arXiv:2010.09368v1 [quant-ph] 19 Oct 2020

Introduction to the Foundations of Quantum Optimal Control

U. Boscain[*], M. Sigalotti[†], D. Sugny[‡]

October 20, 2020

Abstract

Optimal Control Theory is a powerful mathematical tool, which has known a rapid development since the 1950s, mainly for engineering applications. More recently, it has become a widely used method to improve process performance in quantum technologies by means of highly efficient control of quantum dynamics. This review aims at providing an introduction to key concepts of optimal control theory which is accessible to physicists and engineers working in quantum control or in related fields. The different mathematical results are introduced intuitively, before being rigorously stated. This review describes modern aspects of optimal control theory, with a particular focus on the Pontryagin Maximum Principle, which is the main tool for determining open-loop control laws without experimental feedback. The different steps to solve an optimal control problem are discussed, before moving on to more advanced topics such as the existence of optimal solutions or the definition of the different types of extremals, namely normal, abnormal, and singular. The review covers various quantum control issues and describes their mathematical formulation suitable for optimal control. The optimal solution of different low-dimensional quantum systems is presented in detail, illustrating how the mathematical tools are applied in a practical way.

1 Introduction

Quantum technology aims at developing practical applications based on properties of quantum mechanics [1]. This objective requires precise manipulation of quantum objects by means of external electromagnetic fields. Quantum control encompasses a set of techniques to find the time evolution of control parameters which perform specific tasks in quantum physics [37, 28, 24, 7, 31, 48, 40, 75, 49, 27, 36, 77]. In recent years, it has naturally become a key tool in the emergent field of quantum technologies [1, 76, 37], with applications ranging

[*]Laboratoire Jacques-Louis Lions, CNRS, Inria, Sorbonne Université, Université de Paris, France, boscain@gmail.com

[†]Laboratoire Jacques-Louis Lions, CNRS, Inria, Sorbonne Université, Université de Paris, France, mario.sigalotti@inria.fr

[‡]Laboratoire Interdisciplinaire Carnot de Bourgogne (ICB), UMR 6303 CNRS-Université Bourgogne-Franche Comté, 9 Av. A. Savary, BP 47 870, F-21078 Dijon Cedex, France, dominique.sugny@u-bourgogne.fr

from quantum computing [37, 59] to quantum sensing [63] and quantum simulation [32]. In the majority of quantum control protocols, the control law is computed in an open-loop configuration without experimental feedback. In this context, a powerful tool is Optimal Control Theory (OCT) [37] which allows a given process to be carried out, while minimizing a cost such as the control time. This approach has key advantages. Its flexibility makes it possible to adapt to experimental constraints or limitations and its optimal character leads to the physical limits of the driven dynamics. OCT can be viewed as a generalization of the classical calculus of variations for problems with dynamical constraints [55]. Its modern version was born with the Pontryagin maximum principle (PMP) in the late 1950s [61]. Since the pioneering study of Pontryagin and co-workers, OCT has undergone rapid development and is nowadays a recognized field of mathematical research. Recent tools from differential geometry have been applied to control theory, making these methods very effective in dealing with problems of growing complexity. Many reference textbooks have been published on the subject both on mathematical results and engineering applications [3, 2, 22, 65, 55, 19, 42, 52, 25]. Originally inspired by problems of space dynamics, OCT was then applied in a wide spectrum of applications such as robotics or economics. OCT was first used for quantum processes [60, 50] in the context of physical chemistry, the goals being to steer chemical reactions [64, 70, 24, 53] or to control spin dynamics in Nuclear Magnetic Resonance [26, 68, 46, 47]. A lot of results have recently been established for quantum technologies, as for example the minimum duration to generate high-fidelity quantum gates [37].

Two types of approach based on the PMP have been used to solve optimal control problems in low- and high-dimensional systems, respectively. In the first situation, the results can be determined essentially analytically or at least with a very high numerical precision. The PMP allows to deduce the structure of the optimal solutions and, in some cases, a proof of their global optimality can be established. In this context, a series of low-dimensional quantum control problems has been rigorously solved in recent years for both closed [29, 18, 13, 15, 35, 43, 44, 41, 72] and open quantum systems [45, 69, 51, 10, 11, 71]. Specific numerical optimization algorithms have been developed and applied to design control fields in larger quantum systems [46, 62, 32, 58, 57]. Due to the complexity of control landscape, only local optimal solutions are found with this approach.

However, despite the recent success of quantum optimal control theory, the situation is still not completely satisfactory. The difficulty of the concepts used in this field does not allow a non-expert to understand and apply easily these techniques. The mathematical textbooks use a specialized and sophisticated language, which makes these works difficult to access. Very few basic papers for physicists are available in the literature, while having a minimum grasp of these tools will be an important skill in the future of quantum technologies. The purpose of this review is to provide an introduction to the core mathematical concepts and tools of OCT in a rigorous but understandable way by physicists and engineers working in quantum control and in related fields. Thus, a deep analogy can be carried out between OCT and finding the minima of a real function of several variables. This parallel is used throughout the text to qualitatively describe the key aspects of the PMP. The review is based on an advanced course for PhD students in physics taught at Sarrebruken University in Spring of 2019. It assumes a basic knowledge of standard topics in quantum physics and quantum control, but also of mathematical techniques such as linear algebra or differential calculus and geometry. Finally, we hope that this paper will give the reader the prerequisites to access a more specialized literature and to apply these techniques to their own control problems.

Structure of the paper

A review of optimal control is a difficult task because a large number of mathematical results have been obtained and many techniques have been developed over the years for specific applications. Among others, we can distinguish the following problem classes: finite or infinite-dimensional system, open or closed-loop control, linear or nonlinear dynamical system, geometric or numerical optimal control, PMP or Hamilton–Jacobi–Bellmann approach... This means making choices about which topics to include in this paper. We have deliberately selected specific aspects of OCT that are treated rigorously, while others are only briefly mentioned. The choice fell on basic mathematical concepts which are the most useful and the least known in quantum control. We limit our focus on the optimal control of open-loop finite-dimensional system by using the PMP. In particular, we consider only analytical and geometric techniques to solve low-dimensional control problems. To ensure overall consistency and limit the length of the paper, we do not discuss numerical optimization methods and the infinite-dimensional case [12, 17], which are also key points in quantum control. We stress that a precise knowledge of the PMP is an essential skill for numerical optimization, and that the scope of the material of this paper is much broader than the examples presented.

The paper is organized as follows. We start by showing how to formulate an optimal control problem from a mathematical point of view in Sec. 2. Closed and open quantum systems illustrate this discussion. The different steps to solve such a problem are presented in Sec. 3 by using the analogy with finding a minimum of a function of several variables. The review continues with a point which is crucial, but often overlooked in quantum control studies, namely the existence of optimal solutions. We present in Sec. 4 the Filippov test, which is one of the most important techniques to adress this question. The first-order conditions are described in Sec. 5, with a specific attention on the different types of extremals and on the statement of the PMP. Sections 6 and 7 are dedicated to the presentation of two examples in three and two-level quantum systems, respectively. Conclusion and prospective views are given in Sec. 8.

2 Formulation of the control problem

The dynamics. A finite-dimensional control system is a dynamical system governed by an equation of the form

$$\dot{q}(t) = f(q(t), u(t)), \tag{1}$$

where $q : I \to M$ represents the state of the system (here I is an interval in $\mathbb{R}$ and M is a smooth manifold of dimension n), $u : I \to U \subset \mathbb{R}^m$ is the control law, and f is a smooth function such that $f(\cdot, \bar{u})$ is a vector field on M for every

$\bar{u} \in U$. The set U of the possible values of $u(t)$ is usually closed. It can be the entire $\mathbb{R}^m$ if there is no control constraint.

To be sure that Eq. (1) is well-posed from a mathematical viewpoint, we consider the case in which $I = [0, T]$ for some $T > 0$ and u is measurable and essentially bounded, i.e., $u \in L^\infty([0, T], U)$. The space $L^\infty([0, T], U)$ is called the class of *admissible controls*. Piecewise continuous controls form a subset of admissible controls, and in experimental implementations in quantum control they are the only control laws that can be reasonably applied. However, optimal control problems are set for the larger class of measurable and essentially bounded controls in which optimal controls can be shown to exist (under rather general conditions that we discuss below) and can be characterized through suitable necessary conditions. Such conditions often allow to ensure that the optimal controls are indeed piecewise continuous. We should stress, however, that there exist some examples, such as the Fuller's problem [34], for which the optimal control law has infinitely many switches between two values of U in finite time. Such a control law is not piecewise constant, but belongs to $L^\infty([0, T], U)$.

Given an admissible control $u(\cdot)$ and an initial condition $q(0) = q_{\text{in}} \in M$, there exists a unique solution $q(\cdot)$ of Eq. (1), defined at least for small times. Moreover, such a solution is locally Lipschitz continuous. A locally Lipschitz continuous curve $q(\cdot)$ for which there exists and admissible control $u(\cdot)$ such that Eq. (1) is verified, is said to be an *admissible trajectory*.

Typical situations encountered in quantum control are the following.
Consider the time evolution of the wave function of a N-level closed quantum system. In this case, under the dipolar approximation [49, 78, 79], the dynamics are governed by the Schrödinger equation (in units where $\hbar = 1$)

$$i\dot{\psi}(t) = \left(H_0 + \sum_{j=1}^{m} u_j(t) H_j \right) \psi(t),$$

where ψ, the wave function, belongs to the unit sphere in $\mathbb{C}^N$ and $H_0, \ldots, H_m$ are $N \times N$ Hermitian matrices. The control parameters $u_j(t) \in \mathbb{R}$ are the components of the control $u(\cdot)$. This control problem has the form (1) with $n = 2N - 1$, $M = S^{2N-1} \subset \mathbb{C}^N$, $q = \psi$, and $f(\psi, u) = -i(H_0 + \sum_j^m u_j H_j)\psi$. The solution of the Schrödinger equation can also be expressed in terms of the unitary operator $\mathbf{U}(t, t_0)$, which connects the wave function at time t_0 to its value at t: $\psi(t) = \mathbf{U}(t, t_0)\psi(t_0)$. The propagator $\mathbf{U}(t, t_0)$ also satisfies the Schrödinger equation

$$i\dot{\mathbf{U}}(t, t_0) = \left(H_0 + \sum_{j=1}^{m} u_j(t) H_j \right) \mathbf{U}(t, t_0), \tag{2}$$

with initial condition $\mathbf{U}(t_0, t_0) = \mathbb{I}_N$. In quantum computing, the control problem is generally defined with respect to the propagator $\mathbf{U}$. Equation (2) has the form (1) with $M = U(N) \subset \mathbb{C}^{N \times N}$ and $q = \mathbf{U}$.

The wave function formalism is well adapted to describe pure states of isolated quantum systems, but when one lacks information about the system, the correct formalism is the one of mixed-state quantum systems. The state of the system is then described by a density operator ρ, which is a $N \times N$ positive Hermitian matrix of unit trace. For a closed quantum system the density operator is solution of the von Neumann equation

$$i\dot{\rho}(t) = [H, \rho(t)],$$

with $H = H_0 + \sum_{j=1}^{m} u_j(t) H_j$. For an open N-level quantum system interacting with its environment, the dynamics of ρ are governed in some cases by the following first-order differential equation, called the Kossakowski–Lindblad equation [38, 56]:

$$i\dot{\rho}(t) = [H, \rho(t)] + \mathcal{L}[\rho(t)]. \tag{3}$$

This equation differs from the von Neumann one in that a dissipation operator $\mathcal{L}$ acting on the set of density operators has been added. This linear operator which describes the interaction with the environment cannot be chosen arbitrarily. Its expression can be derived from physical arguments based on a Markovian regime and a small coupling with the environment [5, 23]. From a mathematical point of view, the problem of finding dynamical generators for open systems that ensure positivity of the density matrix was solved in finite- and infinite-dimensional Hilbert spaces [38, 56]. The operator $\mathcal{L}$ is a generator of a quantum semi-group which can be expressed for a N-level quantum system as

$$\mathcal{L}[\rho(t)] = \frac{1}{2} \sum_{k,k'=1}^{N^2-1} a_{kk'} ([V_k \rho(t), V_{k'}^\dagger] + [V_k, \rho(t) V_{k'}^\dagger])$$

where the matrices V_k, $k = 1, \ldots, N^2 - 1$, are trace-zero and orthonormal. The density operator is completely positive if and only if the matrix $a = (a_{kk'})_{k,k'=1}^{N^2-1}$ is positive [67]. The density operator ρ can be represented as a vector $\vec{\rho}$ by stacking its columns. The corresponding time evolution is generated by super-operators in the Schrödinger-like form

$$i\dot{\vec{\rho}} = \mathbf{H}\vec{\rho}. \tag{4}$$

Equation (4) has the form (1) with $M = \mathbb{B}^{N^2-1} \subset \mathbb{R}^{N^2-1}$, $q = \vec{\rho}$, and $f : \vec{\rho} \mapsto \mathbf{H}\vec{\rho}$. Here $\mathbb{B}^{N^2-1}$ denotes the ball of radius 1 in $\mathbb{R}^{N^2-1}$. Notice that even if M is here a manifold with a boundary ∂M, the forward dynamics are well defined because the admissible vector fields at ∂M points are either directed towards the interior of M or are tangent to ∂M.

