Optimal Control of Single Spin 1/2 Quantum Systems

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Abstract

The purpose of this study is to explore the optimal control problems for a class of single spin 1/2 quantum ensembles. The system in question evolves on a manifold in $\mathbb{R}^3$ and is modeled as a bilinear control form whose states are represented as coherence vectors. An associated matrix Lie group system with state space $SO(3)$ is introduced in order to facilitate solving the given problem. The controllability as well as the reachable set of the system is first analyzed in detail. Then, the maximum principle is applied to the optimal control for system evolving on the Lie group of special orthogonal matrices of dimension 3, with cost that is quadratic in the control input. As an illustrative example, the authors apply our result to perform a reversible logic quantum operation NOT on single spin 1/2 system. Explicit expressions for the optimal control are given which are linked to the initial state of the system.

Keywords. Spin 1/2 System, Optimal Control, Right Invariance, Maximum Principle

1 Introduction

Quantum control has drawn much attention in the control community since it has numerous potential applications in many fields [1], such as physical chemistry, quantum optics, nanotechnology, etc. The descriptions for the dynamics of classical and quantum systems coupling to the surrounding environment are essentially distinct owing to the different intrinsic nature reacting to observations between the macroscopic objects and microscopic particles [2], and thus the classical control theory cannot be indiscriminately applied to the quantum systems. It is necessary to establish and develop new control strategies and theory in order to bring us better emerging applications of quantum technology.

In recent years, many reports on the control of the spin 1/2 quantum systems have appeared in the literature [3–9]. The spin 1/2 particle with two spin states: "spin up" and "spin down" is a good instance of an implementation of qubits for a quantum computer, and has been discussed and utilized for many years in the nuclear magnetic resonance (NMR) spectroscopy. Moreover, the design of quantum logic gate has been becoming an area of research focus among the field of quantum information processing, in which the spin 1/2 systems also are playing an important role, and has been used as a building block for the construction of quantum computers. Currently, there are some prototype which have been invented using different types of spin 1/2 systems. Over the last four decades, various and universally accepted set of tools have been developed to achieve control and state manipulation. Nevertheless, there are still a number of practical issues such that further investigations are needed to deal with them in practical applications.

By employing the principles of optimal control theory, a variety of techniques [4,5,7,11,12,15] have been proposed for determining the control actions to steer the dynamical systems described by the Schrödinger equation and to acquire a good performance in an optimal manner. D'Alessandro *et al.* [4] studied the

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optimal control problem of a two-level quantum system. The system considered was modeled as a bilinear system based on the Schrödinger equation. The optimal controls were provided which could steer the system from an initial state to a prescribed target state with a minimum cost. Khaneja *et al.* [5] investigated the design of controls as the pulse sequences to implement a unitary transfer between states in a minimum time. An analytical characterization of such time optimal pulse sequences for two-spin systems was given, in which the problem of obtaining the minimum time to generate a unitary propagator was converted to finding the shortest length paths on certain coset spaces. Specifically, Boscain *et al.* [7] tackled the problem of minimizing the population transfer time for spin 1/2 particles with control amplitude bounded. This problem was settled with approaches of optimal syntheses on two-dimensional manifolds.

The aim of this paper is to investigate an optimal control problem for a class of mixed-state single spin 1/2 system whose dynamics are evolving on a manifold. The description of the system is modeled as a right invariant system and there are many existing literature on the right invariant systems. Brockett [17] investigated some fundamental issues of the right invariant systems whose state space is the Lie groups generated by the right invariant vector field associated with the system. Necessary and sufficient conditions of controllability, observability and realization problems were presented by exploiting the properties of Lie groups and Lie algebras, which laid a foundation for the studies of this kind of systems. Using the topological properties of Lie groups, alternative conditions for controllability and observability of right invariant systems were given in [16]. The reachable set was characterized from both the topological and algebraic perspectives. In [18], some general criteria for testing the controllability, observability and realization were established for a special class of system, whose state space is defined on spheres. The optimal control problems in both deterministic and stochastic cases were discussed, and Pontryagin's maximum principle was applied to derive the necessary conditions for the optimal control.

More specifically, we are interested in the optimal control problem of the single spin 1/2 quantum ensembles modeled as bilinear systems whose states are represented as coherence vectors. The main contribution of this paper is to extend the existing result to a larger class of system, generalizing existing wave-function-based results to single spin 1/2 quantum ensembles whose states are represented by density matrices such that it allows the inclusion of mixed states. Controlling the evolution of coherence vector is equivalent to controlling the state of an associated matrix Lie group system. Thus, the optimal control problem for single spin 1/2 systems can be transformed to steer state of the matrix Lie group system from the identity matrix to a final matrix corresponding to an target state of single spin 1/2 system in an optimal fashion. The main tool we shall use is the maximum principle for systems on matrix Lie groups. Rather than computing the numerical results for the optimal control based on the necessary conditions obtained by the maximum principle, as an illustrative example, we derive the explicit expressions that the optimal control law must follow for specified initial condition.

The organization of this paper is as follows. In Section 2, we derive the mathematical model for a mix-state single spin 1/2 quantum system in a typical NMR setting and give the state-space representation. The optimal control problem that we shall investigate is formulated. In Section 3, we present our main results of this paper. The controllability for the associated matrix Lie group system is first analyzed, and then by applying the maximum principle of Pontryagin, the necessary conditions for the optimal control are presented with only single input involved. The characterization of the optimal control for an specified operation is further revealed explicitly in view of the necessary conditions. Concluding remarks are given in Section 4.

Throughout this paper, we use fairly standard notations listed as follows:

$\mathbb{R}$	The real field.
A'	The transpose of matrix A.
$A^\dagger$	The conjugate transpose of matrix A.
$[A, B]$	$AB - BA$ commutator of operators A and B.
$SO(3)$	The special orthogonal group of 3×3 real matrices.
$\mathfrak{so}(3)$	The Lie algebra of $SO(3)$.
$\mathrm{Tr}(A)$	Trace of matrix A.

