A general formulation of time-optimal quantum control and optimality of singular protocols

Hiroaki Wakamura¹ and Tatsuhiko Koike¹,²,³,⁴
¹ Department of Physics, Keio University, Yokohama 223-8522, Japan
² Quantum Computing Center, Keio University, Yokohama 223-8522, Japan
³ Research and Education Center for Natural Sciences, Keio University, Yokohama 223-8521, Japan
⁴ Author to whom any correspondence should be addressed.
E-mail: hwakamura@rk.phys.keio.ac.jp and koike@phys.keio.ac.jp

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Abstract
We present a general theoretical framework for finding the time-optimal unitary evolution of the quantum systems when the Hamiltonian is subject to arbitrary constraints. Quantum brachistochrone (QB) is such a framework based on the variational principle, whose drawback is that it only deals with equality constraints. While inequality constraints can be reduced to equality ones in some situations, they usually cannot, especially when a drift field, an uncontrollable part, is present in the Hamiltonian. We first develop a framework based on Pontryagin’s maximum principle (MP) in order to deal with inequality constraints as well. The new framework contains QB as a special case, and their detailed correspondence is given. Second, we address the problem of singular controls, which satisfy MP trivially so as to cause a trouble in determining the optimal protocol. To overcome this difficulty, we derive an additional necessary condition for a singular protocol to be optimal by applying the generalized Legendre–Clebsch condition. Third, we discuss general relations among the drift, the singular controls, and the inequality constraints. Finally, we demonstrate how our framework and results work in some examples. We also discuss the physical meaning of singular controls.

1. Introduction
In quantum mechanics one can change a given state to another by applying a suitable Hamiltonian on the system. It is often desirable to know the pathway in the shortest time. Fundamental interests include the quantum speed limit [1] originated from the time-energy uncertainty relation [2]. Fast evolution is important for reducing decoherence in any quantum mechanical experiments including information processing, metrology, etc. In particular, as small-scale quantum computers are becoming feasible [3], designing time-efficient quantum gates is crucial for performing larger computations. Time efficiency is also pursued for error correction [4], cooling [5, 6], and quantum battery [7]. Shortcuts to adiabatic passages [8] may speed up quantum annealing [9] and adiabatic quantum computation [10]. Time optimality, as a growing branch of quantum optimal control [11], is studied for systems with fast local control [12–14], for those with close-level controllable couplings [15, 16], for spin chains [37–39], for the Zermelo navigation problem [17–20], and for linear networks [21]. A close relation between time complexity and gate complexity has been suggested [22, 23]. Various analyses have been done on specific one-qubit systems [24–33]. We note that the time optimality depends heavily on the class of quantum processes in consideration.

Quantum brachistochrone (QB) [34–36] is a natural formulation of time-optimal quantum control in that one first specifies the set of available Hamiltonians and then discusses the fastest possible way of realizing a certain quantum process. The formulation has been given for the pure [34] and mixed [35] state transition and the realization of unitary operations [36]. Analytic solutions are obtained in low dimensional
systems [34–39]. Numerical techniques for QB have been developed [23, 40]. The validity of QB is experimentally demonstrated [41]. QB may serve as a basic framework of time-optimal quantum control which provides a fair comparison between various time-efficient algorithms and a unified understanding of individual results. For example, the Zermelo navigation is seen as an easily solvable class of QB (section 3).

However, QB has a weakness. It cannot treat problems with inequality constraints on the system Hamiltonian, which are natural in usual physical and theoretical setups. QB cannot properly treat protocols with jumps, e.g. the ‘bang-bang’ control, either.

In this paper, we present a more general time-optimal control theory in quantum systems, which can handle controls with inequality constraints and jumps. Instead of directly extending QB, we employ an alternative approach, Pontryagin’s maximum principle (MP), which is a modern variational calculus for optimal control. In fact, MP has been applied in many studies [15, 16, 24, 25, 27–33] on time-optimal control in quantum systems. There, MP is usually applied after individual quantum control problems are cast in a standard form in classical control theory with real variables. Instead, we directly formulate the time-optimal quantum control problem on the basis of MP. The resulting framework is applicable to virtually all situations that we encounter in practice and in theoretical investigations; for example, it is relevant for the construction of the fastest quantum gates in specific quantum computers and for the understanding of the quantum speed limits in various setups.

Applying the framework, we investigate the basic structure of time-optimal quantum control itself. First, we address the problem of singular controls, which satisfy MP trivially even if they are non-optimal (e.g. [15, 16, 30–32]). To overcome this difficulty, we derive a condition beyond MP for time-optimal singular controls by introducing the generalized Legendre–Clebsch (GLC) condition [42]. We can thus rule out (at least some of) non-optimal singular controls. Second, we clarify general relations between the drift fields, the singular controls, and the reduction of inequality constraints into equality ones, which serve as a prescription for finding time-optimal controls in specific problems. We will demonstrate how the GLC condition and the obtained results work for identifying singular optimal controls in examples.

The paper is organized as follows. We present the time-optimal quantum control problem that we discuss in section 2. In section 3, we review QB with a refinement and derive some direct results. We present a general framework for the time-optimal control of quantum systems based on MP and discuss its relation to QB in section 4. In section 5, we give the definition of singular controls and derive the GLC condition for quantum control. In section 6, we discuss a general relation among the drift fields, the singular controls, and the reduction of inequality constraints into equality. In section 7, we discuss optimality of singular controls in examples, applying our framework and its results. Section 8 is devoted to conclusion and discussions.

2. Time-optimality problem for realizing unitary operation

We consider the problem of finding the time-optimal control protocol that generates a desired unitary evolution of a quantum system in the least possible time. The optimal control protocol largely depends on the form of available Hamiltonians, which is usually restricted due to the experimental or theoretical setup. We shall formulate the problem and introduce some notations.