The initial and final states. When considering a quantum control problem, the goal in most situations is not to bring the system from an initial state q_{in} to a final state q_{fi}, but rather to reach at time T a smooth submanifold $\mathcal{T}$ of M, called *target*:

$$q(0) = q_{\text{in}}, \qquad q(T) \in \mathcal{T}. \tag{5}$$

This issue arises, for instance, in the population transfer from a state ψ_{in} to an eigenstate ψ_{fi} of the field-free Hamiltonian H_0. In this case, since the phase of the final state is not physically relevant, $\mathcal{T}$ is characterized by $\{e^{i\theta}\psi_{\text{fi}} \mid \theta \in [0, 2\pi]\}$. It can also happen that the initial condition $q(0) = q_{\text{in}}$ is generalized to $q(0) \in \mathcal{S}$, where $\mathcal{S}$ is a smooth submanifold of M. However, for the sake of presentation, we will not treat this case here, the changes to be made to the method being straightforward. Finally, note that the time T can be fixed or free, as, for instance, in a time-minimum control problem.

The optimal control problem. Two different optimal control approaches can be used to steer the system from $q_{\rm in}$ to a target $\mathcal{T}$.

• Approach A: Prove that the target $\mathcal{T}$ is reachable from $q_{\rm in}$ (in time T if the final time is fixed or in any time otherwise) and then find the best possible control realizing the transfer. This approach requires to solve the preliminary step of controllability. Essentially, we need to show that:

$$\begin{aligned}
&\mathcal{T}\cap\mathcal{R}(q_{\rm in})\neq\emptyset \text{ if } T \text{ is free where}\\
&\mathcal{R}(q_{\rm in}):=\{\bar q\in M\mid \exists\ T \text{ and}\\
&\text{an admissible trajectory } q:[0,T]\to M\\
&\text{ such that } q(0)=q_{\rm in},\ q(T)=\bar q\}
\end{aligned}$$

or that

$$\begin{aligned}
&\mathcal{T}\cap\mathcal{R}^T(q_{\rm in})\neq\emptyset \text{ if } T \text{ is fixed where}\\
&\mathcal{R}^T(q_{\rm in}):=\{\bar q\in M\mid \exists \text{ an admissible trajectory}\\
&q:[0,T]\to M \text{ such that } q(0)=q_{\rm in},\ q(T)=\bar q\},
\end{aligned}$$

and then solve the minimization problem

$$\int_0^T f^0(q(t),u(t))\,dt \longrightarrow \min, \tag{6}$$

where $f^0: M\times U\to\mathbb{R}$ is a smooth function, which in many quantum control applications depends only on the control. The control time T is fixed or free.

The test of controllability is sometimes easy (as, for instance, for low-dimensional closed quantum systems [4, 66]) and sometimes extremely difficult. When the test of controllability can be performed, this approach is to be preferred since it permits to reach exactly the final state.

A general and useful sufficient condition for controllability is the following.

Proposition 1. *Let M be a smooth manifold and U be a subset of $\mathbb{R}^m$ containing a neighborhood of the origin. Consider a control system of the form $\dot q = F_0(q)+\sum_{j=1}^m u_j(t)F_j(q)$, with $F_0,\dots,F_m$ smooth vector fields on M and $u(t)=(u_1(t),\dots,u_m(t))\in U$. Let $\mathcal{L}_0$ be the Lie algebra generated by the vector fields $F_0,\dots,F_m$ and $\mathcal{L}_1$ be the Lie algebra generated by the vector fields $F_1,\dots,F_m$. The system is controllable if at least one of the following conditions is satisfied:*

1. *F_0 is a recurrent vector field and $\dim(\mathcal{L}_0(q))$ is equal to the dimension of M at every $q\in M$;*
2. *$U=\mathbb{R}^m$ and $\dim(\mathcal{L}_1(q))$ is equal to the dimension of M at every $q\in M$.*

For a definition of Lie algebra generated by a set of vector fields and for the notion of recurrent vector field we refer to [3, 21]. For our purposes, it is sufficient to recall that:

- if $F_0(q)=A_0q,\dots,F_m(q)=A_mq$ are linear vector fields then $G\in\mathcal{L}_0$ if and only if $G(q)=Bq$ with B in the matrix Lie algebra (for the commutator product) generated by $A_0,\dots,A_m$.

Table 1: Summary of the different optimal control approaches.

Approach A When one can prove that: $\mathcal{T} \cap \mathcal{R}(q_{\mathrm{in}}) \neq \emptyset$ if T is free or $\mathcal{T} \cap \mathcal{R}^T(q_{\mathrm{in}}) \neq \emptyset$ if T is fixed	$\dot{q}(t) = f(q(t), u(t))$ $q(0) = q_{\mathrm{in}},\ q(T) \in \mathcal{T}$ $\int_0^T f^0(q(t), u(t))\, dt \to \min$ T fixed or free
Approach B When controllability cannot be verified	$\dot{q}(t) = f(q(t), u(t))$ $q(0) = q_{\mathrm{in}},\ q(T)$ free $\int_0^T f^0(q(t), u(t))\, dt + d(\mathcal{T}, q(T)) \to \min$ T fixed or free

- vector fields whose integral curves are all periodic are recurrent.

• Approach B: Find a control that brings the system as close as possible to the target, while minimizing the cost. This approach is used for systems for which the controllability step cannot be easily verified. In this case, the initial point is fixed and the final point is free, but the cost contains a term (denoted $d(\cdot, \cdot)$ in the next formula) depending on the distance between the final state of the dynamics and the target:

$$\int_0^T f^0(q(t), u(t))\, dt + d(\mathcal{T}, q(T)) \longrightarrow \min, \tag{7}$$

where T is fixed or free.

An example is given by open quantum systems governed by the Kossakowski–Lindblad equation, for which the characterization of the reachable set is quite involved [6, 30]. If we denote by ρ_{fi} the target state, a cost to minimize penalizing the energy of the control and the distance to the target can be

$$\int_0^T \frac{u(t)^2}{2} dt + \|\rho(T) - \rho_{\mathrm{fi}}\|^2,$$

where $\| \cdot \|$ is the norm corresponding to the scalar product of density matrices $\langle \rho_1 | \rho_2 \rangle = \mathrm{Tr}[\rho_1^\dagger \rho_2]$.

Optimization problem in these two approaches should be of course considered together with the dynamics (1) and the initial and final conditions. They are summarized in Tab. 1.

3 The different steps to solve an optimal control problem

The steps to determine a solution to the minimization problem are similar to finding the minimum of a smooth function $f^0 : \mathbb{R} \to \mathbb{R}$.

0. Find conditions which guarantee the existence of solutions. We recall that among smooth functions $f^0 : \mathbb{R} \to \mathbb{R}$, it is easy to find examples not admitting a minimum (e.g., the function $x \mapsto e^{-x}$ and the function $x \mapsto x$

do not have minima). This step is crucial. If it is skipped, first-order conditions may give a wrong candidate for optimality (see below for details) and numerical optimization schemes may either not converge or converge towards a solution which is not a minimum. For optimal control problems, there exist several existence tests, but they are not always applicable or easy to use. In Sec. 4, we present the Filippov test.

1. Apply first-order necessary conditions. For a smooth function $f^0 : \mathbb{R} \to \mathbb{R}$, this means that if $\bar{x}$ is a minimum then $\frac{d}{dx} f^0(\bar{x}) = 0$. This condition gives candidates for minima, i.e., identifies local minima, local maxima, and saddles. Note that if one does not verify a priori existence of minima, first-order conditions could give wrong candidates. Think for instance to the function $x \mapsto (x^2 + 1/2)e^{-x^2}$. This function has a single local minimum, obtained at $x = 0$, whose value is $1/2$, which is well identified by first-order conditions. However its infimum is zero (for $x \to \pm\infty$, the function tends to zero). For optimal control problems, first-order necessary conditions should be given in an infinite-dimensional space (a space of curves) and they are expressed by the PMP, which is presented in Sec. 5.2. In Approach A, note that the condition that the system reaches exactly the target is a *constraint* leading to the appearance of *Lagrange multipliers (normal and abnormal).* This point is discussed in details in Sec. 5.1.

2. Apply second-order conditions. For instance, for a smooth function $f^0 : \mathbb{R} \to \mathbb{R}$, among the points for which we have $\frac{d}{dx} f^0(\bar{x}) = 0$, a necessary condition to have a minimum is $\frac{d^2}{dx^2} f^0(\bar{x}) \geq 0$. This step is generally used to reduce further the candidates for optimality. For optimal control problems, there are several second-order conditions as higher-order Pontryagin Maximum Principles or Legendre–Clebsch conditions (see for instance [3, 65, 19]). In some cases, this step is difficult and it could be more convenient to go directly to the next one.

3. Among the set of candidates for optimality identified in step 1 and (possibly) further reduced in step 2, one should select the best one. This step is often done by hand if the previous steps have identified a finite number of candidates for optimality. For optimal control problems, one often ends up with infinitely many candidates for optimality and this step is generally very difficult.

There are of course specific examples for which the solution is particularly simple. This is the case of convex problems, for which only first-order conditions should be applied, since the existence step is automatic and first-order conditions are both necessary and sufficient for optimality. This situation is however rare in quantum control and we will not discuss it further.

4 Existence of solutions for Optimal Control Problem: the Filippov test

The existence theory for optimal control is difficult and, unfortunately, there is no general procedure that can be applied in any situation. In this section, we present the most important technique, the Filippov test that allows to tackle several types of problems. We emphasize that it is fundamental to verify the existence of optimal controls before applying first-order conditions (and the PMP). Otherwise, as discussed in the finite-dimensional case, it may occur that the PMP has solutions, but none of them is optimal.

Let us consider the problem in Approach A with T fixed.

Problem P1

$$\begin{aligned}
&\dot{q}(t) = f(q(t), u(t)), \\
&q(0) = q_{\mathrm{in}}, \ q(T) \in \mathcal{T}, \\
&\int_0^T f^0(q(t), u(t))\, dt \to \min, \\
&T > 0 \text{ fixed.}
\end{aligned}$$

Here $q : [0, T] \to M$, where M is a smooth n-dimensional manifold, f, f^0 are smooth functions of their arguments, $u \in L^\infty([0, T], U)$, where $U \subset \mathbb{R}^m$, and $\mathcal{T}$ is a smooth submanifold of M.

In order to tackle the existence problem, we define a new variable q^0 obtained as the value of the cost during the time-evolution, that is,

$$q^0(t) = \int_0^t f^0(q(s), u(s))\, ds,$$

and we denote $\hat{q} = (q^0, q)$. The dynamics of the new state $\hat{q}$ in $\mathbb{R} \times M$ are given by

$$\begin{aligned}
\dot{\hat{q}}(t) &= \begin{pmatrix} \dot{q}^0(t) \\ \dot{q}(t) \end{pmatrix} = \begin{pmatrix} f^0(q(t), u(t)) \\ f(q(t), u(t)) \end{pmatrix} \\
&=: \hat{f}(q(t), u(t)), \\
\hat{q}(0) &= (0, q_{\mathrm{in}}), \ \hat{q}(T) \in \mathbb{R} \times \mathcal{T}.
\end{aligned}$$

This control system is called the *augmented system*. The minimization problem in integral form, $\min \int_0^T f^0(q(t), u(t))\, dt$, becomes a problem of minimization of one of the coordinates at the final time, i.e., $\min q^0(T)$.

We denote by $\hat{\mathcal{R}}(T, (0, q_{\mathrm{in}}))$ the reachable set in time T for the augmented system, starting from $(0, q_{\mathrm{in}})$. The key observation on which optimal control is based is expressed by the following proposition (used both for existence and first-order conditions).

Proposition 2. *If $q(\cdot)$ is an optimal trajectory for problem* **(P1)**, *then $\hat{q}(T) \in \partial\hat{\mathcal{R}}(T, (0, q_{\mathrm{in}}))$.*

Proof. By contradiction, if $\hat{q}(T) = (q^0(T), q(T)) \in \mathrm{int}\hat{\mathcal{R}}(T, (0, q_{\mathrm{in}}))$ then there exists a trajectory reaching a point $(\alpha, q(T))$ with $\alpha < q^0(T)$, i.e., arriving at the same point in M, but with a smaller cost. See Fig. 1. $\square$

It is then clear that the existence of a minimum is guaranteed by the compactness of $\hat{\mathcal{R}}(T, (0, q_{\mathrm{in}})) \cap (\mathbb{R} \times \mathcal{T})$.

Proposition 3. *If $\hat{\mathcal{R}}(T, (0, q_{\mathrm{in}}))$ is compact and $\mathcal{T}$ is closed then there exists a solution to problem* **(P1)**.

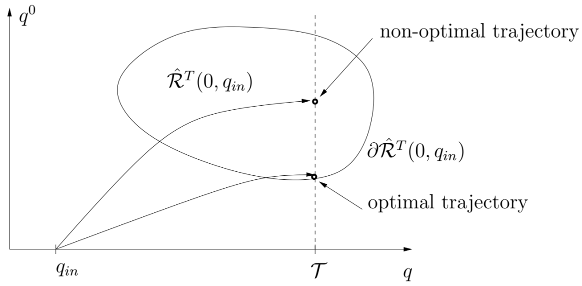

Figure 1: The reachable set of the augmented system

Hence the compactness of $\hat{\mathcal{R}}(T, (0, q_{\rm in}))$ is a key point. A sufficient condition for compactness of the reachable set is given by the following theorem (see, e.g., [55]).