2 Problem Formulation

In quantum mechanics, it is well-known that the Liouville-von Neumann equation is used to describe the time evolution of a quantum system

$$i\hbar\dot{\rho} = [H, \rho], \tag{1}$$

where i denotes the imaginary unit, $\hbar$ is called the reduced Planck constant, H is the system Hamiltonian, ρ is the density operator which represents the state of the system of interest and the bracket $[\cdot, \cdot]$ denotes commutator of two operators. In what follows, we shall take $\hbar = 1$ for the sake of brevity, thus one has a neater form of (1) as follows

$$\dot{\rho} = -i[H, \rho]. \tag{2}$$

We briefly recall some notions and definitions which are necessary for our problem statement. The rescaled Pauli matrices together with the identity matrix are as follows:

$$\lambda_0 = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0\\0 & 1\end{bmatrix}, \qquad \lambda_1 = \frac{1}{\sqrt{2}}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}, \qquad \lambda_2 = \frac{1}{\sqrt{2}}\begin{bmatrix}0 & -i\\i & 0\end{bmatrix}, \qquad \lambda_3 = \frac{1}{\sqrt{2}}\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}. \tag{3}$$

It is well-known that in the case of single spin 1/2 system, any time-dependent density operator $\rho \in SU(2)$ can be expressed in terms of a real linear combination of these four matrices, that is

$$\rho = \upsilon_j\lambda_j = \boldsymbol{\upsilon} \cdot \boldsymbol{\lambda},\ j = 0, 1, 2, 3, \tag{4}$$

in which $\upsilon_j \in \mathbb{R}$ denotes the coefficient with respect to λ_j, $\boldsymbol{\upsilon} = [\upsilon_0, \upsilon_1, \upsilon_2, \upsilon_3]'$ is referred to as the coherence vector for ρ, $\boldsymbol{\lambda}$ is a vector formed by $\lambda_j, j = 0, 1, 2, 3$.

In quantum control, for a system in question the system Hamiltonian H usually consists of two parts: one is the drift or free Hamiltonian H_d (also is known as the Zeeman Hamiltonian), and the other is referred to as the control Hamiltonian H_c, in which the control term is involved; The latter one can be altered externally. The Hamiltonian of a single spin 1/2 system in a static magnetic field B_0 with control actions by applying an electromagnetic field rotating at a frequency ω_c close to the Larmor frequency in the (λ_1, λ_2) plane can be accordingly divided into time-independent and time-dependent parts, which correspond to H_d and H_c, respectively. Referenced to the laboratory frame, these two parts are formulated as follows

$$\begin{aligned} H_d &= -\gamma B_0\lambda_3, && (5)\\ H_c &= -\gamma B_1(\cos(\omega_c t + \phi)\lambda_1 + \sin(\omega_c t + \phi)\lambda_2), && (6) \end{aligned}$$

where γ is the gyromagnetic ratio, B_0 and B_1 are the amplitudes of the static magnetic field and the applied electromagnetic field in the (λ_1, λ_2) plane, respectively. For convenience, we define $\omega_0 = \gamma B_0$ and $\omega_1 = \gamma B_1$, where ω_0 is commonly known as Larmor frequency.

In order to facilitate the solution of Eq. (2), it is necessary to switch H_d and H_c in the laboratory frame into the representations in the rotating frame. In NMR, the reason for this is that experiments are also observed in the rotating frame, which in fact can get rid of the large effects due to the Zeeman Hamiltonian, and at the same time can remove the time dependence of the control Hamiltonian. In our formulation, we take the rotation operator R_z to be $\exp(-i\omega_c\lambda_3 t)$, and let $\tilde{\rho}$ denote the density operator in the rotating frame corresponding to ρ. To obtain the time evolution equation of $\tilde{\rho}$ in the rotating frame, one has

$$\begin{aligned}
\frac{d}{dt}\tilde{\rho} &= \frac{d}{dt}[R_z\rho R_z^\dagger] \\
&= \left[\frac{d}{dt}R_z\right]\rho R_z^\dagger + R_z\left[\frac{d}{dt}\rho\right]R_z^\dagger + R_z\rho\left[\frac{d}{dt}R_z^\dagger\right] \\
&= -i\omega_c\lambda_3 R_z\rho R_z^\dagger + R_z\left[\frac{d}{dt}\rho\right]R_z^\dagger + R_z\rho(i\omega_c\lambda_3)R_z^\dagger \\
&= -i\omega_c\lambda_3\tilde{\rho} + R_z\left[\frac{d}{dt}\rho\right]R_z^\dagger + \tilde{\rho}(i\omega_c\lambda_3) \\
&= -i[\omega_c\lambda_3,\tilde{\rho}] + R_z\left[\frac{d}{dt}\rho\right]R_z^\dagger. \qquad (7)
\end{aligned}$$

Then, by Eq. (2), one can expand the right-hand side of Eq. (7),

$$\begin{aligned}
\frac{d}{dt}\tilde{\rho} &= -i\{[\omega_c\lambda_3,\tilde{\rho}] + R_z[H,\rho]R_z^\dagger\} \\
&= -i\{[\omega_c\lambda_3,\tilde{\rho}] + [R_z H R_z^\dagger, R_z\rho R_z^\dagger]\} \\
&= -i\{[\omega_c\lambda_3,\tilde{\rho}] + [\widetilde{H},\tilde{\rho}]\} \\
&= -i[\widetilde{H} + \omega_c\lambda_3,\tilde{\rho}], \qquad (8)
\end{aligned}$$

in which $\widetilde{H} = R_z H R_z^\dagger$.

In terms of Eq. (8), the Hamiltonians in the rotating frame with $\widetilde{H}_d$ and $\widetilde{H}_c$ denoting the Zeeman Hamiltonian and control Hamiltonian respectively become

$$\begin{aligned}
\widetilde{H}_d &= \exp(-i\omega_c\lambda_3 t)H_d\exp(i\omega_c\lambda_3 t) = -(\omega_0-\omega_c)\lambda_3 = \hat{\omega}\lambda_3, \qquad (9) \\
\widetilde{H}_c &= -\omega_1(\cos\phi\lambda_1 + \sin\phi\lambda_2), \qquad (10)
\end{aligned}$$

where $\hat{\omega} = \omega_c - \omega_0$ and ϕ represents the direction in which the control acts. In what follows, it is assumed that $\phi = 0$, thus we have

$$\widetilde{H}_c = u\lambda_1, \qquad (11)$$

in which $u = -\omega_1$ and is taken as the control input of the system.

