High Fidelity Quantum State Transfer by Pontryagin Maximum Principle

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Abstract: High fidelity quantum state transfer is an essential part of quantum information processing. In this regard, we address the problem of maximizing the fidelity in a quantum state transformation process satisfying the Liouville-von Neumann equation. By introducing fidelity as the performance index, we aim at maximizing the similarity of the final state density operator with the one of the desired target state. Optimality conditions in the form of a Maximum Principle of Pontryagin are given for the matrix-valued dynamic control systems propagating the probability density function. These provide a complete set of relations enabling the computation of the optimal control strategy.

Keywords: quantum optimal control, quantum fidelity measures, Pontryagin maximum principle

1. INTRODUCTION

Quantum control theory, (Dehaghani and Lobo Pereira, 2021), studies how the dynamics of an atomic or subatomic-level system can be manipulated by means of appropriate external electromagnetic fields or forces, designated by control, in order to maximize a given performance criterion to the system. For many quantum control protocols, the control law is required to be open-loop, that is, only a function of time and does not require state feedback data provided, for example, by measurements. In this context, optimal control theory provides powerful tools, (Glaser et al., 2015). By means of Quantum Optimal Control (QOC) theory, it is possible to formulate quantum control problems in order to seek a set of admissible controls satisfying the system dynamics while minimizing a cost functional in order to obtain a control law. In other words, QOC aims to compute the shape and sequence of control pulses to achieve a given task in an optimum way. Moreover, the high versatility of the optimal control problem formulation provides advantages such as the incorporation of diverse experimental constraints or limitations, while the optimality leads to the exploitation of physical limits of the driven dynamics, (Boscain et al., 2021). The investigation of optimal controls to quantum systems has been done through adaptation of traditional optimal control tools such as the variational method, (Kogut and Leugering, 2011), Pontryagin maximum principle, (Lin et al., 2019; Yang et al., 2017; D’alessandro and Dahleh, 2001), converge iterative algorithms, (Wilhelm et al., 2020), among others.

The power of QOC has been instrumental in the design of several experiments, such as preparation of motional states of Bose-Einstein condensate with optimized control sequences, (van Frank et al., 2014), and loading improvement of ultracold atoms in an optical lattice, (Rosi et al., 2013), to name just a few. Pulses computed by using QOC allowed for error-resistant single qubit gates, (Timoney et al., 2008). QOC of a single qubit also led to the design of high-dynamic-range imaging of nanoscale magnetic fields, (Häberle et al., 2013). Virtual transitions and leakage outside the qubit manifold was also overcome in quantum processors based on superconducting circuits by means of QOC results, (Lucero et al., 2010; Motzoi et al., 2009). QOC has proved to be a key tool for quantum engineering in complex Hilbert spaces, (Larrouy et al., 2020). These experiments and several others were preceded by a large number of theoretical considerations on how QOC may impact on the control design of quantum operations including state preparation, (Rojan et al., 2014; Günther et al., 2021), ranging from squeezed states, (Grond et al., 2009), and cluster-states, (Fisher et al., 2009), to many-body entangled state, (Caneva et al., 2012), state transfer problem, (Ying-Hua et al., 2016; Zhang et al., 2016; Guo et al., 2018), and quantum gate synthesis, (Huang and Goan, 2014; Chou et al., 2015; Berrios et al., 2012).

Amongst the above-mentioned problems, quantum state transfer has received considerable attention due to the high importance of trustworthy information transfer in quantum networks. In this regard, high-quality quantum information transport is crucial for practical models used in quantum computation, (DiVincenzo, 1995). A protocol for performing fast and high fidelity quantum state transfer in quantum spin $-\frac{1}{2}$ chains has been proposed in...
as a linear combination of the so-called Pauli matrices can be represented by a Dirac representation, (Dirac, 1981). In quantum information theory, information is coded by means of qubits, which can be is represented by

$$|\psi\rangle = \cos \frac{\theta}{2} |0\rangle + e^{i\varphi} \sin \frac{\theta}{2} |1\rangle \tag{1}$$

where $\theta \in [0, \pi]$, and $\varphi \in [0, 2\pi]$. Here, $|0\rangle$ and $|1\rangle$ correspond to the states 0 and 1 for a classical bit, respectively, (Paul, 2007). Such quantum state represented by the wave function $|\psi\rangle$ is called a pure state.