Theorem 4 (Filippov)**.** *Consider the control system $\dot{q}(t) = f(q(t), u(t))$, $q \in M$, $u \in L^\infty(\mathbb{R}, U)$, where M is a n-dimensional manifold and $U \subset \mathbb{R}^m$. Fix an initial condition $q_{\rm in} \in M$. Assume the following conditions:*

- *the set U is compact,*
- *the set $\mathbf{F}(q) = \Big\{ f(q, u) \mid u \in U \Big\}$ is convex for every $q \in M$,*
- *for every $T > 0$ and $u \in L^\infty([0, T], U)$, the solution of $\dot{q}(t) = f(q(t), u(t))$, $q(0) = q_{\rm in}$, is defined on the whole interval $[0, T]$.*

Then for every $T > 0$ the sets $\mathcal{R}^T(q_{\rm in})$ and $\mathcal{R}^{\leq T}(q_{\rm in})$ are compact.

Here

$$\begin{aligned}
&\mathcal{R}^{\leq T}(q_{\rm in}) := \{\bar{q} \in M \mid \exists\, T' \in [0, T] \\
&\quad \text{and an admissible trajectory } q : [0, T'] \to M \\
&\quad \text{such that } q(0) = q_{\rm in},\ q(T') = \bar{q}\}.
\end{aligned}$$

Note that the third hypothesis of Th. 4 is automatically satisfied when M is compact. By applying this theorem to the augmented system for problem **(P1)**, one obtains:

Proposition 5. *Assume that*

- *$\mathcal{T}$ is closed and $\mathcal{R}(T, q_{\rm in}) \cap \mathcal{T} \neq \emptyset$,*
- *the set U is compact,*
- *the set $\hat{\mathbf{F}}(q) = \left\{ \begin{pmatrix} f^0(q, u) \\ f(q, u) \end{pmatrix} \mid u \in U \right\}$ is convex for every $q \in M$,*
- *for every $T > 0$ and $u \in L^\infty([0, T], U)$ the solution of $\dot{q}(t) = f(q(t), u(t))$, $q(0) = q_{\rm in}$, is defined on the whole interval $[0, T]$.*

Then there exists a solution to problem **P1**.

The idea of reducing the problem of existence of an optimal control to the compactness of the reachable set of the augmented system can be used for more general problems. For instance, if we add a terminal cost $\phi(q(T))$ to the cost $\int_0^T f^0(q(t), u(t))\, dt$, where ϕ is a smooth function (as for instance in Approach B, or in the general formulation given in Sec. 5.2), we get a similar result adding to $f^0(q(t), u(t))$ the directional derivative of ϕ along $f(q(t), u(t))$, that is, replacing $f^0(q(t), u(t))$ by $f^0(q(t), u(t)) + \langle d\phi(q(t)), f(q(t), u(t))\rangle$, where $\langle\cdot,\cdot\rangle$ denotes the duality product between covectors of T^*M (in this case, the differential of ϕ evaluated at $q(t)$) and vectors of TM (in this case, the evaluation of the vector field $f(\cdot, u(t))$ at $q(t)$). We leave the details as an exercise.

When the final time is free, it is more difficult to get the existence of optimal trajectories. However, the compactness of $\mathcal{R}^{\leq T}(q_{\text{in}})$ in the Filippov theorem can be used to find conditions for the existence of optimal controls in minimum time. We state this result in the case where M is compact and we leave its proof as an exercise. Note that the problem of minimizing time can be written in the form of problem **P1** with T free and $f^0 = 1$.

Proposition 6. *Consider problem* **P1** *with T free, $f^0 = 1$, and M compact. Assume that*

- *$\mathcal{T}$ is closed and $\mathcal{R}(T, q_{\text{in}}) \cap \mathcal{T} \neq \emptyset$,*
- *the set U is compact,*
- *the set $\mathbf{F}(q) = \{f(q,u) \mid u \in U\}$ is convex for every $q \in M$.*

Then there exists a solution to the problem.

5 First-order conditions

For a smooth real-valued function of one variable $f^0 : \mathbb{R} \to \mathbb{R}$, first-order optimality conditions are obtained from the observation that, at points where $\frac{df^0}{dx} \neq 0$, the function f^0 is well approximated by its first-order Taylor series and hence cannot be optimal since it behaves locally as an affine (non-constant) function. In this way, one obtains the necessary condition: *If $\bar{x}$ is minimal for f^0 then $\frac{df^0}{dx}(\bar{x}) = 0$.* First-order conditions in optimal control are derived in the same way. We have to require that for a small control variation, there is no cost variation at first order.

More precisely, if $J(u(\cdot))$ is the value of the cost for a reference admissible control $u(\cdot)$ (for instance $J(u(\cdot)) = \int_0^T f^0(q(t), u(t))\, dt$ in Approach A or $J(u(\cdot)) = \int_0^T f^0(q(t), u(t))\, dt + d(\mathcal{T}, q(T))$ in Approach B), and $v(\cdot)$ is another admissible control, one would like to consider a condition of the form

$$\left.\frac{\partial J(u(\cdot) + hv(\cdot))}{\partial h}\right|_{h=0} = 0. \tag{8}$$

But difficulties may arise for the following reasons.

We work in an infinite-dimensional space (the space of controls) and hence condition (8) should be required for infinitely many $v(\cdot)$. It may very well happen that if $u(\cdot)$ and $v(\cdot)$ are admissible controls then $u(\cdot) + hv(\cdot)$ is not admissible for every h close to 0 (think, for instance, to the case in which $m = 1$ and $U = [a, b]$). Hence, one should be very careful in choosing the admissible variations of the control. In Approach A, one should restrict only to variations of the control for which the corresponding trajectory reaches the target. More precisely, if $\tilde{q}(\cdot)$ is the trajectory corresponding to the control $\tilde{u}(\cdot) := u(\cdot)+hv(\cdot)$, one should add the condition

$$\tilde{q}(T) \in \mathcal{T}, \tag{9}$$

with T either free or constrained to be the fixed final time depending on the problem under study. Condition (9) should be considered as a *constraint* for the minimization problem, which results in the use of *Lagrange multipliers (normal and abnormal)*.

The occurrence of Lagrange multipliers in optimal control is not due to the fact that the optimization takes place in an infinite-dimensional space, but is rather a general feature of constrained minimization problems, as explained in Sec. 5.1.

5.1 Why Lagrange multipliers appear in constrained optimization problems

We first recall how to find the minimum of a function of n variables $f^0(x)$, where $x = (x_1, \dots, x_n)$, under the constraint $f(x) = 0$, with the method of Lagrange multipliers. Here f^0 and f are two smooth functions $\mathbb{R}^n \to \mathbb{R}$. We have two cases.

• If $\bar{x}$ is a point such that $f(\bar{x}) = 0$ with $\nabla f(\bar{x}) \neq 0$, then the implicit function theorem guarantees that $\{x \mid f(x) = 0\}$ is a smooth hypersurface in a neighborhood of $\bar{x}$. In this case, a necessary condition for f^0 to have a minimum at $\bar{x}$ is that the level set of f^0 is not transversal to the set $\{x \mid f(x) = 0\}$ at $\bar{x}$. See Figure 2. More precisely, this means that

$$\exists \lambda \in \mathbb{R} \text{ such that } \nabla f^0(\bar{x}) = \lambda \nabla f(\bar{x}). \tag{10}$$

This statement can be proved by assuming, for instance, that $\partial_{x_n} f(\bar{x}) \neq 0$ (in such a way to be able to write the set $\{x \mid f(x) = 0\}$ locally around $\bar{x}$ as $x_n = g(x_1, \dots, x_{n-1})$). The requirement that

$$\begin{aligned}
&\partial_{x_i} f(x_1, \dots, x_{n-1}, g(x_1, \dots, x_{n-1})) \equiv 0, \\
&i = 1, \dots, n-1, \\
&\partial_{x_i} f_0(x_1, \dots, x_{n-1}, g(x_1, \dots, x_{n-1}))|_{x=\bar{x}} = 0, \\
&i = 1, \dots, n-1,
\end{aligned}$$

provides immediately condition (10) with $\lambda = \frac{\partial_{x_n} f_0(\bar{x})}{\partial_{x_n} f(\bar{x})}$.

Notice that λ could be equal to zero. This case corresponds to the situation in which f^0 has a critical point at $\bar{x}$ even in absence of the constraint.

• If $\bar{x}$ is a point such that $f(\bar{x}) = 0$ with $\nabla f(\bar{x}) = 0$ then the set $\{x \mid f(x) = 0\}$ could be very complicated in a neighborhood of $\bar{x}$ (typical examples are a single point, two crossing curves, ... but it could be any closed set). In general the value of f^0 at these points cannot be compared with neighboring points by

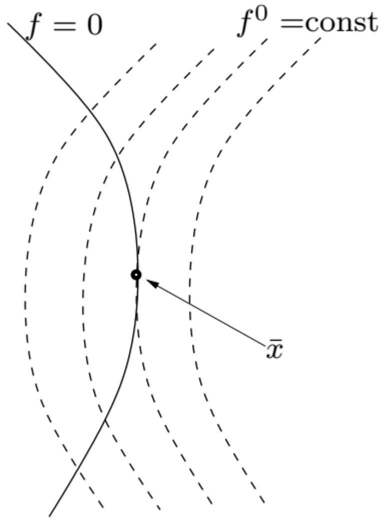

Figure 2: Lagrange multipliers

requiring that a certain derivative is zero (think for instance to the case in which $\{x \mid f(x) = 0\}$ is an isolated point). However, they are candidates to optimality. As an illustrative example, consider the case where $n = 2$, $f^0(x_1, x_2) = x_1^2 + (x_2 - 1/4)^2$, and $f(x_1, x_2) = (x_1^2 + x_2^2)(x_1^2 + x_2^2 - 1)$.

These results can be rewritten in the following form.

Theorem 7 (Lagrange multiplier rule in $\mathbb{R}^n$)**.** *Let f^0 and f be two smooth functions from $\mathbb{R}^n$ to $\mathbb{R}$. If f^0 has a minimum at $\bar{x}$ on the set $\{x \mid f(x) = 0\}$, then there exists $(\bar{\lambda}, \bar{\lambda}_0) \in \mathbb{R}^2 \setminus \{(0,0)\}$ such that, setting $\Lambda(x, \lambda, \lambda_0) = \lambda f(x) + \lambda_0 f^0(x)$, we have*

$$\nabla_x \Lambda(\bar{x}, \bar{\lambda}, \bar{\lambda}_0) = 0, \ \nabla_\lambda \Lambda(\bar{x}, \bar{\lambda}, \bar{\lambda}_0) = 0. \tag{11}$$

To show that this statement is equivalent to what we just discussed, we observe that the second equality in (11) gives the constraint $f(\bar{x}) = 0$. For the first equation, we have two cases. If $\bar{\lambda}_0 \neq 0$ then we can normalize $\bar{\lambda}_0 = -1$ and we get $\bar{\lambda} \nabla_x f(\bar{x}) - \nabla_x f^0(\bar{x}) = 0$, i.e., Eq. (10) with the change of notation $\lambda \to \bar{\lambda}$. If $\bar{\lambda}_0 = 0$ then $\bar{\lambda} \neq 0$ and we get $\nabla_x f(\bar{x}) = 0$, that is, the second case studied above.

The quantities $\bar{\lambda}$ and $\bar{\lambda}_0$ are respectively called *Lagrange multiplier* and *abnormal Lagrange multiplier*. If $(\bar{x}, \bar{\lambda}_0, \bar{\lambda})$ is a solution of Eq. (11) with $\bar{\lambda}_0 \neq 0$ (resp., $\bar{\lambda}_0 = 0$) then $\bar{x}$ is called a *normal extremal* (resp., *abnormal extremal*). An abnormal extremal is a candidate for optimality and occurs, in particular, when we cannot guarantee (at first order) that the set $\{x \mid f(x) = 0\}$ is a smooth curve. Abnormal extremals are candidates for optimality regardless of cost f^0. Note that if $\bar{x}$ is such that $\nabla_x f(\bar{x}) = 0$ and $\nabla_x f^0(\bar{x}) = 0$ then $\bar{x}$ is both normal and abnormal. This is the case in which $\bar{x}$ satisfies the first-order condition for optimality even without the constraint, but we cannot guarantee that the constraint is a smooth curve.

In the (infinite-dimensional) case of an optimal control problem, normal and abnormal Lagrange multipliers appear in a very similar way.

5.2 Statement of the Pontryagin Maximum Principle

In this section, we state the first-order necessary condition for optimal control problems, namely the PMP. The theorem is stated in a more general form that unifies and slightly generalizes optimal control problems of Approaches A and B. In particular, we add to the cost $\int_0^T f^0(q(t), u(t))$ a general terminal cost $\phi(q(T))$. In Approach A, we have $\phi = 0$, while in Approach B, ϕ represents the distance from $q(T)$ to the target $\mathcal{T}$. We allow the target $\mathcal{T}$ to coincide with M. This corresponds to leave the final point $q(T)$ free in Approach B.