The time-optimality problem for realizing unitary operation is specified by \((U_f, A)\), where \(U_f \in SU(N)\) is the target unitary, \(A \subset su(N)\) is the set of available Hamiltonians, and \(N\) is the dimension of the Hilbert space. The problem is to find the minimum time \(T \geq 0\) and the control \(H(t) \in A\), \(0 \leq t \leq T\), such that \(U(0) = 1\) and \(U(T) = U_f\), where the unitary operator \(U(t)\) is driven by the Schrödinger equation

\[
i \frac{d}{dt} U(t) = H(t) U(t).
\] (1)

Here, \(SU(N)\) and \(su(N)\) denote \(N\)-dimensional special unitary group and its Lie algebra \((SU(N) = \exp(-i \cdot su(N)))\). The set \(A\) of available Hamiltonian is the set of all Hamiltonians which are realizable under the given experimental or theoretical setup. We assume that \(A\) is time independent. The reason why we restrict ourselves to \(SU(N)\) and \(su(N)\) is that the global phase of unitary operator does not affect the observables.

We give a simplest example of the time-optimality problem in a qubit system. We assume that a z-directional magnetic field is fixed and that we can manipulate a magnetic field in the xy plane with the maximum magnitude \(\Omega\). The Hamiltonian is given by

\[
H(t) = \omega_0 \sigma_z^2 + \omega^4(t) \sigma_x^2 + \omega^6(t) \sigma_y^2, \quad (\omega^4)^2 + (\omega^6)^2 \leq \Omega^2,
\] (2)
where \( \omega_0 \) is a real constant. Since this Hamiltonian can generate arbitrary unitary operator in \( SU(2) \) with suitable control variables \( u'(t) \) and \( u''(t) \), we can consider the time-optimal control for any \( U_f \in SU(2) \). In this case, we can write the set \( \mathcal{A} \) of available Hamiltonians as
\[
\mathcal{A} = \left\{ \mathcal{H} \in \text{su}(N) \mid f^j(\mathcal{H}) = 0, \quad j = 1, \ldots, p \right\},
\]
where \( f^j \) are real functions. Then the time-optimality problem in section 2 is: minimize the functional
\[
S := \int_0^T dt \left( 1 + L_S + L_C \right),
\]
where \( L_S := \text{tr} \left[ F(t) \left( i\dot{U}^\dagger U - H(t) \right) \right], \quad L_C := \sum_j \lambda_j(t) f^j(H),
\]
with the condition (10) merely determines the overall scale of \( F \) which does not affect the solution for \( H(t) \) and \( U(t) \) satisfy the Schrödinger equation (1). The term \( L_S \) ensures that \( H(t) \) and \( U(t) \) satisfy the Schrödinger equation (1). The term \( L_C \) ensures the constraints \( f^j(H) = 0 \).

We require that the variations of \( S \) with respect to \( H(t), U(t), F(t), \lambda_j(t), \) and \( T \) vanish, where we impose the following relation to keep the final unitary operator \( U(T) = U_f \) unchanged:
\[
\delta U(T) + \dot{U}(T) \delta T = 0.
\]
The variations of \( S \) with respect to \( F(t), \lambda_j(t), H(t), \) and \( U(T) \) give the Schrödinger equation (1), the constraint (4), the formula
\[
F(t) = \sum_j \lambda_j(t) \frac{\partial f^j(H)}{\partial H},
\]
and the QB equation
\[
i\dot{F}(t) = [H(t), F(t)],
\]
respectively [36]. The variations with respect to \( T \) and \( U(T) \), which must be considered at the same time because of (7), yield \( \delta S = \text{tr} \left[ F(T) \delta U(T) U(T)^\dagger \right] + \delta T \), where we have performed integration by parts and have used \( \delta U(0) = 0 \) and \( L_S(T) = L_C(T) = 0 \) implied by (1) and (4) (after taking the variation). Because (1) and (7) imply \( \delta U(T) = i[H(T), U(T)] \delta T \), the condition \( \delta S = 0 \) leads to
\[
\text{tr} \left[ H(t) F(t) \right] = 1.
\]
The time-optimal protocol \( H(t) \) for given \( (U_f, \mathcal{A}) \) is the solution to the equations (8)–(10) with the boundary conditions \( U(0) = 1 \) and \( U(T) = U_f \).

This result is the same as reference [36] except for (10). Since \( \text{tr} \left[ H(t) F(t) \right] \) is constant because of (9), the condition (10) merely determines the overall scale of \( F \) which does not affect the solution for \( H(t) \). We will discuss the role of this condition in section 4 and 5. Note that this condition is compatible with the previous studies [34–36, 40, 41] as is shown in appendix A.

### 3.2. Some direct results
We shall see two important results which can be shown by QB immediately.

The first result is (see also [34]) that the time-optimal Hamiltonian is constant when the Hamiltonians are constraint free except for the normalization \( f^0(H) := \frac{1}{2} \text{tr} \left[ H^2 \right] - \Omega^2 = 0 \). In this case, we have
We generalize QB so that it can treat inequality constraints as well as equality constraints, using Pontryagin’s MP. This is suitable for both general discussions and applications, as will be seen in the subsequent sections.

4. Pontryagin’s maximum principle for time-optimal control in quantum systems

We generalize QB so that it can treat inequality constraints as well as equality constraints, using Pontryagin’s MP. There have been many studies [15, 16, 24, 25, 27–33] using MP. There, specific problems are transformed to control systems with concrete real variables, e.g. the Bloch vectors or the Euler angles, and then MP is applied. Such transformations depend on the physical system and the control setup. Here, we define the interaction-picture operator \( A(t) \) by suitably rescaling the operator \( H(t) \), namely, \( H(t) = H_d + H_c(t) \), where \( H_d \) and \( H_c(t) \) are the drift-free, constraint-free case in the first result, with \( H(t) \). Because \( \tilde{H}^0(H_d) = \tilde{H}^0(H_c) \), equations (1), (8) and (9) are equivalent to

\[
i \tilde{U}_t = H_{d,t} U_t, \quad F_t = \lambda_0 H_{d,t}, \quad i \tilde{F}_t = [H_{d,t}, F_t].
\] (12)

These are nothing but the equations for the drift-free, constraint-free case in the first result, with \( H(t) \), \( F(t) \) and \( U(t) \) being replaced by \( H_{d,t} \), \( F_t \) and \( U(t) \). We immediately obtain the constant solution \( H_{d,t}(t) = H_{d,t}(0) = H_d(0) \) and \( U(t) = e^{-iH_d(0)t} \). In terms of the original variables, we have

\[
H(t) = H_d + e^{-iH_d} H_c(0) e^{iH_d}, \quad U(t) = e^{-iH_d} e^{-iH_d(0)t}.
\] (13)

This is the same as the result of references [18, 20]. The derivation here is simpler and more intuitive. We have only appealed to the invariance of the constraint \( \tilde{f}^0(H_c) = 0 \) under transition to the interaction picture. This observation provides a generalization of the result (appendix B).

