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Optimal Control of Quantum Systems by Pontryagin Maximum Principle

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Abstract

Optimal control provides powerful tools and concepts that can be applied to control quantum systems. It has been used extensively to improve the performance of quantum processes in a variety of active areas in quantum technologies. This paper reviews the necessary conditions of optimality in the form of a Pontryagin Maximum Principle (PMP), and introduces its formulations for quantum systems. After formulating an optimal control problem for a two-level quantum system, we then study the application of PMP to obtain an optimal control strategy.

Author Keywords. Quantum Optimal Control, Pontryagin Maximum Principle, Two-level Quantum Systems.

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1. Introduction

Quantum mechanics theory has been one of the most important areas of research for many years now. Developing practical applications based on quantum mechanics laws require the study of their properties and the ways to control and manipulate quantum systems. This science area is highly connected to the works concentrated on integration of concepts and methods of Quantum Optimal Control (QOC) into the fields of quantum information processing. A common feature for all quantum information processing implementations is the need for an extremely precise control of quantum dynamics with much better accuracy than ever before. Quantum systems and control engineering has become increasingly useful for steering quantum devices with high precision (Goerz et al. 2017; Shan et al. 2018; Basilewitsch, Koch, and Reich 2019; Lin, Sels, and Wang 2020).

QOC has proved to be a powerful tool for implementing significant tasks including quantum state preparation and implementation of quantum operations in a number of experiments. These achievements have been enabled due to the optimal control theoretical developments, methods and algorithms which either improve or enable quantum state operations and preparation protocols, such as cold atom hollow-core fiber interface through an optical conveyor belt (Langbecker et al. 2018), ion interactions (Barry et al. 2014), and also state transfer in a Heisenberg spin chain (Shan et al. 2018). For additional examples, we can point out the use of QOC to maximize squeezing in cavity optomechanics (Basilewitsch, Koch, and Reich 2019), as well as controlling quantum many body systems and entanglements (Platzer, Mintert, and Buchleitner 2010), or high-fidelity spin entangled states (Dolde et al. 2014).

Another fundamental task in quantum technologies is the design of robust quantum control systems which ensure reliability in the, generally, fragile quantum context (Ge et al. 2020; Guo

et al. 2019). Quantum system operations may be degraded due to a wide range of perturbations such as laser fluctuations in quantum optics or faulty operations on the generators of quantum resources which may produce inappropriate signals, thereby deteriorating the performance of the system or even causing its instability (De Jesus Napolitano et al. 2021; Nigmatullin and Schirmer 2009). QOC supports the development of fault-tolerant control approaches for quantum systems with faulty signals (Glaudell, Ross, and Taylor 2021). Moreover, QOC proved to be a powerful tool to address decoherence. Recently, a formalism based on Pontryagin's maximum principle (PMP) was applied to determine the time-optimal protocol driving a general initial state to a desired target state by a Hamiltonian with bounded control signals (Lin, Sels, and Wang 2020; Zhou and Jiang 2020).

The above mentioned results and a great number of other successfully done experiments, follow from the adaptation of Optimal Control methods to quantum systems and technologies e.g., see Goerz et al. (2017), Larrouy et al. (2020), Van Frank et al. (2016), Li et al. (2017). The optimization of specific algorithms for specific hardwares has been the most prominent level of quantum computing (Alexeev et al. 2021). Optimization algorithms were derived for quantum gates (Zhou and Jiang 2020), unitary operation under dissipative evolution (Goerz, Reich, and Koch 2014; Nigmatullin and Schirmer 2009), and system-bath models with the aim of decoupling the system from its environment (Grace et al. 2010; De Jesus Napolitano et al. 2021). Moreover, optimization algorithms could determine the best entangling two qubit gates for a physical set (Wu, Wang, and Duan 2018; Zhou et al. 2018). From the above, it is clear that QOC proved to be the tool of choice to get the most efficient performance in the presence of imperfections and decoherence, thus bridging the gap between quantum control and quantum technologies.