Theorem 8. *Consider the optimal control problem*

$$\begin{aligned}
&\dot{q}(t) = f(q(t), u(t)),\\
&q(0) = q_{\text{in}},\ q(T) \in \mathcal{T},\\
&\int_0^T f^0(q(t), u(t))\, dt + \phi(q(T)) \longrightarrow \min,
\end{aligned}$$

where

- *M is a smooth manifold of dimension n, $U \subset \mathbb{R}^m$,*
- *$\mathcal{T}$ is a (non-empty) smooth submanifold of M. It can be reduced to a point (fixed terminal point) or coincide with M (free terminal point).*
- *f, f^0 are smooth,*
- *$u \in L^\infty([0, T], U)$,*
- *$q : [0, T] \to M$ belongs to the set of Lipschitz continuous curves.*

Define the function (called pre-Hamiltonian*)*

$$\mathcal{H}(q, p, u, p^0) \quad = \quad \langle p, f(q, u)\rangle + p^0 f^0(q, u), \tag{12}$$

with

$$(q, p, u, p^0) \in T^*M \times U \times \mathbb{R}.$$

If the pair $(q, u) : [0, T] \to M \times U$ is optimal, then there exists a never vanishing Lipschitz continuous pair $(p, p^0) : [0, T] \ni t \mapsto (p(t), p^0) \in T^*_{q(t)}M \times \mathbb{R}$ where $p^0 \leq 0$ is a constant and such that for a.e. $t \in [0, T]$ we have

i) $\dot{q}(t) = \frac{\partial \mathcal{H}}{\partial p}(q(t), p(t), u(t), p^0)$ *(Hamiltonian equation for q);*

ii) $\dot{p}(t) = -\frac{\partial \mathcal{H}}{\partial q}(q(t), p(t), u(t), p^0)$ *(Hamiltonian equation for p);*

iii) *the quantity $\mathcal{H}_M(q(t), p(t), p^0) := \max_{v \in U} \mathcal{H}(q(t), p(t), v, p^0)$ is well-defined and*

$$\mathcal{H}(q(t), p(t), u(t), p^0) = \mathcal{H}_M(q(t), p(t), p^0)$$

which corresponds to the maximization condition.

Moreover,

iv) *there exists a constant $c \geq 0$ such that $\mathcal{H}_M(q(t), p(t), p^0) = c$ on $[0, T]$, with $c = 0$ if the final time is free (value of the Hamiltonian);*

v) *for every $v \in T_{q(T)}\mathcal{T}$, we have $\langle p(T), v\rangle = p^0\langle d\phi(q(T)), v\rangle$ (transversality condition).*

Comments.

• By T^*M we denote, as usual, the cotangent bundle, whose fibers T_q^*M are made of covectors. An element of T^*M is given by (q, p) with $p \in T^*M$. In local coordinates, one can think of p as a row vector and $f(q, u)$ as a column vector, with $\langle p, f(q, u)\rangle = pf(q, u)$. The covector p is called *adjoint state* in control theory.

• The quantities $p(\cdot)$ and p^0 play the role of Lagrange multipliers for the constrained optimization problem. We point out the similarity between the expressions of $\mathcal{H}$ and of Λ in Th. 7 (with the change of notation $q \to x$ and $p \to \lambda$).

• A trajectory $q(\cdot)$ for which there exist $p(\cdot)$, $u(\cdot)$ and p^0 such that $(q(\cdot), p(\cdot), u(\cdot), p^0)$ satisfies all the conditions given by the PMP is called an *extremal trajectory* and the 4-uple $(q(\cdot), p(\cdot), u(\cdot), p^0)$ an *extremal.* Such an extremal is called *normal* if $p^0 \neq 0$ and *abnormal* if $p^0 = 0$. It may happen that an extremal trajectory $q(\cdot)$ admits both a normal extremal $(q(\cdot), p_1(\cdot), u(\cdot), p^0)$ and an abnormal extremal $(q(\cdot), p_2(\cdot), u(\cdot), 0)$. In this case, we say that the extremal trajectory $q(\cdot)$ is a *non-strict abnormal trajectory.* Note that (as in the finite-dimensional case) abnormal trajectories are candidates for optimality regardless of the cost.

• The PMP is only a necessary condition for optimality. It may very well happen that an extremal trajectory is not optimal. The PMP can therefore provide several candidates for optimality, only some of which are optimal (or even none of them if the step of existence has not been verified, see Sec. 4).

• Since the equation for $p(\cdot)$ at point **ii)** of the PMP is linear, if $(q(\cdot), p(\cdot), u(\cdot), p^0)$ is an extremal, then for every $\alpha > 0$, $(q(\cdot), \alpha p(\cdot), u(\cdot), \alpha p^0)$ is an extremal as well. As a consequence, some useful normalizations are possible. A typical normalization for normal extremals is to require $p^0 = -\frac{1}{2}$ but other choices are also possible.

• When there is no final cost ($\phi = 0$), the transversality condition simplifies to:

$$\langle p(T), T_{q(T)}\mathcal{T}\rangle = 0. \tag{13}$$

When the final point is fixed ($\mathcal{T} = \{q_{\text{fi}}\}$), $T_{q(T)}\mathcal{T}$ is a zero-dimensional manifold and hence condition (13) is empty. When the final point is free ($\mathcal{T} = M$) the transversality condition simplifies to $p(T) = p^0 d\phi(q(T))$. Notice that, since $(p(T), p^0) \neq 0$, in this case one necessarily has $p^0 \neq 0$.

5.3 Use of the PMP

The application of the PMP is not so straightforward. Indeed, there are many conditions to satisfy and all of them are coupled. This section is aimed at describing how to use it in practice.

The following points should be followed first for normal extremals (with p^0 normalized for instance to $-1/2$) and then for abnormal extremals ($p^0 = 0$). In the different steps, several difficulties (that are briefly mentioned) may arise.

Most of them should be solved case by case, since they can be of different nature depending on the problem under study.

Step 1. Use the maximization condition **iii)** to express, when possible, the control as a function of the state and of the covector, i.e., $u = w(q,p)$. Note that if we have m controls (e.g., if U is an open subset of $\mathbb{R}^m$) then the first-order maximality conditions give m equations for m unknowns. When the maximization condition permits to express u as a function of q and p, we say that the control is *regular*, otherwise the control is said to be *singular*. In T^*M, we may have regions where the control is regular and regions where it is singular. For singular controls, finer techniques have to be used to derive the expression of the control. This point is discussed in the examples.

Step 2. Insert the control found in the previous step into the Hamiltonian equations **i)** and **ii)**:

$$\begin{cases} \dot{q}(t) = \frac{\partial \mathcal{H}}{\partial p}(q(t), p(t), w(q(t), p(t)), p^0) \\ \dot{p}(t) = -\frac{\partial \mathcal{H}}{\partial q}(q(t), p(t), w(q(t), p(t)), p^0). \end{cases} \tag{14}$$

In case the previous step provides a smooth $w(\cdot,\cdot)$, this is a well-defined set of $2n$ equations for $2n$ unknown. Note, however, that the boundary conditions are given in a non-standard form since we know $q(0)$ but not $p(0)$. Instead of $p(0)$, we have a partial information on $q(T)$ and $p(T)$ depending on the dimension of $\mathcal{T}$ (see the next step to understand how these final conditions are shared between $q(T)$ and $p(T)$). We then solve Eq. (14) for *fixed* $q(0) = q_{\rm in}$ and *any* $p(0) = p_{\rm in} \in T^*_{q_{\rm in}}M$. Let us denote the solution as

$$q(t; p_{\rm in}, p^0), \qquad p(t; p_{\rm in}, p^0). \tag{15}$$

We stress that when $w(\cdot,\cdot)$ is not regular enough, solutions to the Cauchy problem (14) with $q(0) = q_{\rm in}$ and $p(0) = p_{\rm in}$ may fail to exist or to be unique.

Step 3. Find $p_{\rm in}$ such that

$$q(T; p_{\rm in}, p^0) \in \mathcal{T}. \tag{16}$$

Note that if $\mathcal{T}$ is reduced to a point and T is fixed, we get n equations for n unknown (the components of $p_{\rm in}$). If T is free then an additional equation is needed. This condition is given by the relation **iv)** in the PMP. If $\mathcal{T}$ is a k-dimensional submanifold of M ($k \le n$) then Eq. (16) provides only $n-k$ equations and the remaining ones correspond to the transversality condition **v)** of the PMP.

Step 4. If Eq. (16) (together with the transversality condition and condition **iv)** of the PMP if T is free) has a unique solution $p_{\rm in}$ and if we have verified a priori the existence step, then the optimal control problem is solved. Unfortunately, in general there is no reason for Eq. (16) to provide a unique solution. Indeed, the PMP is only a necessary condition for optimality. If several solutions are found, one should choose among them the best one by a direct comparison of the value of the cost. This is, in general, a non-trivial step, complicated by the difficulty of solving explicitly Eq. (16). For this reason, several techniques have been developed to select the extremals. Among others, we mention the sufficient conditions for optimality given by Hamilton–Jacobi–Bellman theory and synthesis theory. We refer to [20] for a discussion. In Example 1 (Section 6), we are able to select the optimal solution without the use of sufficient conditions for optimality, while it is not the case in Example 2 (Section 7).

6 Example 1: A three-level quantum system with complex controls

In this section, we mainly use the results of [15], see also [14, 13, 73].

6.1 Formulation of the quantum control problem

We consider a three-level quantum system whose dynamics are governed by the Schrödinger equation. The system is described by a pure state $\psi(t)$ belonging to a three-dimensional complex Hilbert space. The system is characterized by three energy levels E_1, E_2 and E_3 in the absence of external fields [74] and is controlled by the Pump and the Stokes pulses which couple, respectively, states one and two and states two and three. Note that there is no direct coupling between levels one and three. The time evolution of $\psi(t)$ is given by

$$i\dot{\psi}(t) = H(t)\psi(t),$$

where

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

Here $\Omega_1(t), \Omega(t) \in \mathbb{C}$ are the two time-dependent complex control parameters. We denote by $\psi_1(t)$, $\psi_2(t)$, and $\psi_3(t)$ the coordinates of $\psi(t)$ in the eigenbasis of the field-free Hamiltonian. They satisfy

$$|\psi_1(t)|^2 + |\psi_2(t)|^2 + |\psi_3(t)|^2 = 1,$$

leading to $M = S^5$, a manifold of real dimension 5. The goal of the control process is to transfer population from the first eigenstate to the third one in a fixed time T. In other words, the aim is to find a trajectory in M going from the submanifold $|\psi_1|^2 = 1$ to the one with $|\psi_3|^2 = 1$. The system is completely controllable thanks to Point 2 in Proposition 1 and the approach A can be chosen. The optimal control problem is defined through the cost functional

$$C = \int_0^T (|\Omega_1(t)|^2 + |\Omega_2(t)|^2)dt,$$

to be minimized. The cost C can be interpreted as the energy of the control laws used in the control process. We consider the specific case in which the control parameters are in resonance with the energy transition. More precisely, we assume that the pulses $\Omega_1(t)$ and $\Omega_2(t)$ can be expressed as

$$\begin{cases} \Omega_1(t) = u_1(t)e^{i(E_2-E_1)t} \\ \Omega_2(t) = u_2(t)e^{i(E_3-E_2)t} \end{cases}$$

with $u_1(t), u_2(t) \in \mathbb{R}$. Note that this assumption is not restrictive since it can be shown that the resonant case corresponds to the optimal solution [14]. The uncontrolled part, called the drift, together with the imaginary unit in the Schrödinger equation, can be eliminated through a unitary transformation $Y(t)$ given by

$$Y(t) = \mathrm{diag}(e^{-iE_1 t}, e^{-i(E_2 t+\pi/2)}, e^{-i(E_3 t+\pi)}).$$

Defining a new wave function x such that $\psi(t) = Y(t)x(t)$, we obtain that $x(t)$ solves the Schrödinger equation

$$i\dot{x}(t) = H'(t)x(t),$$

where $H' = Y^{-1}HY - iY^{-1}\dot{Y}$. Since Y only modifies the phases of the coordinates, $\psi(t)$ and $x(t)$ correspond to the same population distribution, i.e., setting $x = (x_1, x_2, x_3)$ we have $|x_j(t)|^2 = |\psi_j(t)|^2$, $j = 1, 2, 3$.

Computing explicitly H' we arrive at

$$\begin{pmatrix} \dot{x}_1 \\ \dot{x}_2 \\ \dot{x}_3 \end{pmatrix} = \begin{pmatrix} 0 & -u_1(t) & 0 \\ u_1(t) & 0 & -u_2(t) \\ 0 & u_2(t) & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}. \tag{17}$$

Without loss of generality, the optimal control problem can be restricted to the submanifold $S^2 \subset M$ defined by $\{(x_1, x_2, x_3) \in \mathbb{R}^3 \mid x_1^2 + x_2^2 + x_3^2 = 1\}$. This statement is trivial if the initial condition belongs to S (i.e., if $x(0)$ is real). Otherwise, a straightforward change of coordinates allows to come back to this condition. Equation (17) can be expressed in a more compact form as

$$\dot{x} = u_1(t)F_1(x) + u_2(t)F_2(x), \tag{18}$$

where

$$F_1(x) = \begin{pmatrix} -x_2 \\ x_1 \\ 0 \end{pmatrix}, \; F_2(x) = \begin{pmatrix} 0 \\ -x_3 \\ x_2 \end{pmatrix}.$$

Notice that F_1 and F_2 are two vector fields defined on the sphere S^2 representing respectively a rotation along the x_3- axis and along the x_1- axis. Since $\Omega_1(t)$ and $\Omega_2(t)$ differ from $u_1(t)$ and $u_2(t)$ only for phase factors, the minimization problem becomes

$$C = \int_0^T (u_1(t)^2 + u_1(t)^2)dt \to \min, \tag{19}$$

with T fixed. Concerning initial and final conditions, since the goal is to go from the submanifold $|\psi_1|^2 = 1$ to the submanifold $|\psi_3|^2 = 1$, we can assume without loss of generality that $x(0) = (1, 0, 0)$ (again, a straightforward change of coordinates allows to come back to this condition if it is not the case). Since we are now restricted to real variables, the target is $\mathcal{T} = \{(0, 0, +1), (0, 0, -1)\}$.