4.1. Formulation

We state the result of MP-QB here and put a derivation in section 4.3.

We consider the time-optimality problem in section 2 specified by \( (U_f, A) \), where \( U_f \) is the target unitary operator and \( A \) is the set of available Hamiltonians. Let \( H(t), 0 \leq t \leq T \), be the time-optimal Hamiltonian for given \( (U_f, A) \), namely, \( H(t) \in A \) drives the unitary operator \( U(0) = 1 \) to \( U(T) = U_f \) through the Schrödinger equation (1) in the minimum time \( T \). Then, there exists a Hermitian operator \( F(t) \in \text{su}(N) \) which satisfies

\[
i \tilde{F}(t) = [H(t), F(t)],
\] (14)

\[
\text{tr} [KF(t)] \leq \text{tr} [H(t)F(t)] \quad \text{for any} \quad K \in A \quad \text{at each} \ t,
\] (15)

\[
\text{tr} [H(t)F(t)] = -p_0,
\] (16)

where \( p_0 \leq 0 \) is a constant. A control protocol \( H(t), F(t) \) is called normal if \( p_0 < 0 \) and abnormal if \( p_0 = 0 \) (e.g. [44]). In this paper, we treat normal controls only leaving the analysis of abnormal ones in MP-QB for future works. Thus, we replace (16) with

\[
\text{tr} [H(t)F(t)] = 1,
\] (17)

by suitably rescaling the operator \( F \). The QB equation (14) ensures that the LHS of (17) is constant in time. To summarize, the time-optimality problem is transformed to the problem of finding a pair \( (H(t), F(t)) \in (A, \text{su}(N)) \) satisfying (14), (15), and (17).

In the theory of MP, \( H_{MP} (H(t), F(t)) = -1 + \text{tr} [H(t)F(t)] \) is called the Pontryagin Hamiltonian. Equation (15) states that the optimal control Hamiltonian \( H(t) \) is the maximizer of the Pontryagin Hamiltonian at each \( t \).
Reachability set determined by an evolution of a unitary operator reveals the origin of MP-QB. We provide a derivation of the statement of MP-QB in section 4.1. Although it is an adaptation of protocols (e.g. [45] and [46, theorem 74.1]), though we have not considered such cases in our derivation of QB in section 3 for simplicity. In such cases, equation (10) in QB would be replaced by the maximum condition (15) in MP-QB, while the Schrödinger equation (1) with initial quantum state must have an extremum. We thus obtain (8).

We remark that a strict application of the method of Lagrange multipliers also admits abnormal control protocols (e.g. [34], where state evolution [34], where $H(t)$ drives a given initial quantum state $|\psi(0)\rangle = |\psi_i\rangle$ to a given final one $|\psi(T)\rangle = |\psi_f\rangle$ in the least possible time. For this problem, we obtain the same conditions (equations (14), (15) and (17)) and an additional condition $F = FP + PF$, where $P(t) := |\psi\rangle\langle\psi|$.

### 4.2. Relation between QB and MP-QB

MP-QB includes QB as a special case in which the constraints on $H(t)$ are expressed by equalities. MP-QB has the same equations (14) and (17) as QB does, equations (9) and (10). The operator $F$ is determined implicitly by the maximum condition (15) in MP-QB, while $F$ is given explicitly by (8) in QB. In the case of equality constraints, equation (15) implies (8). To see this, let us assume that the set $\mathcal{A}$ of available Hamiltonians is given by (4). From (15), the time-optimal Hamiltonian $H(t)$ maximizes $\text{tr}[H(t)F(t)]$ at each time $t$, subject to the constraints $F^i(H) = 0$. By the method of Lagrange multipliers, the function of $H$, 

$$\text{tr}[H(t)F(t)] - \sum_j \lambda_j f^j(H),$$

must have an extremum. We thus obtain (8).

We remark that a strict application of the method of Lagrange multipliers also admits abnormal control protocols (e.g. [45] and [46, theorem 74.1]), though we have not considered such cases in our derivation of QB in section 3 for simplicity. In such cases, equation (10) in QB would be $\text{tr}[HF] = -p_0$ with a Lagrange multiplier $p_0$, the same as (16).

### 4.3. Derivation

We provide a derivation of the statement of MP-QB in section 4.1. Although it is an adaptation of Pontryagin’s MP (e.g. [43]), it clarifies some subtle points of MP-QB, including its difference from QB, and reveals the origin of $F(t)$.

Consider an augmented system $\mathcal{M} := \mathbb{R} \times SU(N)$ (see figure 1), in which a trajectory $(t, U(t))$ represents an evolution of a unitary operator $U(t)$ with the time cost $t$. For a given protocol $H(t)$, the trajectory is determined by

$$i = 1, \quad \dot{U}(t) = -iH(t)U(t). \quad (19)$$

The reachability set $\mathcal{R}$ is defined by $\mathcal{R} := \bigcup_{t \in [0, \infty)} \mathcal{R}_t$, where $\mathcal{R}_t := \{ (t, U(t)) | H(t) \in \mathcal{A} \}$, and $U(t)$ satisfies the Schrödinger equation (1) with $U(0) = 1$. The set $\mathcal{R}_t$ consists of the reachable points at time $t$.