2. The Maximum Principle of Pontryagin

Optimal control theory can be regarded as the generalization of classical calculus of variations for problems subject to dynamical constraints with closed velocity sets (Liberzon 2011), whose modern version has been presented through Pontryagin Maximum Principle (PMP), (Pontryagin 1986). An optimal control problem in its general form can be expressed as follows: Given a set X of state functions $x(t)=(x_1,x_2,...,x_n)\in R^n$ and a set U of control functions $u(t)\in U\subset R^m$, find functions $x\in X$ and $u\in U$ such that the dynamical constraint $\dot{x}=f\left(t,x(t),u(t)\right)$, $x_u(0)=x_0$ is satisfied, and the cost functional $J:X\times U\to R$ is minimized, (D'Alessandro 2021). For a system with state vector $x_u(t)$ influenced by control function $u(t)$ over the time interval $t\in[0,T]$, the cost functional J in the form of Bolza is expressed as

$$J:=\Phi\left(x_u(T),T\right)+\int_0^T L\left(x_u(t),u(t),t\right) \tag{1}$$

where Φ and L are smooth functions in R; $\Phi:R^n\times R\to R$, $L:R^n\times R^m\times R\to R$. However Φ only depends on final state and time, while L depends on the whole trajectory $x_u(t)$. Hence, the Pontryagin-Hamilton function, involving the time-varying Lagrange-multiplier vector λ, is written as

$$h\left(x(t),u(t),\lambda(t),t\right)=\lambda^T(t)\,f\left(x(t),u(t),t\right)-L\left(x(t),u(t),t\right). \tag{2}$$

The necessary conditions of optimality in the form of a PMP entails that the maximum condition

$$h\left(x^*,u^*,\lambda,t\right)\geq h\left(x^*,u,\lambda,t\right),\ \forall u\in U \tag{3}$$

and the costate differential equation with its transversality condition, which in this case involves only the terminal condition, must be satisfied so

$$\begin{aligned}\dot{\lambda}^T\left(t\right)&=-\nabla_x h\left(x^*\left(t\right),u^*\left(t\right),\lambda\left(t\right),t\right)\\ \lambda^T\left(T\right)&=\nabla_x\Phi\left(x\left(T\right)\right)\end{aligned}. \tag{4}$$

In the case of free final state problems, there is an additional condition $\frac{\partial\Phi\left(x\right)}{\partial T}\Big|_{x=x(T)}+h\left(T\right)=0$.

3. Optimal Control Formulation for Quantum Systems

The state of quantum systems can be described by pure state vector, density operator or the evolution operator. Here, for the sake of simplicity, we consider the pure quantum state $\vec{\psi}$, whose dynamics can be described through the Schrödinger equation

$$\hbar\frac{d}{dt}\vec{\psi}=-iH\left(u\right)\vec{\psi} \tag{5}$$

where $\vec{\psi}=\vec{\psi}_R+i\vec{\psi}_I$ denotes a column vector corresponding to $\left|\psi\right\rangle$ in a given basis using the Dirac representation (Dirac 1981), with both $\vec{\psi}_R$ and $\vec{\psi}_I$ real vectors, and $-iH\left(u\right)=R\left(u\right)+iI\left(u\right)$ being $R\left(u\right)$ and $I\left(u\right)$ real valued $n\times n$ matrices, which are skew-symmetric and symmetric, respectively. Here, we consider the reduced Planck's constant, $\hbar$, as a unit. Note that the quantum mechanical Hamiltonian in the Schrödinger equation is not the same as the Pontryagin-Hamilton function. According to what we obtained, we can write the following real differential equations

$$\begin{aligned}\frac{d}{dt}\vec{\psi}_R&=R\left(u\right)\vec{\psi}_R-I\left(u\right)\vec{\psi}_I\\ \frac{d}{dt}\vec{\psi}_I&=I\left(u\right)\vec{\psi}_R+R\left(u\right)\vec{\psi}_I\end{aligned} \tag{6}$$

which can be written as $\dot{x}=\tilde{H}\left(u\right)x$, by defining

$$x:=\left[\vec{\psi}_R^T,\vec{\psi}_I^T\right]^T \tag{7}$$

$$\tilde{H}\left(u\right)=\begin{bmatrix}R\left(u\right) & -I\left(u\right)\\ I\left(u\right) & R\left(u\right)\end{bmatrix} \tag{8}$$

the general cost indicated in Equation (1) is then $J:=\tilde{\Phi}\left(x\left(T\right),T\right)+\int_0^T\tilde{L}\left(x\left(t\right),u\left(t\right),t\right)$, so the Pontryagin Hamiltonian is

$$h\left(\lambda,x,u\right)=\lambda^T\tilde{H}\left(u\right)x-\tilde{L}\left(x,u\right) \tag{9}$$

which must satisfy $h(\lambda,x^*,u^*)\geq h(\lambda,x^*,u)$ for every λ, and x^*. The adjoint equation and its boundary condition imply

$$\begin{aligned}\dot{\lambda}^T&=-\lambda^T\tilde{H}(u^*)+\nabla_x\tilde{L}\\ \lambda(T)&=-\nabla_x\tilde{\Phi}^T\left(x^*(T)\right).\end{aligned} \tag{10}$$