In the density operator formalism, quantum states are described by density operators $\rho : \mathbb{H} \to \mathbb{H}$ on the system’s Hilbert space $\mathbb{H}$. For an ensemble $\{p_j, |\psi_j\rangle\}$ of pure states, the density operator is defined as

$$\rho \equiv \sum_j p_j |\psi_j\rangle \langle \psi_j| \tag{2}$$

in which $\langle \psi_j| = (|\psi_j\rangle)^\dagger$ and $\sum_j p_j = 1$, (Cong, 2014). For a pure quantum state, $\rho = |\psi\rangle \langle \psi|$ and $tr (\rho^2) = 1$, while for a mixed state $tr (\rho^2) < 1$. Here $tr A$ denotes the trace of the matrix $A$. An arbitrary state $\rho$ of a qubit can be written as a linear combination of the so-called Pauli matrices $\sigma = (\sigma_x, \sigma_y, \sigma_z)$, which provide a basis for $2 \times 2$ self-adjoint matrices as

$$\rho = \frac{1}{2} (I + r \sigma) \tag{3}$$

where the real vector $r = (r_x, r_y, r_z)$ forms the coordinates of a point within the Bloch Sphere, and $J$ indicates the $2 \times 2$ identity matrix. Hence, for pure states $|r| = 1$, while $|r| < 1$ represents mixed states, (Wilde, 2011).

There are several approaches for modeling a quantum system to be controlled. In the Schrödinger model of quantum mechanics, bilinear models, including Schrödinger and quantum Liouville equations, are used to describe closed quantum systems. Schrödinger equation implies the evolution of the state vector $|\psi(t)\rangle$ as

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H(t) |\psi(t)\rangle, \quad |\psi(t)\rangle_{|t=0} = |\psi_0\rangle \tag{4}$$

where $H(t)$, the Hamiltonian of the system, is a Hermitian operator on $\mathbb{H}$, and $\hbar$ is the reduced Planck’s constant, considered as a unit for convenience. The system control can be realized by a set of control functions $u_k(t) \in \mathbb{R}$, which is coupled to the quantum system via time independent interaction Hamiltonians $H_k (k = 1, 2, \ldots)$. Therefore, the total Hamiltonian $H(t) = H_d + \sum_k u_k(t) H_k$ determines the controlled evolution. Here, $H_d$ indicates the drift Hamiltonian, and the $H_k$‘s are the interaction Hamiltonians.

For systems in mixed states, quantum statistical ensemble can be characterized via the statistical operator $\rho (t) = U (t, t_0) \rho (t_0) U^\dagger (t, t_0)$, in which $\rho (t_0) = \sum_\alpha u_\alpha |\psi_\alpha (t_0)\rangle \langle \psi_\alpha (t_0)|$ with $u_\alpha$ indicating positive weights and $|\psi_\alpha (t)\rangle$ being the normalized state vector evolving in time according to (4). By differentiating $\rho (t)$ with respect to time, the equation of motion for density operator, referred to as Liouville-von Neumann equation,

$$\dot{\rho} (t) = -i \hbar [H (t), \rho (t)] \tag{5}$$

is obtained, where $\rho (t)$ is the variable to be controlled. Equation (5) can be written in a form analogous to the classical Liouville equation as $\dot{\rho} (t) = \mathcal{L} (t) \rho (t)$, in which $\mathcal{L}$ is Liouville super-operator, (Cong, 2014; Breuer et al., 2002).

3. Short Overview on Quantum Optimal Control

The question that we address is: how we can drive (4) from an initial state $|\psi_0\rangle$ to a desired target state $|\psi_f\rangle$ while minimizing the cost functional? There are several methods to design the optimal controller in quantum systems, which vary according to the choice of the cost function, the construction of the Pontryagin-Hamilton function, and the computation scheme using the Maximum Principle conditions, (Cong, 2014).