Let the final time $T$ and the protocol $H(t)$ be optimal for given $(U_f, \mathcal{A})$, so that $U(T) = U_f$. The terminal point $(T, U(T))$ of the trajectory $(t, U(t))$ lies at the boundary of $\mathcal{R}$ because of its reachability and optimality. We shall discuss the changes of the point $(T, U(T))$ caused by the changes of the protocol $H(t)$ and the final time $T$. We employ the needle variation for $H(t)$, in which the change can be finite but is
on infinitesimal intervals. This is particularly useful when the optimal protocols may have jumps, or when
$H(t)$ is on the boundary of $\mathcal{A}$ where $\delta H(t)$ is allowed but $-\delta H(t)$ is not. A simple needle variation
$M(\tau; \delta \tau; K) : H(t) \mapsto H'(t)$ at $t = \tau \in (0, T)$ where $H(t)$ is continuous is defined by

$$H'(t) = \begin{cases} K, & \tau - \delta \tau < t \leq \tau, \\ H(t), & 0 \leq t \leq \tau - \delta \tau \text{ and } \tau < t \leq T, \end{cases}$$

(20)

where $\delta \tau \geq 0$ is infinitesimal and $K \in \mathcal{A}$. By appropriately defining addition and nonnegative scalar
multiplication, which are essentially operations on the time intervals, the needle variations form a space
that is closed under those operations, though the ‘addition’ is noncommutative (appendix C).

The variation $H(t) \mapsto H'(t)$ with respect to $T$ is defined as follows. If $\delta T \leq 0$, $H'(t)$ is simply
the restriction of $H(t)$ on the shortened domain, i.e., $H'(t) = H(t)$, $0 \leq t \leq T - \delta T$. If $\delta T > 0$, $H'(t)$ is defined
on the extended domain by the value at $t = T$, i.e., $H'(t) = H(t)$, $0 \leq t \leq T$ and $H'(t) = H(T)$, $t > T$. It can
be seen that the combination of the two kinds of variations (of $H(t)$ and $T$) again form a space that is closed
under addition and nonnegative scalar multiplication. Furthermore, though the ‘addition’ is noncommutative, they become commutative in the resulting first-order variation of the final unitary
operator $U(T)$ (appendix C). Thus, $\delta \{ U(T) \}$ form a convex cone contained in $T_{(T, U(T))} \mathcal{M}$. This cone
is called the tent $\mathcal{T}_{(T, U(T))}$ of $R$ at $(T, U(T))$.

If the tent $\mathcal{T}_{(T, U(T))}$ would contain the downward vector $(-1, 0)$ in its interior, the protocol $(H(t), F(t))$
would be non-optimal because $R$ would intersect the segment $[0, T] \times \{ T \}$. Thus, if $(H(t), F(t))$ is time
optimal, there is a hyperplane that separates the tangent space $T_{(T, U(T))} \mathcal{M}$ into a closed half-space containing
the tent and a closed half-space containing the vector $(-1, 0)$. There is a normal vector $(p_0, P) \in T_{(T, U(T))} \mathcal{M}$
to the hyperplane such that

$$\langle (p_0, P), (-1, 0) \rangle \geq 0 \geq \langle (p_0, P), (\delta T, i \delta [U(T)] U(T)^\dagger) \rangle,$$

(21)

where $\delta \{ U(T) \}$ is the first-order variation and the bracket denotes the inner product
$\langle q_0, Q \rangle (t_0, R) := q_0 R_0 + tr [QR]$. The first inequality in (21) implies $p_0 \leq 0$.

The first-order variation of $U(T)$ caused by $M(\tau; \delta \tau; K)$ in (20) is

$$\delta U(T) = U(T, \tau) (-i \delta \tau [K - H(\tau)]) U(\tau),$$

(22)

where $U(t, \tau)$ is the time evolution operator satisfying the the Schrödinger equation (1) with the initial
condition $U(\tau, \tau) = 1$. Let us define a Hermitian operator

$$F(t) := U(t, T) P U(T, t).$$

(23)

It is immediately seen that $F$ satisfies the QB equation (14). From (21) and (22), we have
$tr [KF(\tau)] \leq tr [H(\tau) F(\tau)]$, the maximum condition (15). The first-order variation of $U(T)$ with respect to $T$ is given by $\delta \{ U(T) \} = -i \delta T H(T) U(T)$. From (21), and because $\delta T$ can be of both signs, we have
$tr [H(T) F(T)] = -p_0 \geq 0$. This is the algebraic condition (17).

5. Singular controls and the GLC condition

We shall introduce singular controls and derive the condition for them to be optimal. Since singular
controls are trivial solutions of MP, we cannot determine optimal one from MP-QB. The GLC condition, a
condition beyond MP, can exclude some singular controls from being optimal. The problem and the
formulation are the same as in sections 2 and 4.1.

5.1. Drift, control Hamiltonian, and singular controls

We first define the drift and the control Hamiltonians. Let $A \subset \text{su}(N)$ be a general constraint (set of
available Hamiltonians). Consider the smallest hyperplane that contains $A$, which we call the control plane$^6$. Take an arbitrary fixed Hamiltonian $H_0 \in A$ and regard the hyperplane as a linear subspace $C$ of $\text{su}(N)$
whose origin is $H_0$, which we call the control subspace. Then, we can write $H(t) \in A$ as

$$H(t) = H_0 + H_c(t), \quad H_c(t) \in A - H_0 (\subset C),$$

(24)

$^5$ We express the tangent vector $P$ at $U \in \text{su}(N)$ as a Hermitian operator such that the change of $U$ caused by $\epsilon P$, where $\epsilon \in \mathbb{R}$ is infinitesimal, is $-i\epsilon PU$.

$^6$ Mathematically, the control plane is the intersection of all hyperplanes of arbitrary dimensions that contain $A$. 


where $H_d$ is time independent. We call $H_d$ and $H_c(t)$ the *drift* and *control* Hamiltonians, respectively, and the constraint $H_c(t) \in \mathcal{C}$ a *subspace constraint*. Physically, the drift Hamiltonian $H_d$ describes the fields intrinsic to the system such as a fixed magnetic field or an interaction between the particles with a fixed coupling, while the control Hamiltonian $H_c(t)$ describes the controllable fields such as an adjustable magnetic field or a pulse sequence of electromagnetic waves.