Now, being the target made of two points only, one should compute separately the optimal trajectories going from $(1,0,0)$ to $(0,0,1)$ and those going from $(1,0,0)$ to $(0,0,-1)$. Finally between all these trajectories, one should take the ones having the smaller cost. Because of the symmetries of the system the two families of optimal trajectories have precisely the same cost (this will be clear in the explicit computations later on). As a consequence, without loss of generality, we can fix the final condition as $x(T) = (0,0,1)$.

The problem (18)–(19) with fixed initial and final conditions is actually a celebrated problem in OCT called the Grushin model on the sphere [9, 13, 39].

6.2 Existence

For convenience, let us re-write our optimal control problem as follows:

Problem $\mathbf{P}^{\text{Grushin}}(T)$

$$
\begin{aligned}
&\dot{x} = u_1(t)F_1(x) + u_2(t)F_2(x),\\
&\int_0^T (u_1(t)^2 + u_1(t)^2)dt \to \min, \quad T \text{ fixed},\\
&x(0) = (1,0,0), \quad x(T) = (0,0,1),\\
&u_1, u_2 \in L^\infty([0,T],\mathbb{R}).
\end{aligned}
$$

To prove the existence of $\text{P}^{\text{Grushin}}$, one could be tempted to use Proposition 5. However u_1 and u_2 take values in $\mathbb{R}$ and hence the second hypothesis of the proposition is not verified.

Instead we are going to use the following fact.

Claim. If $u_1(t), u_2(t)$ are optimal controls for $\text{P}^{\text{Grushin}}(T)$, then $u_1(t)^2 + u_2(t)^2$ is almost everywhere constant and positive on $[0,T]$. Moreover, for every $\alpha > 0$, we have that $\alpha u_1(t)$, $\alpha u_2(t)$ are optimal controls for $\text{P}^{\text{Grushin}}(T/\alpha)$.

This claim can be proved using the fact that, due to the absence of the drift, a reparameterization of an admissible trajectory is still admissible and the Cauchy-Schwartz inequality [2, 13, 15]. Notice that, as a consequence of the claim, if T is not fixed then there is no existence of optimal solutions.

In the following, it is convenient to normalize T in such a way that $u_1(t)^2 + u_2(t)^2 = 1$. Usually, when one makes this choice one says that trajectories are *parameterized by arc length.* If the objective is to arrive at the target in time T', it is sufficient to use the controls $(\alpha\, u_1(\alpha\, t), \alpha\, u_2(\alpha\, t))$, where $\alpha = \frac{T}{T'}$.

When T is fixed in such a way that $u_1(t)^2 + u_2(t)^2 = 1$, we call problem $\text{P}^{\text{Grushin}}(T)$ simply $\text{P}^{\text{Grushin}}$. With the choice of parameterizing trajectories by arc length, problem $\text{P}^{\text{Grushin}}$ is equivalent to the problem of minimizing T under the constraint $u_1(t)^2 + u_2(t)^2 = 1$. It is not difficult to show that this problem is equivalent to minimize T under the constraint $u_1(t)^2 + u_2(t)^2 \leq 1$. This choice is useful since now the control takes values in the convex and compact set $U = \{(u_1,u_2) \in \mathbb{R}^2 \mid u_1(t)^2 + u_2(t)^2 \leq 1\}$.

We can then apply Proposition 6 and deduce the existence of an optimal trajectory for $\text{P}^{\text{Grushin}}$ (as well as $\text{P}^{\text{Grushin}}(T)$ for every $T > 0$).

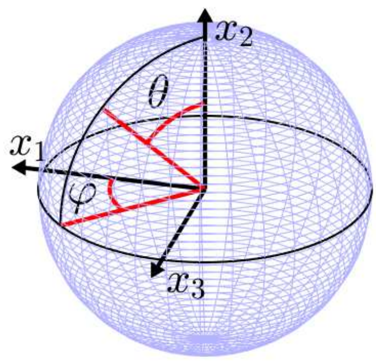

Figure 3: (Color online) Picture of the sphere with the spherical coordinates θ and φ.

6.3 Application of the PMP

Before applying the PMP, it is convenient to reformulate the problem in spherical coordinates. Indeed, one can prove the following statement.

Claim. Consider an optimal control problem as in the statement of the PMP (Theorem 8). If all admissible trajectories starting from $q_{\rm in}$ are contained in a submanifold of M of dimension strictly smaller than n, then all extremal trajectories admit an abnormal lift.

As a consequence, since in our case all trajectories are contained in the sphere S^2, if we apply the PMP in $\mathbb{R}^3$, all optimal trajectories admit an abnormal lift. This creates additional difficulties that can be avoided working directly on S^2 in spherical coordinates.

Let us introduce the coordinates (θ, φ) as displayed in Fig. 3 such that:

$$x_1 = \sin\theta\cos\varphi, \quad x_2 = \cos\theta, \quad x_3 = \sin\theta\sin\varphi.$$

In these coordinates, the starting point $x(0) = (1, 0, 0)$ and the final point $x(T) = (0, 0, 1)$ become $(\theta, \varphi)(0) = (\pi/2, 0)$, $(\theta, \varphi)(T) = (\pi/2, \pi/2)$. Notice that these coordinates are singular for $\theta = 0$ and $\theta = \pi$ but such a singularity does not create any problem, as can be verified by using a second system of coordinates around the singularity. The control system takes then the form:

$$\begin{cases} \dot\theta = -u_1(t)\cos\varphi + u_2(t)\sin\varphi \\ \dot\varphi = \cot(\theta)(u_1(t)\sin\varphi + u_2(t)\cos\varphi). \end{cases}$$

It can be simplified by using the controls v_1 and v_2 defined by

$$\begin{cases} v_1 = -u_1\cos\varphi + u_2\sin\varphi \\ v_2 = u_1\sin\varphi + u_2\cos\varphi, \end{cases} \tag{20}$$

which do not modify the expression of the cost C since $u_1^2 + u_2^2 = v_1^2 + v_2^2$. The control system becomes now

$$\begin{pmatrix} \dot\theta \\ \dot\varphi \end{pmatrix} = v_1(t)X_1(\theta, \varphi) + v_2(t)X_2(\theta, \varphi),$$

where

$$X_1(\theta,\varphi) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \; X_2(\theta,\varphi) = \begin{pmatrix} 0 \\ \cot(\theta) \end{pmatrix}.$$

Let us now apply the PMP. Set $q = (\theta, \varphi)$ and let $p = (p_\theta, p_\varphi)$. The pre-Hamiltonian (12) has the form

$$\begin{aligned} \mathcal{H}(q,p,v,p_0) &= v_1 \langle p, X_1(q)\rangle + v_2 \langle p, X_2(x)\rangle \\ &\quad + p_0(v_1^2 + v_2^2) \\ &= v_1 p_\theta + v_2 p_\varphi \cot(\theta) + p_0(v_1^2 + v_2^2). \end{aligned}$$

We consider the steps of Section 5.3 first for abnormal ($p_0 = 0$) and then for normal ($p_0 = -\frac{1}{2}$) extremals.

Step 1. In this step, we have to apply the maximization condition to find the control as a function of q and p. Since the controls are unbounded and the Hamiltonian is concave, the maximization condition is equivalent to:

$$\begin{cases} \frac{\partial \mathcal{H}}{\partial v_1}(q(t),p(t),v(t),p_0) \equiv 0 \\ \frac{\partial \mathcal{H}}{\partial v_2}(q(t),p(t),v(t),p_0) \equiv 0. \end{cases} \tag{21}$$

For abnormal extremals, we obtain

$$\begin{cases} \langle p(t), X_1(q(t))\rangle = p_\theta(t) \equiv 0 \\ \langle p(t), X_2(q(t))\rangle = p_\varphi(t)\cot(\theta(t)) \equiv 0. \end{cases}$$

These conditions do not permit to obtain the control as a function of q and p. Hence, for this problem, abnormal extremals correspond to singular controls.

Since p and p_0 cannot be simultaneously zero, the only possibility to have an abnormal extremal is that $\theta(t) \equiv \pi/2$ on $[0,T]$. In this case, $\varphi(t)$ should be constant since a trajectory moving on the great circle $\theta = \pi/2$ is not admissible. As a consequence, an abnormal extremal trajectory starting from the initial condition $(\theta,\varphi)(0) = (\pi/2, 0)$ will never reach the final condition $(\theta,\varphi)(T) = (\pi/2, \pi/2)$ and we can disregard these trajectories.

For normal extremals, condition (21) gives:

$$\begin{cases} v_1(t) = \langle p(t), X_1(q(t))\rangle = p_\theta(t) \\ v_2(t) = \langle p(t), X_2(q(t))\rangle = p_\varphi(t)\cot(\theta(t)). \end{cases} \tag{22}$$

Hence, we obtained the controls as a function of q and p and we can conclude that normal extremals correspond to regular controls.

Step 2. Let us insert (22) into the Hamiltonian equations **i)** and **ii)** of Theorem 8.

We have to consider the case $p_0 = -1/2$ only. We obtain:

$$\begin{aligned}
\dot\theta(t) &= \frac{\partial \mathcal{H}}{\partial p_\theta}(q(t), p(t), v(t), -1/2) \\
&= v_1(t) = p_\theta(t), \qquad (23) \\
\dot p_\theta(t) &= -\frac{\partial \mathcal{H}}{\partial \theta}(q(t), p(t), v(t), -1/2) \\
&= v_2(t) p_\varphi(t)(1 + \cot(\theta(t))^2) \\
&= p_\varphi(t)^2 \cot(\theta(t))(1 + \cot^2(\theta(t))), \qquad (24) \\
\dot\varphi(t) &= \frac{\partial \mathcal{H}}{\partial p_\varphi}(q(t), p(t), v(t), -1/2) \\
&= v_2(t)\cot(\theta(t)) = p_\varphi(t)\cot^2(\theta(t)), \qquad (25) \\
\dot p_\varphi(t) &= -\frac{\partial \mathcal{H}}{\partial \varphi}(q(t), p(t), v(t), -1/2) = 0. \qquad (26)
\end{aligned}$$

Equation (26) tells us that p_φ is a constant of the motion denoted a. We are then left with the differential equations

$$\dot\theta = p_\theta,\ \dot p_\theta = a^2 \cot(\theta)(1 + \cot^2(\theta)). \qquad (27)$$

Once these are solved, φ is obtained by integrating in time equation (25) which now has the form:

$$\dot\varphi = a \cot^2(\theta). \qquad (28)$$

Equations (27) and (28) should be solved for every value of $a \in \mathbb{R}$ with the initial conditions

$$\theta(0) = \pi/2, \quad \varphi(0) = 0, \quad p_\theta(0) = \pm 1.$$

The last condition comes from the requirement that the maximized Hamiltonian is now fixed to $\frac{1}{2}$ (corresponding to the choice of taking T in such a way that optimal trajectories are parameterized by arc length). More precisely:

$$\begin{aligned}
\frac{1}{2} &= \mathcal{H}(q(t), p(t), v(t), -1/2) \\
&= v_1(t) p_\theta(t) + v_2(t) a \cot(\theta(t)) \\
&\quad - \frac{1}{2}(v_1(t)^2 + v_2(t)^2) \\
&= \frac{1}{2}(p_\theta(t)^2 + a^2 \cot^2(\theta(t))).
\end{aligned}$$

Requiring this condition at $t = 0$, one gets $p_\theta(0) = \pm 1$.

The system of equations (27) can be solved using again that the maximized Hamiltonian is equal to $\frac{1}{2}$ which implies

$$\dot\theta(t)^2 = 1 - a^2 \cot^2(\theta(t)).$$

Using a separation of variables, we arrive at (with the initial condition $\theta(0) = \pi/2$):

$$\begin{cases} \theta(t) = \arccos\left(\dfrac{\sin(\sqrt{1+a^2}\,t)}{\sqrt{1+a^2}}\right) & \text{if } p_\theta(0) = -1, \\ \theta(t) = \pi - \arccos\left(\dfrac{\sin(\sqrt{1+a^2}\,t)}{\sqrt{1+a^2}}\right) & \text{if } p_\theta(0) = 1. \end{cases} \tag{29}$$

These expressions lead to a simple formula for $x_2(t)$, namely:

$$x_2(t) = \pm\left(\frac{\sin(\sqrt{1+a^2}\,t}{\sqrt{1+a^2}}\right). \tag{30}$$

As already explained, the expression for φ can be obtained by integrating in time equation (28) using the expression (29) with the initial condition $\varphi(0) = 0$. The final result is easier expressed in Cartesian coordinates:

$$\begin{aligned} x_1(t) = {} & \frac{a\sin(a\,t)\sin\left(\sqrt{1+a^2}\,t\right)}{\sqrt{1+a^2}} \\ & + \cos(a\,t)\cos\left(\sqrt{1+a^2}\,t\right), \end{aligned} \tag{31}$$

$$\begin{aligned} x_3(t) = {} & \sin(a\,t)\cos\left(\sqrt{1+a^2}\,t\right) \\ & - \frac{a\sin\left(\sqrt{1+a^2}\,t\right)\cos(a\,t)}{\sqrt{1+a^2}}. \end{aligned} \tag{32}$$

The corresponding controls can be obtained via formulas (23), (24), and (20), or from equation (17), providing

$$\begin{aligned} u_1(t) &= -\dot{x}_1(t)/x_2(t) = \pm\cos(at), \\ u_2(t) &= \dot{x}_3(t)/x_2(t) = \mp\sin(at). \end{aligned}$$

Step 3. In this step, we have to find the initial covector (i.e., $p_\theta(0) \in \{-1, +1\}$ and $a = p_\varphi \in \mathbb{R}$) whose corresponding trajectory arrives at the final target $(x_1, x_2, x_3)(T) = (0, 0, 1)$.