A general optimal control problem can be formulated as follows: Given a set $\mathcal{X}$ of state functions $x : \mathbb{R} \to \mathbb{R}^n$, and a set $\mathcal{U}$ of control functions $u : \mathbb{R} \to \mathbb{R}^m$, find the functions $x \in \mathcal{X}$ and $u \in \mathcal{U}$, which minimize a cost functional $J : \mathcal{X} \times \mathcal{U} \to \mathbb{R}$ and satisfy the dynamical constraint $\dot{x} = f (x, u)$. We can formulate any optimal control problem as a specific case of the mentioned general problem, (d’Alessandro, 2021). Hence, for a system with state vector $x$ driven by controls $u$ over a certain (fixed or variable) time interval $[0, T]$, the scalar real-valued objective functional $J$ in the form of a problem of Bolza, is expressed by

$$(Zhang et al., 2016), by using QOC based on the Krotov algorithm. Another research has shown that QOC allows a success rate of more than 98% in an arbitrary state transfer process for a non-Markovian system implemented with an optimal control, (Ying-Hua et al., 2016). However, despite a number of researches based on QOC algorithms, the Pontryagin Maximum Principle is still far from being fully exploited for quantum systems, and, even more for the case when the dynamics described the evolution of the matrix-valued probability density function are considered. In this context, we consider a closed system described by Liouville-von Neumann equation, and formulate the control problem of quantum state transfer aiming at the maximization of the fidelity criterion. Moreover, we derive a shooting algorithm to solve the two point boundary value problem entailed by the Maximum Principle of Pontryagin by using a multiple shooting method.

The paper is organized as follows. In Section 2, after a brief description of pure and mixed quantum states, we describe the models used for closed quantum systems. The current state of the art concerning the use of the Pontryagin Maximum Principle in the context of quantum systems are described in Section 3. In the next section, we formulate a quantum state transfer in the context of optimal control subjected to Liouville-von Neumann equation with the aim of maximizing fidelity. In section 5, we present an iterative algorithm to solve the optimal control problem. The article ends with brief conclusions on the reported research as well as a brief overview on prospective research challenges.
\[ J := \Phi(x(T), T) + \int_0^T L(x(t), u(t), t) \, dt \]  

(6)

with \( \Phi \) and \( L \) smooth functions \( \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}, \mathbb{R}^n \times \mathbb{R}^m \times \mathbb{R} \to \mathbb{R} \), respectively. The task is to maximize \( J \) subject to the condition that the system dynamics are satisfied, with \( x(0) = x_0 \), and \( u(t) \) restricted to the set of admissible controls \( U \). (Dehaghi and Lobo Pereira, 2021).

For many practical control problems in quantum setting, optimal control theory is a powerful tool to achieve quantum control objectives, (Peirce et al., 1988; Werschkun and Gross, 2007). The key concept of optimal control is that the control law will be obtained by minimizing a cost function that drives system (4) from \( \psi(0) = |\psi_0\rangle \) to the desired \( \psi(T) = |\psi_f\rangle \). Let consider the problem of determining the control fields \( u \in L^2(\mathbb{C}, [0, T]) \) while satisfying equation (4). Suppose that we want to fulfill the following optimal criteria:

- The control sequence brings the system at time \( T \) to the desired state \( \psi_d \in \mathbb{C}^n \).
- The limited laser resources are taken into account through a minimization of the control field effort.
- The population of intermediate states that suffer strong environment losses may need to be suppressed.

The above mentioned constraints can be summarized in the cost functional, (Peirce et al., 1988; James, 2021; Borzi et al., 2002),

\[ J(|\psi\rangle, u) = \frac{1}{2} \| \psi(T) \rangle - |\psi_f\rangle \|^2_{C^*} + \sum_{j=1}^n \alpha_j \| \psi_j \|^2_{L^2([0, T])} \]

in which \( \gamma > 0 \) and \( \alpha_j \geq 0 \) are the weighting factors. We also may add further constraints in the same way. The problem of optimal control for minimizing cost functional (6) subject to equation (4) under normal conditions admits a solution \( (\psi, u) \in H^1(\mathbb{C}^n, [0, T]) \times L^2(\mathbb{C}, [0, T]) \), (Peirce et al., 1988; James, 2021; Borzi et al., 2002; Fattorini et al., 1999). In order to calculate the necessary optimality conditions of first order, the method of Lagrange multipliers is used. Hence, the Lagrangian function is defined as

\[ L(|\psi\rangle, |p\rangle, u) = J(|\psi\rangle, u) + \text{Re} \langle p, i\dot{\psi} - H\psi \rangle \]

(8)

where \( \langle \phi, \psi \rangle = \int_0^T \dot{\phi}^* \psi \, dt \). Here, \( \psi^* \) means the complex conjugate and \( \langle \cdot, \cdot \rangle \) is the usual vector-scalar product in \( \mathbb{C}^n \).