The subspace constraint can be expressed by equality constraints in a simple manner. Namely, the condition $H_c(t) \in \mathcal{C}$ is equivalent to

$$\text{tr} \left[ H_c(t) \tau_j \right] = 0, \quad j = \text{dim } \mathcal{C} + 1, \ldots, N^2 - 1,$$

where $\{ \tau_j \}_{j=1}^{N^2-1}$ is an orthonormal basis on $\text{su}(N)$ such that $\tau_1, \ldots, \tau_{\text{dim } \mathcal{C}} \in \mathcal{C}$ and $\tau_{\text{dim } \mathcal{C} + 1}, \ldots, \tau_{N^2-1} \in \mathcal{C}^\perp$, with $\mathcal{C}^\perp$ being the orthogonal complement of $\mathcal{C}$ (with respect to the inner product $(1/2)\text{tr} [AB]$). The total Hamiltonian is written as

$$H(t) = H_d + \sum_{j=1}^{\dim \mathcal{C}} u_j(t) \tau_j,$$

with some real variables $u_j(t)$.

We shall define a class of constraints which is practically common and theoretically useful. We say that a constraint $\mathcal{A}$ is *planar* if $\mathcal{A}$ is a closed region in $H_d + \mathcal{C}$ and $\dim \mathcal{A} = \dim \mathcal{C}$ holds, more precisely, if

$$\mathcal{A} = \text{closure} (\text{interior} (\mathcal{A}))$$

in the topology of the hyperplane $H_d + \mathcal{C}$ (see figure 2). We also define a further restricted class; a constraint $\mathcal{A}$ is *typical* if $\mathcal{A}$ is defined by a subspace constraint $H_c(t) \in \mathcal{C}$ and a single inequality

$$\frac{1}{2} \text{tr} [H_c(t)^2] \leq \Omega^2,$$

where $\Omega > 0$. This gives an upper bound of the (Hilbert–Schmidt) norm of the control Hamiltonian, so that the control field has a finite energy bandwidth. We can express a typical constraint $\mathcal{A}$ by

$$\sum_{j=1}^{\dim \mathcal{C}} (u_j)^2 \leq \Omega^2$$

together with (26) (see figure 2).

A control $(H(t), F(t))$ for a general constraint $\mathcal{A}$ is said *singular* at time $t$ if $\text{tr} [KF(t)] = \text{constant}$ for all $K \in \mathcal{A}$, or equivalently,

$$\text{tr} [CF(t)] = 0.$$

A non-singular control is called *regular*. For singular controls, the maximum condition (15) is trivially satisfied so that MP-QB cannot determine the optimal protocol. A singular control smooth at $t$ satisfies the time derivatives of (29), e.g.,

$$\frac{d}{dt} \text{tr} [CF] = \text{tr} [[\mathcal{C}, H]F] = 0,$$

where the QB equation (14) is used.

Existence of singular controls causes two difficulties in finding the time-optimal control. First, MP-QB admits any sequence of singular and optimal regular controls as candidates of the optimal protocol. We do not know in advance how to determine the number and the order of them. Second, we cannot identify the optimal singular control by MP-QB. We will partly overcome the second difficulty in the next subsection.

7 The definition of singularity may be slightly different in some literature. See the final remark in this subsection.
5.2. GLC condition

We shall derive a necessary condition beyond MP for singular controls to be optimal, which is one of the main results of this paper. This condition excludes some of the singular controls from candidates of the optimal ones.

Let \( H(t) \) be parametrized by the control variables \( u'(t), 1 \leq j \leq l, \) in a certain subset \( \mathcal{U} \subset \mathbb{R}^l. \) We assume that the control variables \( u' \) are in the interior of \( \mathcal{U} \) so that we can take an arbitrary infinitesimal variation of the control variables \( u'(t) \rightarrow u'(t) + \delta u'(t). \) If \( u' \) are on the boundary of \( \mathcal{U}, \) we can regard \( u' \) to be in the interior of the boundary of \( \mathcal{U} \) by defining new control variables \( u'j \) with reduced dimensionality. Such a condition will appear in section 7 (and in appendix G).

A necessary condition for optimality beyond MP is provided by the GLC condition [42], which comes from the positive semidefiniteness of the second-order variation of the cost functional. We define an \( l \times l \) matrix \( Q(m), m = 0, 1, 2, \ldots, \) whose \((i,j)\) element is given by

\[
Q_{ij}^{(m)} = \frac{\partial}{\partial u^i} \left[ \left( \frac{\partial}{\partial u^j} H_{\text{MP}}(H(t), F(t)) \right) w^m \right].
\]  

We denote by \( M \) the smallest value of \( m \) for which \( Q_{ij}^{(m)} \) has at least one nonzero element. Any optimal control must satisfy the following two conditions:

(a) The integer \( M \) is even.
(b) If \( M = 2k, \) then \((-1)^k Q^{(2k)}\) is negative semidefinite.

When \( M = 0, \) these reduce to the negative semidefiniteness of \( Q_{ij}^{(0)} \) implied by MP. When the control is singular, \( Q_{ij}^{(0)} = 0 \) and \( M > 0 \) follow. It can also be shown that the matrix \( Q_{ij}^{(m)} \) is symmetric if \( m \) is even and antisymmetric if \( m \) is odd. We remark that the GLC condition does not depend on the parametrization (see appendix D for a proof).

We shall go back to time-optimal quantum control. We give the expressions of \( Q_{ij}^{(m)} \) for singular protocols, whose derivation is in appendix E, so that we can examine the GLC condition step by step. The singularity condition implies \( Q_{ij}^{(0)} = (\partial^2 / \partial u^i \partial u^j) \text{tr}[HF] = 0. \) Assume that \( Q^{(k)} = 0 \) hold for \( k = 0, 1, \ldots, m - 1. \) Then, \( Q_{ij}^{(m)} \) is given by

\[
Q_{ij}^{(m)} = -i \text{tr} \left[ [h_j, F] R_{ij}^{(m-1)} \right],
\]  

where \( h_i := \partial H / \partial u^i \) and \( R_{ij}^{(m)} \) satisfies the recurrence relation,

\[
R_{ij}^{(m)} = \frac{d}{dt} R_{ij}^{(m-1)} - i [R_{ij}^{(m-1)}, H], \quad R_{ij}^{(0)} = h_i.
\]  

We can perform the GLC test for time-optimal quantum control as follows:

(a) Let \( m = 0. \) We have \( Q_{ij}^{(m)} = 0. \)
(b) Increase \( m \) by one and calculate \( Q_{ij}^{(m)} \) by equations (32) and (33).
(c) If \( Q_{ij}^{(m)} \) is identically zero, with the help of the previously obtained conditions, go to (b).
(d) If \( m \) is odd, impose a condition \( Q_{ij}^{(m)} = 0 \) and go to (b).
(e) Impose negative semidefiniteness on \((-1)^k Q^{(2k)}\) and halt.