4. Application of Pontryagin Maximum Principle for Two-level Quantum Systems

By means of the PMP, we can transform an infinite dimensional optimization problem into a finite dimensional one, which means that the search over a set of functions is replaced by the search for a set of parameters in a finite dimensional space. The optimal control problem for two-level quantum systems has been studied in D'Alessandro and Dahleh (2000), and generalized to n-level quantum systems in Boscain (2003). Here, we review the problem, and

consider a single spin particle $\vec{S} := \frac{1}{2}\{\sigma_x, \sigma_y, \sigma_z\}$, being σ_x, σ_y, and σ_z the so-called Pauli matrices. Spin is an intrinsic property of fundamental particles in quantum mechanics, and a spin-$\frac{1}{2}$ shows that the particle has to be rotated by two full turns before getting to the initial configuration. In nuclear magnetic resonance (NMR) analysis, a spin-$\frac{1}{2}$ is typically controlled through interacting with an electromagnetic field $\vec{B} := \{B_x, B_y, B_z\}$, which is supposed to vary in time while being constant in space. Two components of the field, usually B_x and B_y, are considered to vary in time so that they can change the spin's direction, and the B_z component is considered time invariant (See Figure 1).

The quantum mechanical Hamiltonian is a Hermitian matrix function that is time dependent through controls $u_k(t) \in R$ and, thus, it can be expressed as

$$H(u) = H_0 + \sum_k H_k u_k(t) \tag{11}$$

in which H_0 and H_k are called drift and control Hamiltonians, respectively. By setting the components of the magnetic field as controls, and also by scaling the magnetic field and time, the dynamics of the system can be expressed as

$$\frac{\partial}{\partial t}|\psi\rangle = \frac{1}{2}\left(\bar{\sigma}_z u_z + \bar{\sigma}_x u_x(t) + \bar{\sigma}_y u_y(t)\right)|\psi\rangle \tag{12}$$

In which the matrices $\bar{\sigma}_{x,y,z}$ are the multiples of Pauli matrices spanning the Lie algebra $su(2)$ defined as

$$\bar{\sigma}_x = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix},\ \bar{\sigma}_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix},\ \bar{\sigma}_z = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} \tag{13}$$

with the commutator bracket satisfying

$$[\bar{\sigma}_z, \bar{\sigma}_x] = 2\bar{\sigma}_y,\ [\bar{\sigma}_x, \bar{\sigma}_y] = 2\bar{\sigma}_z,\ [\bar{\sigma}_y, \bar{\sigma}_z] = 2\bar{\sigma}_x \tag{14}$$

Following the same procedure explained in the previous section, we can obtain a Lie algebra isomorphism mapping $\bar{\sigma}_x \leftrightarrow \tilde{H}_x(u)$, $\bar{\sigma}_y \leftrightarrow \tilde{H}_y(u)$, $\bar{\sigma}_z \leftrightarrow \tilde{H}_z(u)$ as following

$$\bar{\sigma}_x = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} + i\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \rightarrow \tilde{H}_x = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{15 a}$$

$$\bar{\sigma}_y = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} + i\begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} \rightarrow \tilde{H}_y = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \tag{15 b}$$

$$\bar{\sigma}_z = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 0 & 0 \end{pmatrix} + i\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \rightarrow \tilde{H}_z = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \tag{15 c}$$

satisfying the commutation relations $\left[\tilde{H}_x,\tilde{H}_y\right]=2\tilde{H}_z$, $\left[\tilde{H}_y,\tilde{H}_z\right]=2\tilde{H}_x$, $\left[\tilde{H}_z,\tilde{H}_x\right]=2\tilde{H}_y$. Hence, the problem transformation to a real one, and also considering that $x:=\left[\vec{\psi}_R^T,\vec{\psi}_I^T\right]^T$, results in the following dynamics

$$\dot{x}=\frac{1}{2}\left(\tilde{H}_x u_x(t)+\tilde{H}_y u_y(t)+\tilde{H}_z u_z\right)x\,. \tag{16}$$

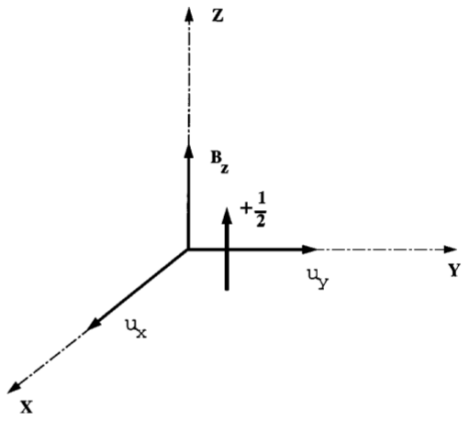

Figure 1: Spin-$\frac{1}{2}$ controlled by an electromagnetic field in NMR experiments (D'Alessandro and Dahleh 2000)