Consider the minimization problem

\[ L(|\tilde{\psi}|, |\tilde{p}|, \tilde{u}) = \inf_{|\psi\rangle \in X^0, |p\rangle \in U} L(|\psi\rangle, |p\rangle, u) \]

\[ U = L^2(\mathbb{C}^n, [0, T]) \]

\[ X^0 = \{ \psi : \psi(0) = \psi_0 \} \]

(9)

The necessary conditions for problem (9) are obtained by equating to zero the Fréchet derivative of \( L \) with respect to \( |\psi\rangle \), \( |p\rangle \), and \( u \), Dehaghi and Lobo Pereira (2021).

Therefore, the optimality system entails:

\[ |\dot{\psi}\rangle = -i (H_d + H_k u) |\psi\rangle, \quad |\psi(0)\rangle = |\psi_0\rangle \]

\[ |\dot{p}\rangle = -i (H_d + H_k u) |p\rangle - q, \quad |p(T)\rangle = -i (|\psi(T)\rangle - |\psi_d\rangle) \]

(10)

where \( q_j = \alpha_j \psi_j \), and \( u = u_{Re} + i u_{Im} \). (Cong, 2014; Borzi et al., 2002; Zhu and Rabitz, 1998).

4. FORMULATION OF THE OPTIMAL CONTROL PROBLEM

Consider the following optimal control problem \( (P_1) \)

Minimize \( -F(\rho, \sigma) \)

subject to \( \dot{\rho}(t) = F(\rho(t), u(t)) \)

\[ \rho(0) = \rho_0 \in \mathbb{R}^{n \times n} \]

\[ u(t) \in U := \{ u \in L_\infty : u(t) \in \Omega \subset \mathbb{R}^m \} \]

where \( \dot{\rho} := \frac{d\rho}{dt}, t \in [0, 1] \) determines the time variable, \( \rho \) is the state variable in \( \mathbb{R}^n \times \mathbb{R}^n \) supposed to satisfy the differential constraints \( \dot{\rho} = F(\rho, u) \) according to Liouville-von Neumann equation (5), and \( \rho_0 \) is the so-called initial quantum state. \( u(\cdot) \) is the measurable bounded function termed as control. Here, we aim to maximize fidelity \( F \) so that the density operator \( \rho \) has the maximum overlap with the target \( \sigma \). The most widely-used generalization of fidelity that has been indicated in the literature is the Uhlmann-Jozsa fidelity, (Jozsa, 1994), which represents the maximal transition probability between the purification of a pair of density matrices, \( \rho \) and \( \sigma \), (Liang et al., 2019), and is defined as

\[ F(\rho, \sigma) := \max_{|\varphi\rangle, |\varphi'\rangle} \langle |\varphi\rangle, |\varphi'\rangle |^2 \]  

(11)

satisfying the following properties, (Liang et al., 2019),

i. \( F(\rho, \sigma) = F(\sigma, \rho) \)

ii. \( 0 \leq F(\rho, \sigma) \leq 1 \) \( \forall \rho, \sigma, \quad F(\rho, \rho) = 1 \)

iii. \( F(\rho, \sigma) = tr(\sigma \rho) \) if either \( \rho \) or \( \sigma \) is a pure state.

iv. \( F(U\rho U^\dagger, U\sigma U^\dagger) = F(\rho, \sigma) \) for all unitary operations \( U \).

The fidelity criteria signifies a security level for quantum state transformation or the effectiveness of quantum gate synthesis, so is of high importance in quantum systems.

5. NECESSARY CONDITIONS OF OPTIMALITY IN THE FORM OF A MAXIMUM PRINCIPLE

The Pontryagin-Hamilton function \( \mathcal{H} \) is defined for almost all \( t \in [0, T] \) by introducing the adjoint variable \( \pi \), which is a time-varying multiplier vector designated by costate or adjoint variable of the system. Thus,

\[ \mathcal{H}(\rho, u, \pi) = tr(\pi^\dagger F(\rho, u)) \]

(12)