In the special case of planar constraint \( \mathcal{A}, \) the Hamiltonian \( H(t) \) can be written by independent control variables \( \{ u' \} \in \mathcal{U} \) as

\[
H(t) = H_d + H_c(t) = H_d + \sum_{j=1}^{l} u'(t) h_j.
\]  

Then, \( h_j \) appearing in equations (32) and (33) become fixed operators that span the control subspace \( \mathcal{C}. \) We give concrete expressions for the first few \( Q_{ij}^{(m)} \) in this case:

\[
Q_{ij}^{(1)} = -i \text{tr} \left[ [h_j, h_i] F \right],
\]

\[
Q_{ij}^{(2)} = \text{tr} \left[ [[[H, h_j], h_i] F \right],
\]

\[
Q_{ij}^{(3)} = i \text{tr} \left[ [[[H, [H, h_j]], h_i] F \right] + \text{tr} \left[ \left[ \left[ \frac{dH}{dt}, h_i \right], h_i \right] F \right].
\]  

In particular, the GLC condition for \( m = 1 \) reads

\[
\text{tr} \left[ [\mathcal{C}, \mathcal{C}] F \right] = 0.
\]
Figure 3. (a) An example of ‘lollipop’ constraint for $H$. This is characterized by $H_d \in C$, where $H_d$ is the drift Hamiltonian and $C$ is the control subspace. (b) An example of ‘lotus-leaf’ constraint, characterized by $H_d \not\in C$.

Figure 4. Optimal regular control lies on the boundary for planar constraints. For interior $H$, we can enlarge $\text{tr}[HF]$ by stretching $H_c$ along the nonzero projection $P_C(F)$.

Before closing this section, we note that our definition of singularity is narrower than that in reference [42] so that the theorem there implies the assertion here. In a common definition (e.g. [42]), a control $u \in U$ is called singular if there exists a variation $\delta u$, by which $\delta H_{MP}$ vanishes up to the second order. Our definition requires that $\delta H_{MP}$ vanish to all orders and in all directions. We can always regard regular controls with vanishing $\delta H_{MP}$ in some directions $\delta u$ as singular ones by redefining $A$ as the subset of $A$ of the controls that satisfies the maximum condition (15).

6. Drift and inequality constraints

We shall discuss, by applying MP-QB and the GLC condition, the general structure of the time-optimality problem, with a focus on the relations between the drift, the singular controls, and the inequality constraints. We divide the sets $A$ of available Hamiltonians into two types according to whether the drift $H_d$ is in the control subspace $C$ or not. We call $A$ lollipop type if $H_d \in C$, including $H_d = 0$, and lotus leaf type if $H_d \not\in C$ (see figure 3). These conditions are equivalent to $A \subseteq C$ and $A \not\subseteq C$, respectively. We shall show three results.

First, if the constraint $A$ is lollipop type, all optimal controls are regular. Suppose that the control $H(t)$ is singular. Then $H_d \in C$ and the singularity condition (29) imply that the control $H(t) = H_d + H_c(t)$ cannot satisfy the algebraic condition (17) so that $H(t)$ cannot be optimal. Thus, the statement holds. If the constraint is lotus leaf type, optimal controls can contain both regular and singular ones.

Second, for any $A$, all regular optimal controls $H(t)$ must belong to the boundary of $A$ in the control plane $H_d + C$. Moreover, if $A$ is planar, this implies that at least one of the inequality constraints reduces to an equality. Regularity implies that the orthogonal projection $P_C(F)$ of $F$ onto $C$ does not vanish (see figure 4). If a regular optimal control $H = H_d + H_c(t)$ were in the interior of the control plane, then $\text{tr}[HF]$ would become larger by changing $H_c$ to $H_c + \varepsilon P_C(F)$, $\varepsilon > 0$, contradicting the maximum condition (15). We remark that when $A$ is non-planar and when $\dim A < \dim C$ holds, all $H(t)$ are regarded as being on the boundary of $A$. The case of typical lollipop constraint has been shown in reference [40].

Third, though the reduction to equality constraint does not occur in general for lotus-leaf constraints, we observe that it does occur under a certain condition. Consider the case that the drift can be taken such that $H_d \in [C, C]$. Mathematically, this is equivalent to the condition $A \subseteq C \oplus [C, C]$ (where $\oplus$ denotes the direct sum of real vector spaces). We have the following. If $A$ is planar lotus leaf and admits $H_d \in [C, C]$, then all optimal controls are on the boundary of $A$ so that an inequality constraint reduces to an equality. Because of the second result above, it is enough to show the case of singular controls. Suppose that a singular optimal control $(H(t), F(t))$ were in the interior of a planar $A$. Then, the GLC condition would
Table 1. Types of possible optimal controls for each type of constraint $A$. The boundary' denotes the boundary of $A$ in the control plane. For planar $A$, 'on the boundary' implies that an equality is attained among the inequality constraints.

| Types of Available $H_d$          | Constraints on the Boundary | Constraints on the Boundary and Singular Controls |
|-----------------------------------|-----------------------------|-------------------------------------------------|
| Lollipop ($H_d \in C$)            | Regular controls on the boundary | Regular controls on the boundary and singular controls |
| Non-planar                        | Controls on the boundary$^a$  |                                                  |
| Planar                            | $H_d \in [C, C]$             |                                                  |
| Non-planar                        | $H_d \notin [C, C]$           |                                                  |

$^a$For singular controls, do the GLC test after parametrizing the boundary with a smaller number of variables. $^b$For singular controls, do the GLC test.

imply (35). This and $H_d \in [C, C]$ would imply $\text{tr}[H_d F(t)] = 0$, which would contradict the algebraic condition (17). Therefore, all singular control in a planar, lotus leaf $A$ must be on the boundary of $A$.