To facilitate our study on the dynamics of the single spin-1/2 system, the adjoint operators and their matrix representations are introduced. Based on the matrix representations of adjoint operators, the Liouville-von Neumann equation Eq. (1) can be transformed into coordinate differential equations in a bilinear form.

Define the operator "ad" using the matrices of (3) as follows:

$$ad_{\lambda_j}\lambda_k = [\lambda_j,\lambda_k] = \sum_{l=0}^{3} c_{jk}^l\lambda_l,\ \ j,k\in\{0,1,2,3\}. \qquad (12)$$

The structure constants c^l_{jk} in Eq. (12) can be used to construct four 4×4 matrices $ad_{\lambda_j}, j\in\{0,1,2,3\}$, which are given by $(ad_{\lambda_j})_{kl}=c^l_{jk}$. The matrices $ad_{\lambda_j}, j\in\{0,1,2,3\}$ are referred to as matrix representations of the adjoint operators $ad_{\lambda_j}\lambda_k, j,k\in\{0,1,2,3\}$. It will be shown in (14) that these matrices play an important role in depicting the dynamics of single spin 1/2 systems. Following the foregoing construction method of the matrices $ad_{\lambda_j}, j\in\{0,1,2,3\}$, one readily obtains a lemma as below.

Lemma 1. *[10]. The matrices $ad_{\lambda_j},\ j=0,1,2,3$, are given by*

$$ad_{\lambda_0}=0_{4\times 4}, ad_{\lambda_1}=\sqrt{2}i\begin{bmatrix}0&0&0&0\\0&0&0&0\\0&0&0&-1\\0&0&1&0\end{bmatrix}, ad_{\lambda_2}=\sqrt{2}i\begin{bmatrix}0&0&0&0\\0&0&0&1\\0&0&0&0\\0&-1&0&0\end{bmatrix}, ad_{\lambda_3}=\sqrt{2}i\begin{bmatrix}0&0&0&0\\0&0&-1&0\\0&1&0&0\\0&0&0&0\end{bmatrix} \tag{13}$$

Remark 1. *It can be seen that the matrices $ad_{\lambda_j},\ j=1,2,3$ are skew symmetric, as they are all in $\mathfrak{so}(3)$. This observation will be used in our controllability analysis of single spin 1/2 systems. The matrix representations of the adjoint operators for multi-spin 1/2 systems can also be constructed by using the adjoint matrices of single spin 1/2 systems. Exactly as the single spin 1/2 case, these matrices play an important role in modeling the multi-spin 1/2 systems with the coherence vectors alternatively representing the system state.*

For a single spin 1/2 system, we can use the relation (4) and Eq. (2) to derive ordinary differential equations with respect to the real vector $\boldsymbol{\upsilon}\in\mathbb{R}^4$ instead of the density operator $\rho\in SU(2)$. The matrices $ad_{\lambda_j},\ j=0,1,2,3$, play a part in this ordinary differential equations. Then substituting (9) and (11) into (4), one obtains the Bloch equations

$$\dot{\boldsymbol{\upsilon}}=-i\left(\hat{\omega}ad_{\lambda_3}+uad_{\lambda_1}\right)\boldsymbol{\upsilon}, \tag{14}$$

where $\boldsymbol{\upsilon}\in\mathbb{R}^4$, i is the imaginary unit, $\hat{\omega}\in\mathbb{R}$ and $u\in\mathbb{R}$ is the single control input. However, since the entries in the first row and first column of ad_{λ_1} and ad_{λ_3} are all zero, we rewrite (14) in the rest of our treatment as follows

$$\dot{x}=(A+Bu)x, \tag{15}$$

in which $x=[\upsilon_1,\upsilon_2,\upsilon_3]'$, $A_{m,n}=(-i\hat{\omega}ad_{\lambda_3})_{m+1,n+1}$, $B_{m,n}=(-iad_{\lambda_1})_{m+1,n+1}$, $m,n\in\{1,2,3\}$ and $A_{m,n}$, $B_{m,n}$ denotes the mth row and nth column entry in A, B, respectively. In what follows, we take $\hat{\omega}=1$.

Remark 2. *It is noted that the previous work [4] dealt with the optimal problem for systems modeled by the Schrödinger equation whose state space is the Lie group $SU(2)$. Whereas, as shown above, based on the Liouville-von Neumann equation the model for single spin 1/2 quantum ensembles is formulated as a right invariant system whose state space is the Lie group $SO(3)$.*

In this paper, we will investigate an optimal control problem for a single spin 1/2 quantum system described by (15). Such a model is formulated as a bilinear form yet different from the Schrödinger equation. Only the single input case will be considered since the controllability of the system can be achieved even for one input, which implies that just one electromagnetic field is available for control. For a typical optimal control of quantum systems, we need to set up a measure of the total cost of the control for time 0 up to time T, which is represented by the following objective functional

$$J(u)=\frac{1}{2}\int_0^T u^2(t)dt. \tag{16}$$

We will design an optimal control law which can steer the system from an initial state to a specified final state in finite time and simultaneously minimize the cost via the computation of (16).

3 Main Results

In this section, we are interested in solving the optimal control problem of the system (15). The controllability of such system is first analyzed, then the necessary conditions of optimality are obtained by applying the maximum principle. Given prescribed initial and final states, the optimal control input for the single spin 1/2 system is derived using those necessary conditions.