According to the Pontryagin’s Maximum Principle, for the optimal state trajectory \( \rho^* \) and the corresponding
adjoint variable, the matrix \( \pi \), the optimal control \( u^*(t) \),
maximizes the Pontryagin-Hamiltonian function \( \mathcal{H} \), i.e.,
for almost all \( t \in [0, T] \),
\[
\mathcal{H}(\rho^*(t), u, \pi(t)) \leq \mathcal{H}(\rho^*(t), u^*(t), \pi(t))
\]
for all admissible control values \( u \in \Omega \). Additionally, the
adjoint equation, and its terminal conditions imply that,
Lebesgue a.e.,
\[
(\pi^1(t), \dot{\pi}^1(t)) = \nabla_{\rho^1} \rho^1(\rho^1(t), u^*(t), \pi(t))
\]
and the boundary condition at the final time is obtained
\[
\rho^1(1) = \pi^1(1) = \nabla_{\rho^1} F(\rho^1(1), \sigma(1))
\]
From (14) we can obtain
\[
-\dot{\pi}^1(t) = \nabla_{\rho^1} t r(\pi^1(t) F(\rho^1(t), u^*(t)))
\]
\[
= -i \frac{\partial}{\partial \rho} t r(\pi^1(t) [H^*(t), \rho(t)])
\]
\[
= -i \frac{1}{\hbar} (\pi^1(t) H^*(t) - H^*(t) \pi^1(t))
\]
\[
= \frac{1}{\hbar} [H^*(t), \pi^1(t)] .
\]  
Remark that the dependence of \( \mathcal{H} \) on \( t \) is through the
control variable, and, hence, \( H^*(t) \) denotes \( H \) evaluated at
each time along the optimal control \( u^* \). It is straightforward
to conclude that the differential equation (16) has the
formal solution
\[
\pi^1(t) = e^{t \int F(\rho^1(s), u^*(s))ds} \pi^1(0)
\]  
and the boundary condition at the final time is obtained
by computing
\[
\pi^1(1) = \nabla_{\rho} t r(\pi^1(t) F(\rho^1(t), \sigma(1)))
\]
for which by means of Taylor expansion at the point \( \rho = I \),
we have
\[
\sqrt{\rho} = \sum_{k=0}^{n-1} \frac{1}{k!} \frac{d^k}{dp^k} \sqrt{\rho} |_{p=I} (\rho - I)^k
\]
which, in turn, under some conditions, the application of the
Cayley–Hamilton theorem yields, for a certain
coefficients \( \alpha_k, k = 0, \ldots, n - 1 \), being \( n \) the dimension
of the square matrix \( \rho \),
\[
\sqrt{\rho} = \sum_{k=0}^{n-1} \alpha_k (\rho - I)^k.
\]
Thus, by using matrixical calculus, we obtain
\[
\pi^1(1) = 2t \sqrt{\rho(1) \sigma(1)} \nabla_{\rho} t r(\sqrt{\rho(1) \sigma(1)})
\]
\[
= 2t \sqrt{\rho(1)} \sigma(1) \sum_{k=0}^{n-1} \sum_{i=0}^{k-1} \alpha_k \sqrt{\rho(1)} \sigma(1) \rho(1)^{k-i-1}
\]
where \( \rho(1) = \rho(t) - I \).

6. APPLICATION OF THE PONTRYAGIN MAXIMUM PRINCIPLE

Let us consider a spin \(-\frac{1}{2}\) particle in an invariable mag-
netic field \( B_0 \) along z-axis as the controlled system, the
control magnetic fields on the x-y plane is given by
\[
\gamma B_x = u(t) \cos(\omega t + \phi)
\]
\[
\gamma B_y = -u(t) \sin(\omega t + \phi)
\]
where \( \gamma \) is the magnetic ratio of spin particle, and \( u(t) \) is
a real valued number indicating the Rabi frequency of the
particle. Hence, The system Hamiltonian \( H(t) \), composing
of the free Hamiltonian \( H_0 \) and the control Hamiltonian
\( H_c \), is expressed as
\[
H(t) = -\frac{\gamma \hbar}{2} (B_0 \sigma_z + B_x(t) \sigma_x + B_y(t) \sigma_y)
\]
\[
= -\frac{\hbar}{2} \left( u(t) e^{-i(\omega t + \phi)} \right)
\]
in which \( \gamma B_0 = \omega_0 \) and \( \sigma_z, \sigma_y, \) and \( \sigma_x \) are the so-called
Pauli matrices given by
\[
\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}
\]
Once the matrix \( H(t) \) is known, the matrix \( U(t) \) of the system
can be computed by
\[
U(t) = e^{-\frac{\hbar}{\gamma} \int_0^t H(s) ds}
\]
The system dynamics are given by the Liouville equation
whose solution is analogous to the one of the adjoint
system considered in a previous section, that is,
\[
\rho(t) = U(t) \rho(0) U(t)^\dagger
\]
Here, we consider a state transfer problem from \([0|0)\) to \([1|1)\),
so \( \rho(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \) and \( \sigma(1) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \).