The results in this section are summarized in section 8 and in table 1, which serve as a prescription when the constraint $A$ is given.

7. Examples

We shall discuss three examples of systems where singular controls are present. We will see how the methods and the results in the previous sections work. The first two examples are revisits to previously analyzed, simple two-dimensional systems. The first example allows an optimal singular control. The second allows singular controls but they turn out non-optimal thanks to the GLC condition. However, we will observe that consideration of only a single singular control is enough. We remark that the control of simple systems are analyzed also in a different context (e.g. [47–52]).

7.1. Example 1: Landau–Zener model

First, let us seek the time-optimal controls in the Landau–Zener model,

$$H(t) = \omega_0 \sigma^z + u(t) \sigma^x,$$

where $\omega_0 > 0$ is a fixed parameter and $u(t)$ is a control variable satisfying $|u(t)| \leq \Omega$ (e.g. references [16, 28]). We have the drift $H_d = \omega_0 \sigma^z$ and the control subspace $C = \langle \sigma^x \rangle$. The set $\mathcal{A}$ of available Hamiltonians is typical and lotus leaf with $H_d \notin [C, C]$.

We can show that $u(t) = 0$ holds for the optimal singular controls. From (29), a singular control satisfies $\text{tr}[\sigma^z F] = 0$. The first and second time derivatives of this condition are

$$\frac{d}{dt} \text{tr}[\sigma^z F] = -2\omega_0 \text{tr}(\sigma^z F) = 0,$$

$$\frac{d^2}{dt^2} \text{tr}[\sigma^z F] = 4\omega_0 u(t) \text{tr}[\sigma^z F] = 0,$$

respectively. If the singular control is time optimal, we have from (17) that

$$\text{tr}[H_d F] = \omega_0 \text{tr}[\sigma^z F] = 1.$$

Equations (38) and (39) imply $u(t) = 0$. This is the only singular control that is potentially time optimal. The GLC condition does not exclude this control, which can be verified through (35). Reference [16] (see also [28]) actually provides a case, that the ‘bang-off-bang’ control is optimal, where the ‘bang’ control $u(t) = \pm \Omega$ is regular and the ‘off’ control $u(t) = 0$ is singular.

7.2. Example 2: one-qubit system

Next, we discuss the one-qubit example raised at the end of section 2. The Hamiltonian reads

$$H(t) = \omega_0 \sigma^z + u'(t) \sigma^x + u''(t) \sigma^x,$$

where $\omega_0 > 0$ is a fixed parameter and $u'(t)$ and $u''(t)$ are control variables satisfying $(u')^2 + (u'')^2 \leq \Omega$. We have the drift $H_d = \omega_0 \sigma^z$ and the control subspace $C = \langle \sigma^x, \sigma^y \rangle$. The constraint $\mathcal{A}$ is typical and lotus leaf with $H_d \in [C, C]$.

We show that all optimal controls are regular in this system. From the results in section 6 (or from table 1), all optimal controls must attain the equality $(u')^2 + (u'')^2 = \Omega$. On the other hand, the singular controls satisfy $\text{tr}[\sigma^z F] = \text{tr}[\sigma^z F] = 0$ by the definition (29), and $u' \text{tr}[\sigma^z F] = u' \text{tr}[\sigma^z F] = 0$ by its
time derivatives. Then, we have \( u^t = u^r = 0 \), because \( \text{tr} \{ \sigma^2 F \} \neq 0 \) follows from the algebraic condition (17). Thus, the singular controls never satisfy the equality \((u^t)^2 + (u^r)^2 = \Omega\) and must be non-optimal. Although this statement has already been shown in reference [30], the proof has become much easier thanks to the GLC conditions (which is reflected in table 1).

7.3. Example 3: symmetric two-qubit system

Our final example is a quantum control in a three-dimensional Hilbert space. We adopt a representation by two spins. Consider a Hamiltonian in a two-spin Hilbert space \( \mathcal{H} \),

\[
H_2(t) = \omega_0 \sigma_1^x \sigma_2^x + J(t) \sigma_1^y \sigma_2^y + \frac{3}{2} \sum_{i=1}^{3} \frac{b_i(t)}{2} (\sigma_1^i + \sigma_2^i),
\]

where \( \omega_0 > 0 \) is a fixed parameter and \((J, b^1, b^2, b^3) \in \mathbb{R}^4\) are control variables in the region \( J^2 + (b^1)^2 + (b^2)^2 + (b^3)^2 \leq \Omega^2 \) denoted by \( \mathcal{U} \subset \mathbb{R}^4 \). We assume \( \omega_0 < \Omega \).

The Hamiltonian (41) is symmetric under the exchange of the two spins. Thus, the space \( \mathcal{H}_{\text{sym}} \) of the symmetric states, i.e., the triplet states, is invariant under the time evolution by \( U(t) \). We hereafter restrict our attention on \( \mathcal{H}_{\text{sym}} \). This is a control problem on \( \text{SU}(3) \). On \( \mathcal{H}_{\text{sym}} \), we can rewrite the Hamiltonian \( H_2(t) \) as

\[
H(t) = \omega_0 \tilde{\Sigma}_x + J(t) \tilde{\Sigma}_y + \sum_i b_i(t) S_i^z,
\]

where \( \Sigma_x, \Sigma_y, S_1, S_2, \) and \( S^z ) \) are the restrictions on \( \mathcal{H}_{\text{sym}} \) of \( \sigma_1^x \sigma_2^x, \sigma_1^y \sigma_2^y, (\sigma_1^x + \sigma_2^x)/2, (\sigma_1^y + \sigma_2^y)/2, \) and \( (\sigma_1^x + \sigma_2^x)/2 \), respectively, and the tilde denotes the traceless part on \( \mathcal{H}_{\text{sym}} \). Their concrete expressions are in appendix F. For the Hamiltonian (42), we have

\[
H_d = \omega_0 \tilde{\Sigma}_x, \quad H_c(t) = J(t) \tilde{\Sigma}_y + \sum_i b_i(t) S_i^z,
\]

where \( \mathcal{C} = \text{span} \{ \tilde{\Sigma}_z, S_1^z, S_2^z, S_3^z \} = \text{span} \{ \lambda_1 + \lambda_6, \lambda_2 + \lambda_7, \lambda_3, \lambda_8 \} \)

(44)

where \( \{ \lambda_i \}_{i=1}^8 \) are the Gell–Mann matrices. The constraint \( \mathcal{A} \) is planar and lotus leaf with \( H_d \notin [\mathcal{C}, \mathcal{C}] \).