3.1 Controllability

The existing literature on controllability for closed quantum systems is concerned with the Lie algebra $\mathfrak{su}(N)$ generated by matrices corresponding to the drift Hamiltonian and the control Hamiltonians in the Schrödinger equation. The single spin 1/2 quantum ensembles is formulated as a bilinear form, in which the drift term and control term as vector fields generate the Lie algebra $\mathfrak{so}(3)$. The controllability described by (15) is required to be examined before the optimal control design. Some knowledge of Lie algebras and Lie groups acting on spheres is essential in the controllability analysis of right invariant systems (see [13, 14, 16]).

The state space of the system (15) can be described by the Bloch sphere $\mathbb{S}^2$, that is, the system in itself evolves on a manifold in $\mathbb{R}^3$. The controllability analysis of right invariant systems can be facilitated with the introduction of matrix differential equations associated with (15), given by

$$\dot{\Phi}(t) = (A + uB)\,\Phi(t), \Phi(0) = I, \tag{17}$$

and the trajectory $x(t)$ determined by (15) can also be obtained by allowing $\Phi(t)$ to act on the initial state $x(0)$ via usual matrix-vector multiplication. Thus, a new control problem on matrix Lie group can be defined which is in connection with the original problem in question. Given the initial state (namely, the identity matrix) and time T, one needs to find a control law which drives the system (17) to a predetermined final state related to the final state of system (15) in an optimal manner. The system (15) is *controllable* on the Bloch sphere $\mathbb{S}^2$ if for any two point on it they can be connected by a trajectory generated by a Lebesgue integrable control input $u(t)$; correspondingly, the system (17) is *controllable* if the reachable set from the identity matrix can act transitively on Bloch sphere $\mathbb{S}^2$.

It is apparent that the adjoint matrices $ad_{\lambda_j}, j \in \{1, 2, 3\}$ are skew symmetric, and $-iad_{\lambda_j}, j \in \{1, 2, 3\}$ form a basis of the Lie algebra $\mathfrak{so}(3)$, the adjoint representation of $\mathfrak{su}(2)$. Also, we have the following relations among these matrices

$$\begin{aligned}
&[-iad_{\lambda_j}, -iad_{\lambda_j}] = 0,\ j \in \{1, 2, 3\},\\
&[-iad_{\lambda_1}, -iad_{\lambda_2}] = \sqrt{2}(-i)ad_{\lambda_3},\\
&[-iad_{\lambda_2}, -iad_{\lambda_3}] = \sqrt{2}(-i)ad_{\lambda_1},\\
&[-iad_{\lambda_3}, -iad_{\lambda_1}] = \sqrt{2}(-i)ad_{\lambda_2}.
\end{aligned} \tag{18}$$

Then, it can be verified that the generated Lie algebra of $-iad_{\lambda_1}$ and $-iad_{\lambda_3}$ (termed as "generators") obtained by following the way given in [17] is $\mathfrak{so}(3)$, which is the smallest real-involutive linear subspace of $\mathfrak{gl}(3, \mathbb{R})$ containing the generators $-iad_{\lambda_1}$ and $-iad_{\lambda_3}$. The Lie algebra $\mathfrak{so}(3)$ is isomorphic to three-dimensional real space, with the Lie bracket corresponding to the vector product. Using this correspondence, if M and N are any two linearly independent elements of $\mathfrak{so}(3)$, then the set $\{M, N, [M, N]\}$ forms a basis of $\mathfrak{so}(3)$. Since an element M in a connected matrix Lie group $SO(3)$ can be written in the form $M = e^{N_1}e^{N_2}\ldots e^{N_m}$ for some $N_1, N_2, \ldots, N_m$ in the Lie algebra $\mathfrak{so}(3)$, then the system described by

(17) is controllable on the Bloch sphere $\mathbb{S}^2$, which implies the corresponding system (15) is also controllable. For $-iad_{\lambda_1}$ and $-iad_{\lambda_3}$, they satisfy the so-called "Jurdjevic-Qinn conditions" as well, which is a sufficient condition for (15) to be globally stabilizable. It will be necessary in the following to adopt an inner product $\langle \cdot, \cdot \rangle$ in the Lie algebra $\mathfrak{so}(3)$ defined as

$$\langle P, Q \rangle = \mathrm{Tr}(PQ') = -\,\mathrm{Tr}(PQ). \tag{19}$$

We have the following lemmas which will be used in next section.

Lemma 2. *For each pair of matrices P and Q in $\mathfrak{so}(3)$, the following properties hold*

1) $[P, Q]$ *is orthogonal to both P and Q;*

2) $[P, Q]$ *is equal to* 0 *if and only if P and Q are linearly dependent;*

3) *if $[P, Q] \neq 0$, then $P, Q, [P, Q]$ form a basis in $\mathfrak{so}(3)$.*

Proof. **1)** By definition of the inner product in $\mathfrak{so}(3)$ and the Lie bracket, one obtains

$$\langle [P, Q], P \rangle = \langle PQ - QP, P \rangle = \langle PQ, P \rangle - \langle QP, P \rangle = \mathrm{Tr}(PQP') - \mathrm{Tr}(QPP') = 0. \tag{20}$$

Thus, $[P, Q]$ is orthogonal to both P and Q.

2)
- Necessity: It is obvious that if $\alpha P + \beta Q = 0$ for two not both zero real coefficients, then one has $[P, Q] = 0$.
- Sufficiency: Note that $-iad_{\lambda_1}, -iad_{\lambda_2}, -iad_{\lambda_3}$ form a basis of $\mathfrak{so}(3)$, then P and Q is expanded as

$$\begin{aligned} P &= p_1 (-iad_{\lambda_1}) + p_2 (-iad_{\lambda_2}) + p_3 (-iad_{\lambda_3}), \\ Q &= q_1 (-iad_{\lambda_1}) + q_2 (-iad_{\lambda_2}) + q_3 (-iad_{\lambda_3}). \end{aligned} \tag{21}$$

The Lie bracket of P and Q thus can be expanded as follows

$$\begin{aligned} [P, Q] &= (p_1 q_2 - p_2 q_1)[-iad_{\lambda_1}, -iad_{\lambda_2}] + (p_1 q_3 - p_3 q_1)[-iad_{\lambda_1}, -iad_{\lambda_3}] \\ &+ (p_2 q_3 - p_3 q_2)[-iad_{\lambda_2}, -iad_{\lambda_3}]. \end{aligned} \tag{22}$$