From expression (30), requiring $x_2(T) = 0$ we get $\sin(\sqrt{1+a^2}\,T) = 0$. Then from (31), requiring $x_1(T) = 0$ we arrive at $\cos(a\,T) = 0$. We have then the conditions

$$\sqrt{1+a^2}T = n_1\pi,\ aT = \frac{\pi}{2} + n_2\pi, \quad \text{with } n_1, n_2 \in \mathbb{Z}.$$

Notice that $n_1 > 0$ since $T > 0$, and hence

$$\frac{a}{\sqrt{1+a^2}} = \frac{n_2 + \frac{1}{2}}{n_1},$$

from which we deduce that $|n_2 + \frac{1}{2}| < n_1$. It follows that

$$a = \frac{(n_2 + \frac{1}{2})/n_1}{\sqrt{1 - (\frac{n_2+\frac{1}{2}}{n_1})^2}}. \tag{33}$$

The target is reached at time

$$T = \pi n_1 \sqrt{1 - \left(\frac{n_2 + \frac{1}{2}}{n_1}\right)^2}. \qquad (34)$$

Step 4. The previous step provided a discrete set of trajectories reaching the target. The one arriving in shorter time corresponds to $n_1 = 1$ and $n_2 = 0$ or $n_2 = -1$ for which $T = \pi\frac{\sqrt{3}}{2}$ and $a = \pm 1/\sqrt{3}$. The final expression of the optimal trajectories and optimal controls are:

$$\begin{cases} x_1(t) = \cos^3(t/\sqrt{3}) \\ x_2(t) = \pm\frac{\sqrt{3}}{2}\sin(2t/\sqrt{3}) \\ x_3(t) = -\varepsilon\sin^3(t/\sqrt{3}), \end{cases} \qquad (35)$$

and

$$\begin{cases} u_1(t) = \pm\cos(t/\sqrt{3}) \\ u_2(t) = \mp\varepsilon\sin(t/\sqrt{3}), \end{cases} \qquad (36)$$

where $\varepsilon = \pm 1$ is the sign of a.

Notice that there are two trajectories arriving at time T at the point $(0, 0, 1)$ that are those corresponding to $n_2 = 0$ (i.e., to $a = 1/\sqrt{3}$) and to $p_\theta(0) = \mp 1$ (i.e., to the sign $+$ in formula (30)) and two trajectories arriving at time T at the point $(0, 0, -1)$ that are those corresponding to $n_2 = -1$ (i.e., to $a = -1/\sqrt{3}$). See Section 6.1. The four trajectories obtained in this way are optimal since we know that optimal trajectories exist and the ones that we have selected are the best among all trajectories satisfying a necessary condition for optimality. Notice that, in this example, we can select the optimal trajectories by applying the PMP and finding by hand the best extremals, without using second order conditions nor other sufficient conditions for optimality.

Figures 4 and 5 display respectively the two symmetric extremal trajectories reaching the target state $(0, 0, 1)$ at time T and the time evolution of the corresponding controls.

7 Example 2: A minimum time two-level quantum system with a real control

7.1 Formulation of the control problem

We consider the control of a spin-1/2 particle whose dynamics are governed by the Bloch equation in a given rotating frame [33, 54]:

$$\begin{cases} \dot{M}_x = -\omega M_y, \\ \dot{M}_y = \omega M_x - \omega_x(t) M_z, \\ \dot{M}_z = \omega_x(t) M_y, \end{cases}$$

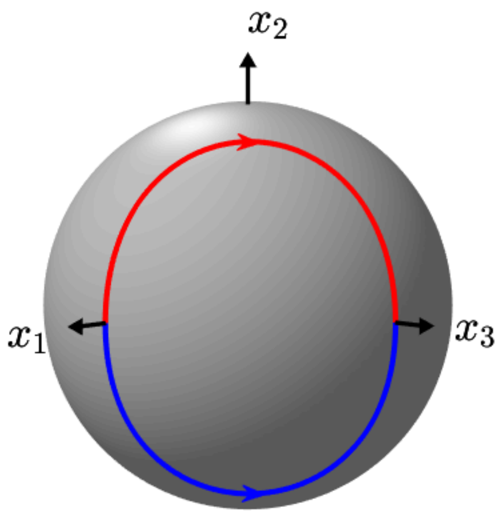

Figure 4: (Color online) Plot of the two extremal trajectories (in red and blue) on the sphere going from the point $(1, 0, 0)$ to the point $(0, 0, 1)$ and minimizing the cost functional C.

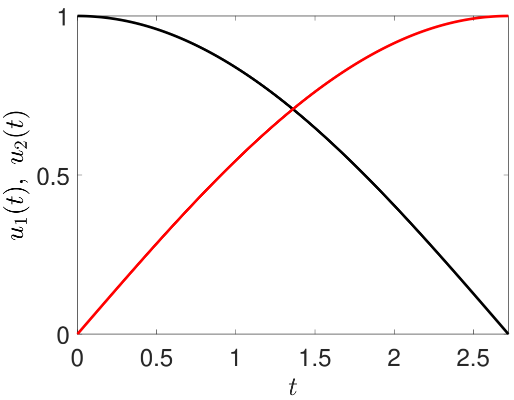

Figure 5: (Color online) Time evolution of the controls u_1 (in black) and u_2 (in red). The control time T and the parameter a are respectively set to $\pi\sqrt{3}/2$ and $-1/\sqrt{3}$.

where $\mathbf{M} = (M_x, M_y, M_z)$ is the magnetization vector and ω the offset term. The system is controlled through a single magnetic field along the x-axis which satisfies the constraint $|\omega_x| \leq \omega_{\max}$. We introduce normalized coordinates $(x, y, z) = \mathbf{M}/M_0$ where M_0 is the thermal equilibrium magnetization, a normalized control $u = \omega_x/\omega_{\max}$ which satisfies the constraint $|u| \leq 1$, and a normalized time $\tau = \omega_{\max} t$ (denoted t below). Dividing the previous system by $\omega_{\max} M_0$, we get that the time evolution of the normalized coordinates is given by the equations

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} -\Delta y \\ \Delta x \\ 0 \end{pmatrix} + u(t) \begin{pmatrix} 0 \\ -z \\ y \end{pmatrix},$$

where $\Delta = \frac{\omega}{\omega_{\max}}$ is the normalized offset. The trajectories of the system lie on the Bloch sphere defined by the equation $x^2 + y^2 + z^2 = 1$. The differential system can be written in a more compact form as

$$\dot{q} = F(q) + u(t)G(q), \tag{37}$$

where $q = (x, y, z)$ is the state of the system, $u(t) \in U = [-1, 1]$, and F, G are vector fields on the sphere, given by

$$F(q) = \Delta \begin{pmatrix} -y \\ x \\ 0 \end{pmatrix}, \qquad G(q) = \begin{pmatrix} 0 \\ -z \\ y \end{pmatrix}$$

The vector fields F and G generate rotations around, respectively, the z- and the x- axes. The bilinear structure of Eq. (37) allows to express the dynamics as

$$\dot{q} = (\mathcal{F} + u\mathcal{G})q,$$

where $\mathcal{F}$ and $\mathcal{G}$ are the skew-symmetric 3×3 matrices

$$\mathcal{F} = \begin{pmatrix} 0 & -\Delta & 0 \\ \Delta & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \mathcal{G} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}.$$

Existence of time-optimal trajectories. By Point 1 in Proposition 1, any initial point q_0 on the Bloch sphere can be connected by an admissible trajectory of the control system to any other point q_1 on the Bloch sphere. In this case the existence of a time-optimal trajectory connecting q_0 to q_1 is a direct consequence of Proposition 6.

7.2 Application of the PMP

The goal of the two control processes that we are considering is to steer the system in minimum time from the north pole $(0, 0, 1)$ of the Bloch sphere to, respectively, the south pole $(0, 0, -1)$ or the state $(1, 0, 0)$. We follow here the results established in [18, 16] (see also [8] for an experimental implementation).

The time-optimal control problem is solved by the application of the PMP. The pre-Hamiltonian can be expressed as

$$\mathcal{H}(q, p, u, p_0) = p(\mathcal{F} + u\mathcal{G})q + p_0,$$

where $p = (p_x, p_y, p_z) \in \mathbb{R}^3$ is the covector and p_0 is a nonpositive constant such that p and p_0 are not simultaneously equal to 0. (Here p is seen as a row vector and q as a column vector.) The value of $\mathcal{H}$ is constantly equal to 0 since the final time is free. The PMP states that the optimal trajectories are solutions of the equations

$$\begin{aligned}
\dot{q}(t) &= \frac{\partial \mathcal{H}}{\partial p}(q(t), p(t), u(t), p_0), \\
\dot{p}(t) &= -\frac{\partial \mathcal{H}}{\partial q}(q(t), p(t), u(t), p_0), \\
\mathcal{H}(q(t), p(t), u(t), p_0) &= \max_{|v| \le 1} \mathcal{H}(q(t), p(t), v, p_0).
\end{aligned}$$

The dynamics of the adjoint state p are given by

$$\dot{p}(t) = -p(t)(\mathcal{F} + u(t)\mathcal{G}). \tag{38}$$

Note that $\|p(t)\|$ is nonzero (since $\mathcal{H} = 0$ and $(p, p_0) \neq 0$) and does not depend on time.

A systematic and geometric approach to identify the extremals of the control problem can be used in this case since the manifold M is of dimension 2 [19]. The first step consists in defining $\Delta_A, \Delta_B : M \to \mathbb{R}$ by

$$\begin{cases} \Delta_A(q) = \det(\mathcal{F}q, \mathcal{G}q) \\ \Delta_B(q) = \det(\mathcal{G}q, [\mathcal{F}, \mathcal{G}]q), \ \ q \in M \end{cases}$$

where

$$\det(v, w) = (v \times w) \cdot q, \quad \text{for } v, w \in T_q M,$$

and $[\cdot, \cdot]$ denotes the matrix commutator operator. We now determine the two sets of points $\Delta_A^{-1}(0)$ and $\Delta_B^{-1}(0)$ on the sphere. The set $\Delta_A^{-1}(0)$ is the circle of equation $y = 0$ on which the two vector fields F and G are parallel. Since $[F, G]$ generates a rotation around the y-axis, we deduce that $\Delta_B^{-1}(0)$ corresponds to the equator $z = 0$. The sphere is thus divided into four parts by the meridian $\Delta_A^{-1}(0)$ and the equator $\Delta_B^{-1}(0)$.

We now come back to the PMP. The maximization condition leads to introduce the switching function

$$\Phi(t) = p(t)\mathcal{G}q(t).$$

In the regular case in which $\Phi(t) \neq 0$, we deduce from the maximization condition that the optimal control is given by the sign of Φ, $u(t) = \text{sign}[\Phi(t)]$. The corresponding trajectory is called a *bang trajectory*. If Φ has an isolated zero in a given time interval, then the control function may *switch* from -1 to 1 or from 1 to -1. A *bang-bang trajectory* is a trajectory obtained after a finite number of switches.

Using the relation (38), we have

$$\dot{\Phi}(t) = p(t)[\mathcal{G}, \mathcal{F}]q(t). \tag{39}$$

In particular, Φ is a C^1 function and, for almost every t,

$$\ddot{\Phi}(t) = p(t)[\mathcal{F}, [\mathcal{F}, \mathcal{G}]]q(t) + u(t)p(t)[\mathcal{G}, [\mathcal{F}, \mathcal{G}]]q(t).$$

Since $[\mathcal{F},[\mathcal{F},\mathcal{G}]] = -\Delta^2\mathcal{G}$ and $[\mathcal{G},[\mathcal{F},\mathcal{G}]] = \Delta\mathcal{F}$, we have, for almost every t,

$$\begin{aligned}\ddot{\Phi}(t) &= -\Delta^2\Phi(t) + u(t)\Delta p(t)\mathcal{F}q(t)\\ &= -\Omega^2\Phi(t) - p_0u(t),\end{aligned} \tag{40}$$

where the second equality follows from the identity $\mathcal{H} = 0$ and $\Omega = \sqrt{1+\Delta^2}$.

Abnormal extremals. Abnormal extremals are characterized by the equality $p_0 = 0$, from which, together with $\mathcal{H} = 0$, we deduce that $\Phi(t) = -p(t)\mathcal{F}q(t)$. In particular, if $\Phi(t) = 0$ at some time t, then $p(t)$ is orthogonal both to $\mathcal{F}q(t)$ and $\mathcal{G}q(t)$. If, moreover, t was not an isolated zero of Φ, then $\dot{\Phi}(t) = 0$, since Φ is C^1. It would follow from (39) that $p(t)$ is orthogonal also to $[\mathcal{G},\mathcal{F}]q(t)$. Since $\mathcal{F}q$, $\mathcal{G}q$, and $[\mathcal{G},\mathcal{F}]q$ span T_qM for every $q \in M$, we would deduce that $p(t) = 0$, contradicting the PMP.

