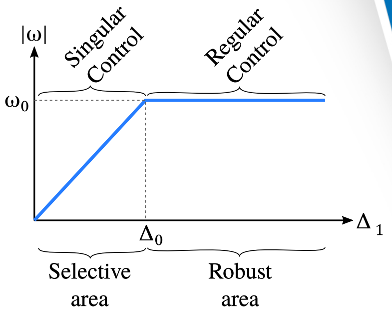


Figure 7: Transition from the area of selective controls characterized by singular solutions of the PMP, to the area of robust controls characterized by regular trajectories.

Outlook

- Using a larger number of offset can improve the selectivity or the robustness.
- For example, we can use the offsets: 0, Δ_1, Δ_2 such that the target states are: $e^{\phi \hat{\epsilon}_x}, \hat{\mathbb{I}}, \hat{\mathbb{I}}$.
- With these more elaborated systems, no analytical expression of the optimal pulses is known in general.

The results presented in this talk are published in: Quentin Ansel & al, J. Phys. A: Math. Theor. 54 085204, 2021.