By substituting (18) into (22), we have

$$\begin{aligned} [P, Q] &= \sqrt{2}(p_1 q_2 - p_2 q_1)(-i)ad_{\lambda_3} + \sqrt{2}(p_1 q_3 - p_3 q_1)(-i)ad_{\lambda_2} \\ &+ \sqrt{2}(p_2 q_3 - p_3 q_2)(-i)ad_{\lambda_1}. \end{aligned} \tag{23}$$

Hence, $[P, Q] = 0$ means $p_1 q_2 - p_2 q_1 = p_1 q_3 - p_3 q_1 = p_2 q_3 - p_3 q_2 = 0$. We then conclude that either all $p_i = 0, i \in \{1, 2, 3\}$ or $q_i = 0, i \in \{1, 2, 3\}$ or P and Q are linearly dependent.

3) If $[P, Q] \neq 0$, then P and Q are linearly independent. There exist some constants c_1, c_2, c_3, not all 0 such that

$$c_1 P + c_2 Q + c_3 [P, Q] = 0. \tag{24}$$

By taking the inner product with $[P, Q]$ in (24), one has $c_3 = 0$ and

$$c_1 P + c_2 Q = 0, \tag{25}$$

which contradicts with the claim that P and Q are linearly independent.

□

For the optimal control problems, we need to analyze the reachable sets in order to ensure the existence of an optimal control for a specified task. Define $\mathcal{R}(\Phi_0, T)$ as the set of matrices reachable from the matrix Φ_0 with the control $u(t)$ at time T. Using the right invariance property, one has $\mathcal{R}(I, T)\Phi_0 = \mathcal{R}(\Phi_0, T)$ for all $\Phi_0 \in SO(3)$ and all T. The following lemma summarizes properties of the reachable sets for the system (17).

Lemma 3. *Consider system (17) and the Lie algebra of $\mathfrak{so}(3)$ generated by A and B together with the corresponding Lie group of $SO(3)$. In addition, consider the subalgebra generated by A and the corresponding Lie subgroup of $SO(3)$, G_A.*

(a). *There exists some time $\widetilde{T}$ such that*

$$\mathcal{R}(I, T) = SO(3), \tag{26}$$

for every $T > \widetilde{T}$.

(b). *The set of states reachable at any arbitrary time is given by*

$$\bigcap_{T>0} \mathcal{R}(I, T) = G_A. \tag{27}$$

From the above lemma, along with (17), the reachable set for the system (14) can also be characterized by applying $\Phi(t)$ to act on the initial state of (14).

3.2 Optimal Control

Consider the system described by (15) defined on the sphere. With the time $T > 0$, the initial state $x(0)$ and the final state $x(T)$ given, suppose that the cost functional $J(u)$ for the given control problem has the form of (16), then we shall address the problem of acquiring the optimal control law which minimizes the cost functional subject to the constraints that the system evolves according to (15) and the boundary conditions are satisfied. As the previous controllability analysis subsection has shown, the controllability of the vector system (15) is linked with that of the matrix Lie group system (17), thus we will attack the problem based on the system (17).

In order to deal with the problem we need to introduce a costate matrix $\Theta(t)$, and define the system Hamiltonian $\mathcal{H}$ as follows

$$\mathcal{H}(\Phi(t), u(t), \Theta(t), t) \triangleq \frac{1}{2}u^2(t) + \langle \Theta(t), A\Phi(t)\rangle + \langle \Theta(t), uB\Phi(t)\rangle, \tag{28}$$

which should be minimized with the optimal control $\hat{u}(t)$.

By applying the Pontryagin's maximum principle, we can write the necessary conditions for the optimal control

$$\begin{cases} \frac{d}{dt}\widehat{\Phi}(t) = (A + u(t)B)\,\widehat{\Phi}(t); \\ \frac{d}{dt}\widehat{\Theta}(t) = -\left(A' - u(t)B'\right)\widehat{\Theta}(t), \end{cases} \tag{29}$$

for all $t \in [0, T]$. Differentiating $\mathcal{H}$ with respect to $u(t)$ yields the optimal control $\hat{u}(t)$, which reads

$$\hat{u}(t) = \langle -\widehat{\Theta}(t), B\widehat{\Phi}(t)\rangle. \tag{30}$$

Since the final time and the final state are specified, one has the boundary condition

$$\widehat{\Phi}(T)x(0) = x(T). \tag{31}$$

Several existing works [4, 18] have discussed the optimal control problems on matrix Lie groups by employing the maximum principle. The following result provides the necessary conditions for problems on matrix Lie group $SO(3)$.

Theorem 1. *Suppose that $\hat{u}(t)$ is the optimal Lebesgue integrable control for the system (17), in the sense that, it transfers the state of system from the initial state Φ_0 (i. e. the identity matrix) to a prescribed terminal state Φ_T, in time T and simultaneously minimizes the cost functional $J(u)$ given in (16). Let $\widehat{\Phi}(t)$ denote the system trajectory generated by the corresponding optimal control. There exists a constant matrix $\Theta \in \mathfrak{so}(3)$ and a nonnegative real scalar μ, such that $\hat{u}(t)$ pointwise minimizes the Hamiltonian function*

$$\mathcal{H}(\Theta, \Phi(t), u(t)) \triangleq \frac{1}{2}\mu\hat{u}^2(t) + \langle\Theta, \widehat{\Phi}'(t)A\widehat{\Phi}(t)\rangle + \langle\Theta, u\widehat{\Phi}'(t)B\widehat{\Phi}(t)\rangle. \tag{32}$$

Proof. It follows from (17) that

$$\frac{d}{dt}\left(\widehat{\Phi}(t)^{-1}\right)' = -\left[A' + \hat{u}(t)B'\right]\left(\widehat{\Phi}(t)^{-1}\right)'.$$