Depending on the problem, we may choose different performance functionals. For instance, we may intend to minimize the energy of the laser electric field in $[0,T]$ used in controlling the quantum system, so the cost functional is

$$J(u)=k\int_0^T u^2(t)\,dt \tag{17}$$

for some constant $k>0$. If the filtration of high frequency elements of control field is of interest, then we can simply choose a cost functional of the type $J(u)=k\int_0^T\left(\frac{du}{dt}\right)^2 dt$. In some cases, it is very important that the control function drives the state of the system towards a desired target state at time T. In this case, it is of interest to maximize the overlap of the desired state $|\psi_f\rangle$ with the final state $|\psi(T)\rangle$, which is called fidelity for pure quantum states.

Moreover, the cost functional may also be a composition of these if it is of interest to choose a trade-off between two distinct goals which, may, for example, transfer the state of the system to some desired target state, while, also minimizing the energy of the applied control field. Hence, the cost functional will have the form

$$J(u_x,u_y)=-\mathrm{Re}\left(\vec{\psi}^{\dagger}(T)\vec{\psi}_f\right)+k\int_0^T\left(u_x^2(t)+u_y^2(t)\right)dt\,. \tag{18}$$

Now, we can reformulate the cost by denoting that x represents the $2n$ dimensional real vector that corresponds to $\vec{\psi}$ as

$$J(u_x,u_y)=-\left(x^T(T)x_f\right)+k\int_0^T\left(u_x^2(t)+u_y^2(t)\right)dt\,. \tag{19}$$

The Pontryagin Hamilton function is then expressed as

$$h=\frac{1}{2}\lambda^T\left(\tilde{H}_x u_x(t)+\tilde{H}_y u_y(t)+\tilde{H}_z u_z\right)x-k\left(u_x^2(t)+u_y^2(t)\right) \quad (20)$$

Now, we can apply the necessary conditions for optimality in the form of the PMP. For this problem, since the cost functional is not dependent on x, the adjoint equation has the same form as state equation, so

$$\dot{\lambda}=\frac{1}{2}\left(\tilde{H}_x u_x(t)+\tilde{H}_y u_y(t)+\tilde{H}_z u_z\right)\lambda \quad (21)$$

To obtain the form of the optimal controls, PMP implies that $u^*=\arg\max h\left(t,x^*,u,\lambda\right)$, so

$$\begin{aligned}\frac{\partial h}{\partial u_x}=0\rightarrow\frac{1}{2}\lambda^T\tilde{H}_x x-2ku_x(t)=0\rightarrow u_x=\frac{1}{4k}\lambda^T\tilde{H}_x x\\ \frac{\partial h}{\partial u_y}=0\rightarrow\frac{1}{2}\lambda^T\tilde{H}_y x-2ku_y(t)=0\rightarrow u_y=\frac{1}{4k}\lambda^T\tilde{H}_y x\end{aligned} \quad (22)$$

We can replace u_x and u_y in both state and costate equations, and, then, solve the obtained two point boundary value problem. However, when the controls are differentiable functions, we can also take the derivatives of the controls, and, then, by means of state and costate equations and also the commutation relations, try to obtain the form of optimal controls. By differentiating the controls, we have

$$\begin{aligned}\dot{u}_x&=\frac{1}{4k}\left(\lambda^T\tilde{H}_z x u_y-u_z u_y\right)\\ \dot{u}_y&=\frac{1}{4k}\left(-\lambda^T\tilde{H}_z x u_x+u_z u_x\right)\end{aligned} \quad (23)$$

Obviously we can write

$$\dot{u}_x=\alpha u_y,\ \ \dot{u}_y=-\alpha u_x \quad (24)$$

where $\alpha=\frac{1}{4k}\left(\lambda^T\tilde{H}_z x-u_z\right)$, so we can conclude the form of controls are sinusoidal functions;

$$u_x(t)=M\cos(\omega t+\gamma),\ \ u_y(t)=M\sin(\omega t+\gamma) \quad (25)$$

for which we can obtain the optimal values of M, ω, and γ by substituting the controls and solving the differential equations. These two controls form the controlling components of the electromagnetic field used in NMR experiments.

5. Conclusions

To conclude, we aimed to provide the basic mathematical techniques that can be used to formulate and solve an optimal control problem for a fundamental quantum system. As seen, by applying the necessary conditions of PMP, we can simply get to the result that the controls obtained by solving the PMP conditions are the ones practically used in NMR experiments. The formulations explained in this work can be used as a starting point and, surely, be extended to address much more complex quantum systems.

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