This means that abnormal extremals are necessarily bang-bang. Moreover, we deduce from (40) that the switching times are the zeros of a nontrivial solution of the equation

$$\ddot{\Phi} + \Omega^2\Phi = 0.$$

The length of an arc between any two successive switching times is then equal to π/Ω.

Singular arcs. When the trajectory is normal, there might exist extremals for which Φ is zero on a nontrivial time interval. The control is singular on such an interval, since it cannot directly be obtained from the maximization condition. We call the restriction of the trajectory to an interval on which $\Phi \equiv 0$ a *singular arc*. Singular arcs are characterized by the fact that the time derivatives of Φ at all orders are zero.

Since $p(t)$ is different from zero, the only possibility to have simultaneously $\Phi(t) = 0$ and $\dot{\Phi}(t) = 0$ is that the vectors $\mathcal{G}q(t)$ and $[\mathcal{G},\mathcal{F}]q(t)$ are parallel, i.e., $\det(\mathcal{G}q(t),[\mathcal{G},\mathcal{F}]q(t)) = 0$. Singular arcs are then contained in the set $\Delta_B^{-1}(0)$.

The singular control law u_s can be calculated from (40) by imposing that Φ and its second time derivative are zero, yielding $u_s(t) = 0$. As it could be expected, this control law generates a rotation along the equator. It is admissible because $|u_s| \leq 1$.

Normal bang-bang extremals. Consider a normal extremal and an interior bang arc of duration T between the switching times t_0 and t_0+T on which the control u is constantly equal to $+1$ or -1. Let us normalize $p_0 = -1$. According to (40), the function $\Psi = \Phi - \frac{u}{\Omega^2}$ is a solution of $\ddot{\Psi} + \Omega^2\Psi = 0$. Moreover, since Φ is non-constant then Ψ is nontrivial. Hence, $\Psi(t) = \nu\cos(\Omega t + \theta_0)$ for some $\nu > 0$ and $\theta_0 \in \mathbb{R}$. Moreover, $\nu > 0$ is uniquely identified by u and $\dot{\Phi}(t_0)$ through the equalities $\Psi(t_0) = -\frac{u}{\Omega^2}$ and $\dot{\Psi}(t_0) = \dot{\Phi}(t_0)$. Switchings occur if $\Phi = \Psi + \frac{u}{\Omega^2}$ vanishes and changes sign. Since, moreover, $\mathrm{sign}[u] = \mathrm{sign}[\Phi]$, it follows that Ψ is larger than the negative value $-\frac{1}{\Omega^2}$ on (t_0, t_0+T) when $u = +1$ and smaller than the positive value $\frac{1}{\Omega^2}$ on (t_0, t_0+T) when $u = -1$. Hence T is larger than π/Ω and

$$\dot{\Phi}(t_0+T) = -\dot{\Phi}(t_0).$$

If $\dot{\Phi}(t_0) = 0$, we deduce that $T = 2\pi/\Omega$. Notice that if u is constant to $+1$ or -1, then the integral curves of the vector field $F+uG$ are $2\pi/\Omega$ periodic rotations around the axis spanned by $(1,0,u\Delta)$. Since a time-optimal trajectory cannot self-intersect, we conclude that $T < 2\pi/\Omega$ and $\dot{\Phi}(t_0) \neq 0$.

If $t_0 + T$ is the starting time of another internal bang arc, then by the above considerations the duration of such internal bang arc is also equal to T.

Given a bang-bang normal trajectory, there exists then $T \in (\pi/\Omega, 2\pi/\Omega)$ such that the trajectory is the concatenation of bang arcs of duration T, except possibly for the first and last bang arc, whose length can be smaller than T.

General extremals. As we have seen in the previous paragraphs, if a trajectory contains an internal bang arc, then it is bang-bang. Otherwise the set of zeros of Φ is connected, that is, either Φ has a single zero or it vanishes on a nontrivial singular arc and is different from zero out of it.

To summarize, extremal trajectories are of two types:

- bang-bang trajectories whose internal bang arcs have all the same length $T \in [\pi/\Omega, 2\pi/\Omega)$ (the case $T = \pi/\Omega$ corresponding to abnormal extremals) and for which the first and last bang arcs have length at most T;
- concatenations of a (possibly trivial) bang arc of length smaller that $2\pi/\Omega$, a singular arc on which $u_s = 0$, and another (possibly trivial) bang arc of length smaller that $2\pi/\Omega$.

7.3 Optimal solutions

We solve in this section two time-optimal control problems. Starting from the north pole $(0, 0, 1)$, the goal is to reach in minimum time the points $(0, 0, -1)$ (problem (P1)) and $(1, 0, 0)$ (problem (P2)). To simplify the derivation of the optimal solutions, we assume that $|\Delta| \leq 1$ [18].

Before solving (P1) and (P2), we first derive analytical results describing the dynamics of the system. Consider a bang extremal trajectory starting from the north pole at time $t = 0$ with control $u(t) = \varepsilon = \pm 1$. The corresponding trajectory is given by

$$\begin{cases} x(t) = \frac{\varepsilon\Delta}{\Omega^2}(1 - \cos(\Omega t)) \\ y(t) = -\frac{\varepsilon}{\Omega}\sin(\Omega t) \\ z(t) = 1 + \frac{1}{\Omega^2}(\cos(\Omega t) - 1). \end{cases}$$

The first two times for which $z(t) = 0$ are $t_1 = \frac{1}{\Omega}(\pi - \arccos(\Delta^2))$ and $t_2 = \frac{1}{\Omega}(\pi + \arccos(\Delta^2))$. Notice that all other times for which $z(t) = 0$ are larger than $2\pi/\Omega$ and cannot be the duration of a bang arc of an optimal trajectory.

The optimal solution of (P1) is a bang-bang trajectory with a first switch on the equator at $t = t_1$. The total duration of the process is $t_1 + t_2 = \frac{2\pi}{\Omega}$. A symmetric configuration is possible with a first switch at $t = t_2$. The two trajectories are displayed in Fig. 6. Let us discuss how the optimality of such a trajectory can be asserted. The proposed trajectory is clearly extremal and connects the chosen initial and final points. Since a bang-bang trajectory with at least two internal bang arcs has duration larger than $2\pi/\Omega$, it follows that any bang-bang trajectory with four or more bang arcs has a duration larger than the candidate optimal trajectory (that is, $\frac{2\pi}{\Omega}$). One is then left to compare $\frac{2\pi}{\Omega}$ with finitely many types of trajectories: bang-bang trajectories with two or three bang arcs, and trajectories obtained by concatenation of a bang, a singular, and a bang arc. By setting the initial and final points, this leaves few competitors to the optimal trajectory, which can be easily excluded by enumeration.

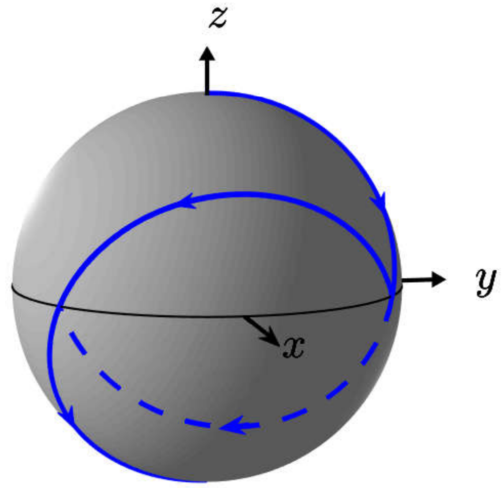

Figure 6: (Color online) Optimal trajectories (in blue) going from the north pole to the south pole of the Bloch sphere. The solid black line indicates the position of the equator. The parameter Δ is set to -0.5.

Let us now discuss the solution of (P2). Using the results of Sec. 7.2, we consider the concatenation of a bang extremal with $u=+1$ during the time t_1 and of a singular extremal during the time t_s. At time $t=t_1$, the trajectory reaches the point $(\Delta,-\sqrt{1-\Delta^2},0)$. We deduce that $t_s=\frac{1}{\Delta}\arctan(\frac{\sqrt{1-\Delta^2}}{\Delta})$. The total duration of the control process is t_1+t_s. The corresponding trajectory is represented in Fig. 7. One can verify that all other candidates for optimality join $(1,0,0)$ in a longer time. The situation is more complicated than for (P1), since here $t_s\to\infty$ as $\Delta\to 0$, so the candidate trajectory should be compared with trajectories with more and more bangs as $\Delta\to 0$. A proof of the optimality of the trajectory described above can be obtained, for instance, using optimal synthesis theory, i.e., describing all the optimal trajectories starting from the north pole, as done in [18].

8 Conclusion and Prospective Views

In this review, we have attempted to give the reader a minimal background on the mathematical techniques of OCT. In our opinion, this is a fundamental prerequisite to rigorously and correctly apply these tools in quantum control.

The objectives of the review are twofold. First, we have highlighted the key concepts of the PMP using ideas based on the finding of extrema of functions of several variables. This analogy gives non-experts an intuition of the tools of optimal control that might seem abstract on first reading. We have then stated the PMP and described in details the different steps to follow in order to solve an optimal control problem. Some are rarely discussed in quantum control such

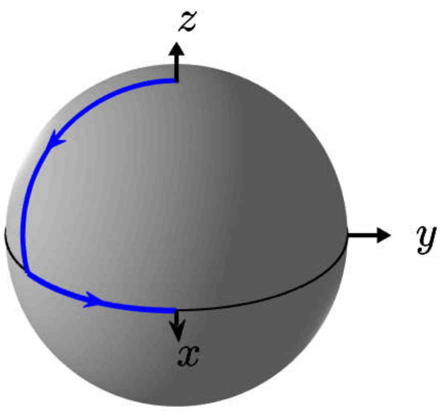

Figure 7: (Color online) Optimal trajectory (in blue) going from the north pole to the point $(1, 0, 0)$ of the x-axis. The solid black line indicates the position of the equator. The parameter Δ is set to 0.5.

as the existence of solutions or abnormal and singular extremals, while they play a crucial role in some problems. Second, we have solved two basics control problems, namely the control of three-level quantum systems by means of two complex resonant fields and the control of a spin 1/2 particle through a real off-resonance driving. The low dimension of the two systems allows us to express analytically the optimal solutions and to give a complete geometric description of the control protocol. Such examples can be used as a starting point by the reader to apply the PMP to more complex quantum systems.

Acknowledgments

The authors have contributed equally to this work. This research has been partially supported by the ANR projects “SRGI” ANR-15-CE40-0018 and “QUACO” ANR-17-CE40-0007-01. This project has received funding from the European Union Horizon 2020 research and innovation program under Marie-Sklodowska-Curie Grant No. 765267 (QUSCO). We gratefully acknowledge useful discussions with Pr. Christiane Koch, who suggested that we write this review and provided advice throughout the project.

References

[1] A. Acín, I. Bloch, H. Buhrman, T. Calarco, C. Eichler, J. Eisert, D. Esteve, N. Gisin, S. J. Glaser, F. Jelezko, S. Kuhr, M. Lewenstein, M. F. Riedel, P. O. Schmidt, R. Thew, A. Wallraff, I. Walmsley, and F. K. Wilhelm. The quantum technologies roadmap: a European community view. *New Journal of Physics*, 20(8):080201, 2018.

[2] A. Agrachev, D. Barilari, and U. Boscain. *A comprehensive introduction to sub-Riemannian geometry*, volume 181 of *Cambridge Studies in Advanced Mathematics*. Cambridge University Press, Cambridge, 2020.

[3] A. A. Agrachev and Y. L. Sachkov. *Control theory from the geometric viewpoint*, volume 87 of *Encyclopaedia of Mathematical Sciences*. Springer-Verlag, Berlin, 2004.

[4] F. Albertini and D. D'Alessandro. Notions of controllability for bilinear multilevel quantum systems. *IEEE Trans. Automat. Control*, 48(8):1399–1403, 2003.

[5] R. Alicki and K. Lendi. *Quantum Dynamical Semigroups*. Springer, Berlin, 1987.

[6] C. Altafini. Controllability properties for finite dimensional quantum Markovian master equations. *J. Math. Phys.*, 44:2357, 2003.

[7] C. Altafini and F. Ticozzi. Modeling and control of quantum systems: an introduction. *IEEE Trans. Automat. Control*, 57(8):1898–1917, 2012.

[8] E. Assémat, M. Lapert, Y. Zhang, M. Braun, S. J. Glaser, and D. Sugny. Simultaneous time-optimal control of the inversion of two spin-$\frac{1}{2}$ particles. *Phys. Rev. A*, 82:013415, 2010.

[9] B. Bonnard and J.-B. Caillau. Metrics with equatorial singularities on the sphere. *Ann. Mat. Pura Appl. (4)*, 193(5):1353–1382, 2014.

[10] B. Bonnard, M. Chyba, and D. Sugny. Time-minimal control of dissipative two-level quantum systems: The generic case. *IEEE Transactions on Automatic Control*, 54(11):2598–2610, 2009.

[11] B. Bonnard, O. Cots, S. J. Glaser, M. Lapert, D. Sugny, and Y. Zhang. Geometric optimal control of the contrast imaging problem in nuclear magnetic resonance. *IEEE Transactions on Automatic Control*, 57(8):1957–1969, 2012.

[12] A. Borzì, G. Ciaramella, and M. Sprengel. *Formulation and numerical solution of quantum control problems*, volume 16 of *Computational Science & Engineering*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2017.

[13] U. Boscain, T. Chambrion, and G. Charlot. Nonisotropic 3-level quantum systems: complete solutions for minimum time and minimum energy. *Discrete Contin. Dyn. Syst. Ser. B*, 5(4):957–990, 2005.