Note that

$$\left(\widehat{\Phi}(0)^{-1}\right)' = I,$$

then there exists some constant matrix K such that

$$\Theta(t) = \left(\widehat{\Phi}(t)^{-1}\right)'\Theta.$$

The Hamiltonian in (28) thus can be written as

$$\left\langle \left(\widehat{\Phi}(t)^{-1}\right)'\Theta, (A + u(t)B)\,\widehat{\Phi}(t)\right\rangle + \frac{1}{2}\mu u^2(t).$$

By the property of trace of a product, the above can be rewritten as

$$\left\langle \Theta, \widehat{\Phi}(t)^{-1}\,(A + u(t)B)\,\widehat{\Phi}(t)\right\rangle + \frac{1}{2}\mu u^2(t).$$

If $\Theta \in \mathfrak{so}(3)$, the value of $\mathcal{H}$ can only affected by any component of Θ lying in $\mathfrak{so}(3)$. Thus, the proof is complete. □

Remark 3. *It is noted that the costate matrix Θ must be in $\mathfrak{so}(3)$ in contrast to $\mathfrak{su}(2)$ for the necessary optimality conditions based on the Schrödinger equation. Although there is a two-to-one correspondence between Lie group $SU(2)$ and $SO(3)$, they are not homeomorphic since the two have different fundamental groups.*

Note that extremals which fulfill (32) with μ nonzero is referred to as normal, otherwise abnormal. In the case of $u(t) \equiv 0$, if the target state lies in the Lie group generated by the matrix A and T is given such that $\Phi(T) = \Phi_T$, then we can also consider it to be controllable. The following result is concerned with the abnormal extremal of the control $u(t) \neq 0$ obtained from Theorem 1 for the single spin 1/2 systems.

Theorem 2. *For the optimal control problem of system (17) which minimizes (16) with a specified final state $\Phi(T) = \Phi_T$ and $u(t) \neq 0$ a. e. (i. e. almost everywhere), there is no abnormal extremal for the control input.*

Proof. It is noticed that the existence and uniqueness of solutions of (17) for Lebesgue integrable control can be verified by the Carathéodory conditions (see [4]). Suppose that there exists an extremal $\hat{u}(t) \neq 0$ a. e. and we shall show that it is a normal extremal. Also assume that $\mu = 0$ in (32). Because the extremal $\hat{u}(t)$ must be bounded, and pointwise minimize the system Hamiltonian (32), we have the following relation in $[0, T]$ by virtue of the necessary conditions for optimality in calculus of variations.

$$\langle \Theta, \widehat{\Phi}'(t) B \widehat{\Phi}(t) \rangle = 0. \text{ a. e.} \tag{33}$$

By continuity, one has

$$\langle \Theta, \widehat{\Phi}'(t) B \widehat{\Phi}(t) \rangle \equiv 0. \tag{34}$$

Define a matrix C, with $C_{m,n} = (-iad_{\lambda_2})_{m+1,n+1}$. Differentiation of (34) leads to

$$\langle \Theta, \widehat{\Phi}'(t) C \widehat{\Phi}(t) \rangle \equiv 0. \tag{35}$$

By differentiating (35), we have

$$\langle \Theta, \widehat{\Phi}'(t) [C, A] \widehat{\Phi}(t) \rangle + \hat{u}(t) \langle \Theta, \widehat{\Phi}'(t) [C, B] \widehat{\Phi}(t) \rangle = 0. \text{ a. e.} \tag{36}$$

Since $[C, A] = \sqrt{2}\hat{\omega} B, [C, B] = -\frac{\sqrt{2}}{\hat{\omega}} A$, we can also obtain

$$\hat{\omega} \langle \Theta, \widehat{\Phi}'(t) B \widehat{\Phi}(t) \rangle - \frac{1}{\hat{\omega}} \hat{u}(t) \langle \Theta, \widehat{\Phi}'(t) A \widehat{\Phi}(t) \rangle = 0. \text{ a. e.} \tag{37}$$

By making use of (34), one has

$$\hat{u}(t) \langle \Theta, \widehat{\Phi}'(t) A \widehat{\Phi}(t) \rangle \equiv 0. \tag{38}$$

Then we must prove that

$$\langle \Theta, \widehat{\Phi}'(t) A \widehat{\Phi}(t) \rangle \equiv 0. \tag{39}$$

Recall that $\hat{u}(t) \neq 0$ a. e. is assumed, then we can obtain (39) as a result of the continuity of $\langle \Theta, \widehat{\Phi}'(t) A \widehat{\Phi}(t) \rangle$. It can be seen from (34), (35), (39) that if we have an extremal which is not normal, then Θ must be zero. However, this contradicts with Theorem 1 and implies that the extremal is normal. The proof is thus complete.

□

Remark 4. *In our treatment, the optimal control is obtained by pointwise minimizing the Hamiltonian function $\mathcal{H}$. Since $\Phi(t)$ is uniformly bounded, it can be shown that the normality indicates the optimal control is smooth.*

In what follows, we shall investigate a specified optimal control problem. Consider the system (15) with the initial state $x(0) = [0\ 0\ 1]'$. It is required that by performing a control action, the system can be steered to the final state $x(T) = [0\ 0\ -1]'$, which corresponds to a reversible logic quantum operation NOT operation. Accordingly, the system (17) needs to be driven from the identity matrix to the final state matrix Φ_T, at time T

$$\Phi_T = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \tag{40}$$

and at the same time the cost functional $J(u)$ is minimized.