In this section, we present a time discretized computational
scheme to solve the optimal control problem associated with
(\(P_1\)) by using an indirect method based on the
Maximum Principle. Let \( N \) be the number of discrete time
subintervals. Given the smooth properties of the problems
data, let us consider a uniform discretization. Thus, we
consider the \( N \) points \( t_k = \frac{k}{N} \) for \( k = 0, \ldots, N - 1 \) and
denote the value of any function \( f(t_k) \) by \( f_k \). We consider
the both the system dynamics, and the adjoint differential
equations approximated by a first order Euler approxima-
ation. Higher order methods yield better approximations
but our option is made to keep the presentation simple.
Let \( j = 0, \ldots \) be the iterations counter, and we denote the
\( j^{th} \) iteration of the function \( f \) at time \( t_k \) by \( f_{jk} \).
The proposed algorithm is as follows:

**Step 1 - Initialization.**
Let \( j = 0 \), and initialize the values of \( u_k^j \) for \( k = 1, \ldots, N - 1 \), \( \omega^j \), and \( \phi^j \) in (22).

**Step 2 - Computation of the state trajectory.**
For \( k = 0, \ldots, N - 1 \), let \( \rho_{k+1}^j = \rho_k^j + \frac{1}{k} \beta_k^j \).

**Step 3 - Computation of the adjoint trajectory.**
Compute \( \pi_{N}^j \) by using (20) with \( \rho_N^j \) computed in Step
2. Compute \( \pi_k^j \) by using the discretized version of (17),
that is, \( \pi_k^j = U_j^j \pi_k^{j+1} \) \( U_j^j = e^{i \sum_{k=0}^{N-1} \pi_k^{j+1}} \)
being \( H_k^j \) the Hamiltonian of the system dynamics
with the value control \( u^j \) at time \( t_k \).
For \( k = 0, \ldots, N - 1 \), let \( \pi_{k+1}^j = \pi_k^j + \frac{1}{k} \beta_k^j \).

**Step 4 - Computation of the Pontryagin Hamilton function**
For $k = 0, \ldots, N - 1$, let
$$\mathcal{H}_k^j (u, \omega, \phi) = \text{tr}(-i \sigma_k^j [H(u, \omega, \phi, t_k), \rho_k^j])$$
where $H(u, \omega, \phi, t_k)$, from (22), is given by
$$-\frac{1}{2} \begin{pmatrix} \omega_0 & u e^{i(\omega t_k + \phi)} \\ u e^{-i(\omega t_k + \phi)} & -\omega_0 \end{pmatrix}$$

**Step 5: Update the control function.**

For $k = 0, \ldots, N - 1$, compute the values $u_k^{j+1}$, $\omega_k^{j+1}$, and $\phi_k^{j+1}$ that maximize the map $(u, \omega, \phi) \rightarrow \mathcal{H}_k^j (u, \omega, \phi)$.

**Step 6: Stopping test.**

For given small positive numbers $\varepsilon_\omega$, $\varepsilon_\phi$, and $\varepsilon_u$ (tolerance errors), check whether all the following inequalities hold:
$$|\omega^{j} - \omega^{j+1}| < \varepsilon_\omega$$
$$|\phi^{j} - \phi^{j+1}| < \varepsilon_\phi$$
$$\max_{k=0,\ldots,N-1} \{|u_k^j - u_k^{j+1}|\} < \varepsilon_u$$
If yes, let $\omega^*=\omega^{j+1}$, $\phi^*=\phi^{j+1}$, for $k = 0, \ldots, N - 1$, $u^*(t_k) = u_k^{j+1}$, and exit the algorithm.
Otherwise, let $j = j + 1$, go to Step 2.

7. CONCLUSION

In this paper we have shown how the Maximum Principle of Pontryagin can be applied in order to compute the optimal control of the problem of maximizing fidelity in the transfer of the state variable, expressed by the matrix-valued probability density function, between two given state values with the dynamics of the system the Liouville-von Neumann equation. This context is not very common neither in Optimal Control nor in Quantum Optimal Control. We obtained a shooting algorithm to solve the two point boundary value problem resulting from the application of the Maximum Principle of Pontryagin. Future challenges consists in exploiting the versatility of the optimal control paradigm further by including state constraints and other types of constraints. More efficient algorithms to solve this problem will also be considered.

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