[14] U. Boscain, T. Chambrion, and J.-P. Gauthier. On the K+P problem for a three-level quantum system: optimality implies resonance. *J. Dyn. Control Syst.*, 8:547, 2002.

[15] U. Boscain, G. Charlot, J.-P. Gauthier, S. Guérin, and H.-R. Jauslin. Optimal control in laser-induced population transfer for two- and three-level quantum systems. *J. Math. Phys.*, 43(5):2107–2132, 2002.

[16] U. Boscain and Y. Chitour. Time-optimal synthesis for left-invariant control systems on SO(3). *SIAM J. Control Optim.*, 44(1):111–139, 2005.

[17] U. Boscain, J.-P. Gauthier, F. Rossi, and M. Sigalotti. Approximate controllability, exact controllability, and conical eigenvalue intersections for quantum mechanical systems. *Comm. Math. Phys.*, 333(3):1225–1239, 2015.

[18] U. Boscain and P. Mason. Time minimal trajectories for a spin 1/2 particle in a magnetic field. *J. Math. Phys.*, 47(6):062101, 29, 2006.

[19] U. Boscain and B. Piccoli. *Optimal syntheses for control systems on 2-D manifolds*, volume 43 of *Mathématiques & Applications (Berlin) [Mathematics & Applications]*. Springer-Verlag, Berlin, 2004.

[20] U. Boscain and B. Piccoli. Synthesis theory in optimal control. In *Encyclopedia of systems and control,* J Baillieul, and T Samad editors, Progr. Math. Springer Publishing Company, Incorporated, 2015.

[21] U. Boscain and M. Sigalotti. Introduction to controllability of nonlinear systems. In *Contemporary research in elliptic PDEs and related topics*, volume 33 of *Springer INdAM Ser.*, pages 203–219. Springer, Cham, 2019.

[22] A. Bressan and B. Piccoli. *Introduction to the mathematical theory of control*, volume 2 of *AIMS Series on Applied Mathematics.* American Institute of Mathematical Sciences (AIMS), Springfield, MO, 2007.

[23] H.-P. Breuer and F. Petruccione. *The theory of open quantum systems.* Oxford University, Oxford, 2002.

[24] C. Brif, R. Chakrabarti, and H. Rabitz. Control of quantum phenomena: past, present and future. *New Journal of Physics*, 12(7):075008, 2010.

[25] A. E. Bryson and Y. C. Ho. *Applied Optimal Control: Optimization, Estimation, and Control.* Taylor and Francis, Philadelphia, 1975.

[26] S. Conolly, D. Nashimura, and A. Macovski. Optimal control solutions to the magnetic resonance selective excitation problem. *IEEE Trans. Med. Imag.*, 5:106, 1986.

[27] D. Daems, A. Ruschhaupt, D. Sugny, and S. Guérin. Robust quantum control by a single-shot shaped pulse. *Phys. Rev. Lett.*, 111:050404, 2013.

[28] D. D'Alessandro. *Introduction to quantum control and dynamics.* Applied Mathematics and Nonlinear Science Series. Boca Raton, FL: Chapman, Hall/CRC., 2008.

[29] D. D'Alessandro and M. Dahleh. Optimal control of two-level quantum systems. *IEEE Transactions on Automatic Control*, 46(6):866–876, 2001.

[30] G. Dirr, U. Helmke, I. Kurniawan, and T. Schulte-Herbrueggen. Lie-semigroup structures for reachability and control of open quantum systems: Viewing Markovian quantum channels as Lie semigroups and GKS-Lindblad generators as Lie wedge. *Rep. Math. Phys.*, 64:93, 2009.

[31] D. Dong and I. R. Petersen. Quantum control theory and applications: a survey. *IET Control Theory & Applications*, 4(12):2651–2671, 2010.

[32] P. Doria, T. Calarco, and S. Montangero. Optimal control technique for many-body quantum dynamics. *Phys. Rev. Lett.*, 106:190501, 2011.

[33] R. R. Ernst, G. Bodenhausen, and A. Wokaun. *Principles of Nuclear Magnetic Resonance in One and Two Dimensions.* Clarendon Press, Oxford, 1987.

[34] A. T. Fuller. Minimization of various performance indices for a system with bounded control. *Int. J. Control*, 41:1, 1985.

[35] A. Garon, S. J. Glaser, and D. Sugny. Time-optimal control of SU(2) quantum operations. *Phys. Rev. A*, 88:043422, 2013.

[36] G. T. Genov, D. Schraft, T. Halfmann, and N. V. Vitanov. Correction of arbitrary field errors in population inversion of quantum systems by universal composite pulses. *Phys. Rev. Lett.*, 113:043001, Jul 2014.

[37] S. J. Glaser, U. Boscain, T. Calarco, C. P. Koch, W. Köckenberger, R. Kosloff, I. Kuprov, B. Luy, S. Schirmer, T. Schulte-Herbrüggen, D. Sugny, and F. K. Wilhelm. Training Schrödinger's cat: quantum optimal control. Strategic report on current status, visions and goals for research in Europe. *European Physical Journal D*, 69:279, 2015.

[38] V. Gorini, A. Kossakowski, and E. C. G. Sudarshan. Completely positive dynamical semigroups of n-level systems. *J. Math. Phys.*, 17:821, 1976.

[39] V. V. Grusin. A certain class of hypoelliptic operators. *Mat. Sb.*, 83:456, 1970.

[40] D. Guéry-Odelin, A. Ruschhaupt, A. Kiely, E. Torrontegui, S. Martínez-Garaot, and J. G. Muga. Shortcuts to adiabaticity: Concepts, methods, and applications. *Rev. Mod. Phys.*, 91:045001, 2019.

[41] G. C. Hegerfeldt. Driving at the quantum speed limit: Optimal control of a two-level system. *Phys. Rev. Lett.*, 111:260501, 2013.

[42] V. Jurdjevic. *Geometric control theory*, volume 52 of *Cambridge Studies in Advanced Mathematics.* Cambridge University Press, Cambridge, 1997.

[43] N. Khaneja, R. Brockett, and S. J. Glaser. Time optimal control in spin systems. *Phys. Rev. A*, 63:032308, 2001.

[44] N. Khaneja, S. J. Glaser, and R. Brockett. Sub-Riemannian geometry and time optimal control of three spin systems: Quantum gates and coherence transfer. *Phys. Rev. A*, 65:032301, 2002.

[45] N. Khaneja, B. Luy, and S. J. Glaser. Boundary of quantum evolution under decoherence. *Proceedings of the National Academy of Sciences*, 100(23):13162–13166, 2003.

[46] N. Khaneja, T. Reiss, C. Kehlet, T. Schulte-Herbrueggen, and S. J. Glaser. Optimal control of coupled spin dynamics: design of NMR pulse sequences by gradient ascent algorithms. *Journal of Magnetic Resonance*, 172(2):296 – 305, 2005.

[47] K. Kobzar, S. Ehni, T. E. Skinner, S. J. Glaser, and B. Luy. Exploring the limits of broadband 90^o and 180^o universal rotation pulses. *Journal of Magnetic Resonance*, 225:142 – 160, 2012.

[48] C. P. Koch. Controlling open quantum systems: tools, achievements, and limitations. *Journal of Physics: Condensed Matter*, 28(21):213001, 2016.

[49] C. P. Koch, M. Lemeshko, and D. Sugny. Quantum control of molecular rotation. *Rev. Mod. Phys.*, 91:035005, 2019.

[50] R. Kosloff, S. Rice, P. Gaspard, S. Tersigni, and D. Tannor. Wavepacket dancing: Achieving chemical selectivity by shaping light pulses. *Chemical Physics*, 139(1):201 – 220, 1989.

[51] M. Lapert, Y. Zhang, M. Braun, S. J. Glaser, and D. Sugny. Singular extremals for the time-optimal control of dissipative spin $\frac{1}{2}$ particles. *Phys. Rev. Lett.*, 104:083001, 2010.

[52] M. M. Lee and L. Markus. *Foundations of Optimal Control Theory.* John Wiley and Sons, New York, 1967.

[53] L. Levin, W. Skomorowski, L. Rybak, R. Kosloff, C. P. Koch, and Z. Amitay. Coherent control of bond making. *Phys. Rev. Lett.*, 114:233003, 2015.

[54] M. H. Levitt. *Spin Dynamics: Basics of Nuclear Magnetic Resonance.* Wiley, New York, 2008.

[55] D. Liberzon. *Calculus of variations and optimal control theory.* Princeton University Press, Princeton, NJ, 2012.

[56] G. Lindblad. On the generators of quantum dynamical semi-groups. *Commun. Math. Phys.*, 48:119, 1976.

[57] S. Machnes, E. Assémat, D. Tannor, and F. K. Wilhelm. Tunable, flexible, and efficient optimization of control pulses for practical qubits. *Phys. Rev. Lett.*, 120:150401, Apr 2018.

[58] S. Machnes, U. Sander, S. J. Glaser, P. de Fouquières, A. Gruslys, S. Schirmer, and T. Schulte-Herbrüggen. Comparing, optimizing, and benchmarking quantum-control algorithms in a unifying programming framework. *Phys. Rev. A*, 84:022305, Aug 2011.

[59] J. P. Palao and R. Kosloff. Quantum computing by an optimal control algorithm for unitary transformations. *Phys. Rev. Lett.*, 89:188301, 2002.

[60] A. P. Peirce, M. A. Dahleh, and H. Rabitz. Optimal control of quantum-mechanical systems: Existence, numerical approximation, and applications. *Phys. Rev. A*, 37:4950–4964, 1988.

[61] L. S. Pontryagin, V. Boltianski, R. Gamkrelidze, and E. Mitchtchenko. *The Mathematical Theory of Optimal Processes.* John Wiley and Sons, New York, 1962.

[62] D. M. Reich, M. Ndong, and C. P. Koch. Monotonically convergent optimization in quantum control using Krotov's method. *The Journal of Chemical Physics*, 136(10):104103, 2012.

[63] P. Rembold, N. Oshnik, M. M. Müller, S. Montangero, T. Calarco, and E. Neu. Introduction to quantum optimal control for quantum sensing with nitrogen-vacancy centers in diamond. *AVS Quantum Science*, 2(2):024701, 2020.

[64] S. A. Rice and M. Zhao. *Optimal Control of Molecular Dynamics.* John Wiley and Sons, New York, 2000.

[65] H. Schättler and U. Ledzewicz. *Geometric optimal control*, volume 38 of *Interdisciplinary Applied Mathematics.* Springer, New York, 2012.

[66] S. G. Schirmer, H. Fu, and A. I. Solomon. Complete controllability of quantum systems. *Phys. Rev. A*, 63:063410, 2001.

[67] S. G. Schirmer and A. I. Solomon. Constraints on relaxation rates for n-level quantum systems. *Phys. Rev. A*, 70:022107, Aug 2004.

[68] T. E. Skinner, T. O. Reiss, B. Luy, N. Khaneja, and S. J. Glaser. Application of optimal control theory to the design of broadband excitation pulses for high-resolution NMR. *Journal of Magnetic Resonance*, 163(1):8–15, 2003.

[69] S. E. Sklarz, D. J. Tannor, and N. Khaneja. Optimal control of quantum dissipative dynamics: Analytic solution for cooling the three-level Λ system. *Phys. Rev. A*, 69:053408, 2004.

[70] J. Somloi, V. A. Kazakov, and D. J. Tannor. Controlled dissociation of I_2 via optical transitions between the X and B electronic states. *Chemical Physics*, 172(1):85 – 98, 1993.

[71] D. Stefanatos, N. Khaneja, and S. J. Glaser. Optimal control of coupled spins in the presence of longitudinal and transverse relaxation. *Phys. Rev. A*, 69:022319, Feb 2004.

[72] D. Stefanatos, J. Ruths, and J.-S. Li. Frictionless atom cooling in harmonic traps: A time-optimal approach. *Phys. Rev. A*, 82:063422, Dec 2010.

[73] D. Sugny and C. Kontz. Optimal control of a three-level quantum system by laser fields plus von Neumann measurements. *Phys. Rev. A*, 77:063420, 2008.

[74] N. V. Vitanov, T. Halfmann, B. W. Shore, and K. Bergmann. Laser-induced population transfer by adiabatic passage techniques. *Annual Review of Physical Chemistry*, 52(1):763–809, 2001.

[75] N. V. Vitanov, A. A. Rangelov, B. W. Shore, and K. Bergmann. Stimulated Raman adiabatic passage in physics, chemistry, and beyond. *Rev. Mod. Phys.*, 89:015006, 2017.

[76] F. K. Wilhelm, S. Kirchhoff, S. Machnes, N. Wittler, and D. Sugny. An introduction into optimal control for quantum technologies. *Lecture notes for the 51st IFF Spring School*, 2020.

[77] S. Deffner and S. Campbell. Quantum speed limits: from Heisenberg's uncertainty principle to optimal quantum control. *Journal of Physics A: Mathematical and Theoretical*, 50:453001, 2017.

[78] M. Lapert, R. Tehini, G. Turinici and D. Sugny. Monotonically convergent optimal control theory of quantum systems under a nonlinear interaction with the control field. *Phys. Rev. A*, 78:023408, 2008.

[79] Y. Ohtsuki and K. Nakagami. Monotonically convergent algorithms for solving quantum optimal control problems of a dynamical system nonlinearly interacting with a control. *Phys. Rev. A*, 77:033414, 2008.