As mentioned in Lemma 3, the states expressible as $e^{A\alpha}, \alpha \in \mathbb{R}$ can be reached in arbitrary short time T. However, there exists a time $\widetilde{T}$ such that the problem in question possesses a solution for the final state

(40) and a final time $T > \widetilde{T}$. For the system (17), this can be demonstrated by an example. Suppose that $u(t)$ is a control input without constraint of its magnitude, and that $\Phi(t)$ is a solution of the evolution equation with respect to $u(t)$ with an initial state $\Phi(0) = I$. Φ is written as $(\phi_{ij})_{i,j=1,2,3}$. Thus, one has

$$\begin{cases} \dot{\phi}_{21} = \sqrt{2}\phi_{11} - \sqrt{2}u\phi_{31}, \\ \dot{\phi}_{32} = \sqrt{2}u\phi_{22}. \end{cases} \tag{41}$$

Multiplying the first equation by ϕ_{21}, the second equation by ϕ_{32} and summing up the obtained two equations, we have

$$\frac{1}{2}\frac{d}{dt}(\phi_{21}^2 + \phi_{32}^2) = \sqrt{2}\phi_{11}\phi_{22}. \tag{42}$$

Because the initial state $\Phi(0) = I$, it is apparent that $(\phi_{21}^2 + \phi_{32}^2)$ must vanish at time $t = 0$. Thus, we obtains

$$(\phi_{21}^2 + \phi_{32}^2)(t) = 2\sqrt{2}\int_0^t \phi_{11}(\tau)\phi_{22}(\tau)d\tau. \tag{43}$$

It is noticed that $\phi_{11}(\tau)$ and $\phi_{22}(\tau)$ are elements of an orthogonal matrix, hence both values are not greater than 1. Consequently, the following inequality is obtained

$$(\phi_{21}^2 + \phi_{32}^2)(t) \le 2\sqrt{2}t, \tag{44}$$

which shows that a matrix (m_{ij}) with $m_{21}^2 + m_{32}^2 = 1$ can not be achieved from the initial state in less than $\frac{1}{2\sqrt{2}}$ unit of time.

For the purpose of illustration, we select $T = \pi/\sqrt{2}$. The optimal control must be in the form of

$$u_o = -\langle \Theta, \widehat{\Phi}^{-1}B\widehat{\Phi}\rangle = Tr(\Theta\widehat{\Phi}^{-1}B\widehat{\Phi}), \tag{45}$$

in which Θ is some matrix in $\mathfrak{so}(3)$ in terms of Theorem 3.1 in [19]. We introduce another two variables u_a, u_b which will be used in deriving the optimal control $u(t)$,

$$u_a \triangleq -\langle \Theta, \widehat{\Phi}^{-1}C\widehat{\Phi}\rangle = Tr(\Theta\widehat{\Phi}^{-1}C\widehat{\Phi}), \tag{46}$$
$$u_b \triangleq -\langle \Theta, \widehat{\Phi}^{-1}A\widehat{\Phi}\rangle = Tr(\Theta\widehat{\Phi}^{-1}A\widehat{\Phi}). \tag{47}$$

Differentiating (45) with respect to time, and substituting (17) in to the derivative of (45) yields

$$\begin{aligned} \dot{u}_o &= -\left\langle \Theta, \left(\frac{d}{dt}\widehat{\Phi}^{-1}\right)B\widehat{\Phi}\right\rangle - \left\langle \Theta, \widehat{\Phi}^{-1}B\left(\frac{d}{dt}\widehat{\Phi}\right)\right\rangle \\ &= -\langle \Theta, \widehat{\Phi}^{-1}(A' + u_oB')A\widehat{\Phi}\rangle - \langle \Theta, \widehat{\Phi}^{-1}B(A + u_oB)\widehat{\Phi}\rangle \\ &= -\langle \Theta, \widehat{\Phi}^{-1}(A'B + BA + u_oB'B + u_oBB)\widehat{\Phi}\rangle \\ &= -\langle \Theta, \widehat{\Phi}^{-1}(-\sqrt{2}C)\widehat{\Phi}\rangle \\ &= \sqrt{2}\langle \Theta, \widehat{\Phi}^{-1}C\widehat{\Phi}\rangle \\ &= -\sqrt{2}u_a. \end{aligned} \tag{48}$$

In a similar way, we can also have

$$\begin{aligned}\dot{u}_a &= -\left\langle \Theta, \left(\frac{d}{dt}\widehat{\Phi}^{-1}\right) C\widehat{\Phi} \right\rangle - \left\langle \Theta, \widehat{\Phi}^{-1} C \left(\frac{d}{dt}\widehat{\Phi}\right) \right\rangle \\ &= -\langle \Theta, \widehat{\Phi}^{-1}(A' + u_o B')B\widehat{\Phi}\rangle - \langle \Theta, \widehat{\Phi}^{-1}C(A + u_o B)\widehat{\Phi}\rangle \\ &= -\langle \Theta, \widehat{\Phi}^{-1}(A'C + CA + u_o B'C + u_o CB)\widehat{\Phi}\rangle \\ &= -\langle \Theta, \widehat{\Phi}^{-1}(\sqrt{2}B - \sqrt{2}u_o A)\widehat{\Phi}\rangle \\ &= -\sqrt{2}\langle \Theta, \widehat{\Phi}^{-1}B\widehat{\Phi}\rangle + \sqrt{2}\langle \Theta, \widehat{\Phi}^{-1}(u_o A)\widehat{\Phi}\rangle \\ &= \sqrt{2}u_o - \sqrt{2}u_o u_b \\ &= \sqrt{2}u_o(1 - u_b). \end{aligned} \tag{49}$$

$$\begin{aligned}\dot{u}_b &= -\left\langle \Theta, \left(\frac{d}{dt}\widehat{\Phi}^{-1}\right) A\widehat{\Phi} \right\rangle - \left\langle \Theta, \widehat{\Phi}^{-1} A \left(\frac{d}{dt}\widehat{\Phi}\right) \right\rangle \\ &= -\langle \Theta, \widehat{\Phi}^{-1}(A' + u_o B')C\widehat{\Phi}\rangle - \langle \Theta, \widehat{\Phi}^{-1}A(A + u_o B)\widehat{\Phi}\rangle \\ &= -\langle \Theta, \widehat{\Phi}^{-1}(A'A + AA + u_o B'A + u_o AB)\widehat{\Phi}\rangle \\ &= -\langle \Theta, \widehat{\Phi}^{-1}(\sqrt{2}u_o C)\widehat{\Phi}\rangle \\ &= -\sqrt{2}u_o\langle \Theta, \widehat{\Phi}^{-1}C\widehat{\Phi}\rangle \\ &= \sqrt{2}u_o u_a. \end{aligned} \tag{50}$$

Since Θ is some element in $\mathfrak{so}(3)$ as mentioned earlier, we can write Θ as

$$\Theta = \begin{bmatrix} 0 & \theta_3 & -\theta_2 \\ -\theta_3 & 0 & \theta_1 \\ \theta_2 & -\theta_1 & 0 \end{bmatrix}. \tag{51}$$

By substituting (51) into (45), (46), (47), and noting that $\widehat{\Phi}(0) = I$, the relations between the initial conditions of $u_o(0), u_a(0), u_b(0)$ and the parameters in Θ are as follows

$$u_o(0) = 2\sqrt{2}\theta_1, \tag{52}$$

$$u_a(0) = 2\sqrt{2}\theta_2, \tag{53}$$

$$u_b(0) = 2\sqrt{2}\theta_3. \tag{54}$$

Further, by substituting (51) into (45), (46), (47), and using the final condition $\widehat{\Phi}(T) = \Phi_T$ given in (40), the relations between the initial conditions of $u_o(0), u_a(0), u_b(0)$ and the parameters in Θ are as follows

$$u_o(T) = 2\sqrt{2}\theta_1, \tag{55}$$

$$u_a(T) = -2\sqrt{2}\theta_2, \tag{56}$$

$$u_b(T) = -2\sqrt{2}\theta_3. \tag{57}$$

The system formed by (48), (49), (50) satisfies the following two prime integrals

$$\mathcal{H}_1 \triangleq u_o^2 + u_a^2 + u_b^2, \tag{58}$$

$$\mathcal{H}_2 \triangleq u_a^2 + (u_b - 1)^2, \tag{59}$$

Hence, one has

$$u_o^2 + 2u_b = \text{constant}. \tag{60}$$

In terms of (52, 54, 55, 57), we have $\theta_3 = u_b(0) = u_b(T) = 0$.

Notice that $u_b(0) = 0$, then it follows from (60) that $u_b = -\frac{1}{2}((u_a)^2 - (u_a(0))^2)$. Combining this and (48), (49), (50) leads to ordinary differential equations in terms of u_a and u_b given by

$$\begin{cases} \dot{u_a} = 2u_o \\ \dot{u_o} = (u_a^2(0) - 2)u_a - u_a^3. \end{cases} \tag{61}$$

Define the function

$$\mathcal{H} \triangleq 4m_o^2 - 2(u_a^2(0) - 2)u_a^2 + u_a^4, \tag{62}$$

as a prime integral for the system (61). It is noted that if the initial conditions of $u_o(0)$ and $u_a(0)$ are chosen such that $\mathcal{H}(u_o(0), u_a(0)) \leq 0$, then $\mathcal{H}(u_o(t), u_a(t)) \leq 0$ for arbitrary t. Due to the fact that the trajectory along the level line of $\mathcal{H}$ must traverse the u_o axis and at this intersection point, it is apparent that u_a should be 0 and hence, $4u_o^2 < 0$, which shows that $u_o = 0$. Although $u_a(t) \equiv 0, u_o(t) \equiv 0$ is a possible trajectory for the system, we are not interested in it because this leads to a control input which is zero all the time and we then can not obtain the prescribed final states. On the basis of the above analysis, one has to choose the initial conditions of $u_a(0)$ and $u_o(0)$ such that

$$\mathcal{H}(u_a(0), u_o(0)) = 4u_o^2(0) - u_a^4(0) + 4u_a^2(0) > 0. \tag{63}$$

For the type of the system (61), with the initial conditions of $u_a(0)$ and $u_o(0)$ satisfying (63), the solutions are as follows

$$\begin{cases} u_a(t) = acn(bt + f, k), \\ u_o(t) = -\frac{ab}{2}sn(bt + f, k)dn(bt + f, k), \end{cases} \tag{64}$$

where $sn(\cdot, k), cn(\cdot, k), dn(\cdot, k)$ are the Jacobi elliptic functions with elliptic modulus $k \in (0, 1)$, and the coefficients are chosen as

$$k^2 = k^2(u_a(0), u_o(0)) = \frac{(u_a^2(0) - 2) + \sqrt{4 + 4u_o^2(0)}}{2\sqrt{4 + 4u_o^2(0)}} \tag{65}$$

$$a = a(u_a(0), u_o(0)) = \sqrt{(u_a^2(0) - 2) + \sqrt{4 + 4u_o^2(0)}} \tag{66}$$

$$b^2 = b^2(u_o(0)) = \frac{a^2}{k^2} = 2\sqrt{4 + 4u_o^2(0)}, \tag{67}$$

and

$$f = cn^{-1}\left(\frac{u_a(0)}{a}, k\right) \tag{68}$$

if $u_o(0) < 0$ and

$$f = -cn^{-1}\left(\frac{u_a(0)}{a}, k\right) \tag{69}$$

if $u_o(0) < 0$.

The above analysis clearly shows that the optimal control input is Jacobi elliptic functions. The unknowns $u_a(0)$ and $u_o(0)$ are required to be chosen such that the final condition (40) is satisfied.

Remark 5. *It is noted that the optimal control expression performing the reversible logic quantum operation NOT for both formulations based on Schrödinger equation Liouville-von Neumann equation exhibit Jacobi elliptic functions since there exists a two-to-one homomorphism between Lie group $SU(2)$ and $SO(3)$. However, in general, one can only obtain numerical solutions to optimal control using the necessary optimality conditions.*

4 Conclusion

The optimal control of quantum systems based on the Schrödinger equations has been discussed since the 1980s. Many existing results formulate the control problem as numerically solving the two-point boundary value problem derived from the maximum principle. We present an explicit formula of the optimal control for single spin 1/2 systems with prescribed initial and final states in finite time. This is an open-loop control which is dependent on the initial state of the system. It is anticipated that the more control inputs, the more complex the practical implementation of the optimal control becomes. The issues that arises for the multi-spin 1/2 systems will be considered in our future work.

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