The results in section 6 (see table 1) imply that the time-optimal controls are either regular ones on the boundary or singular ones.

We focus on the optimality of singular controls \( (H(t), F(t)) \). We expand \( F(t) \) as \( F(t) = \sum_{i=1}^8 f_i(t) \lambda_i \). The singularity condition (29) and its derivative (30) imply that

\[
f^1 + f^6 = f^2 + f^5 = f^3 + f^8 = f^0 = 0.
\]

Under these relations, the algebraic condition (17) leads to

\[
f^4 \neq 0.
\]

Let us perform the GLC test. We discuss here the case that \((J, b^1, b^2, b^3) \) is in the interior of \( \mathcal{U} \), while we show non-optimality of the singular controls on the boundary of \( \mathcal{U} \) in appendix G. The matrix \( Q^{(1)} \) is given by (35) with \( h_j = S_i^z \) for \( j = 1, 2, 3 \) and \( h_4 = \tilde{\Sigma}_z \). The nonzero components are

\[
Q_{41}^{(1)} = -Q_{14}^{(1)} = 4\sqrt{2} f^2, \quad Q_{42}^{(1)} = -Q_{24}^{(1)} = -4\sqrt{2} f^1.
\]

(47)

The GLC condition \( Q_i^{(1)} = 0 \) requires \( f^i = f^2 = 0 \). It follows that \( f^4 = 0 \) except \( i = 4 \). Then, from the conditions \( df^i/dt = -i \text{tr} \{ \lambda_i[H, F] \} = 0 \) for \( i \neq 4 \), we have

\[
b_i = 0, \quad i = 1, 2, 3.
\]

(48)

Therefore, all variables except \( f^4 \) and \( J \) are zero by the GLC condition for \( m = 1 \). Next, we calculate \( Q^{(2)} \) to obtain

\[
Q^{(2)} = 4 \begin{pmatrix}
J f^4 & 0 & 0 & 0 \\
0 & (\omega_0 - J) f^4 & 0 & 0 \\
0 & 0 & 2f^4 \omega_0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}.
\]

(49)

Although the constraint is typical as a two-qubit problem (on \( \mathcal{H} \)), it is not so as a one-qutrit problem (on \( \mathcal{H}_{\text{sym}} \)). If one wants to consider a typical time-optimal control on a qutrit, replace the constraint \( J^2 + (b^1)^2 + (b^2)^2 + (b^3)^2 \leq \Omega^2 \) with \( 8f^2/3 + (b^1)^2 + (b^2)^2 + (b^3)^2 \leq \Omega^2 \), which is equivalent to \( \text{tr} (H_d)^2 \leq \Omega^2 \) in the subsequent discussions.
From the GLC condition, $Q^{(2)}$ must be positive semidefinite, which implies

$$0 \leq f^a, \quad 0 \leq J \leq \omega_0. \quad (50)$$

This is the condition that singular optimal controls must satisfy. As a result, the singular time-optimal Hamiltonian has the form

$$H(t) = \omega_0 \hat{\Sigma}^x + J(t)\hat{\Sigma}^y, \quad (51)$$

where $0 \leq J(t) \leq \omega_0$.

A further observation enables us to focus on the drift-only control

$$H(t) = H_d = \omega_0 \hat{\Sigma}^x. \quad (52)$$

Any optimal singular protocol (51) can be replaced with a regular protocol followed by the protocol (52) without changing the time duration. Assume that a time-optimal protocol $H(t)$ in the interval $[t_1, t_2]$ is given by (51). The corresponding unitary operator in $[t_1, t_2]$ is given by

$$U_{\text{sing}}(t_2, t_1) = e^{-i\omega_0(t_2-t_1)\hat{\Sigma}^x} e^{-i\int_{t_1}^{t_2} dt J(t)\hat{\Sigma}^y}, \quad (53)$$

because $\hat{\Sigma}^x$ and $\hat{\Sigma}^y$ commute. Since $0 \leq J(t) < \Omega$, there exists $t_3 \in [t_1, t_2]$ such that $\int_{t_1}^{t_2} dt J(t) = \Omega(t_3 - t_1)$.

We can realize the same unitary operator (53) by setting $J(t) = \Omega$ on $[t_1, t_3]$ and $J(t) = 0$ on $[t_3, t_2]$. By (50), the control $J(t) = \Omega$ cannot be singular optimal so it must be regular. Therefore, we can deform any time-optimal singular control to a regular control plus the singular control (52). Thus, we can restrict ourselves to seek a sequence consisting of optimal regular solutions to MP-QB and a singular control (52).

In particular, if the target unitary operator $U_f$ has the form

$$U_f = e^{-i\alpha \hat{\Sigma}^x}, \quad (54)$$

then the singular control (52) may be optimal and the time cost is $\alpha/\omega_0$.

8. Conclusion and discussions

The conclusion consists of four parts.

First, we have presented a general framework, based on MP, for finding the time-optimal Hamiltonian $H(t) \in A$ for given $(U_f, A)$, where $U_f$ is the target unitary operation and $A$ is the set of available Hamiltonians. Compared with the older formulation, QB [34, 36], our new framework, MP-QB, can handle not only equality constraints but also inequality ones, which is essential in practical and theoretical applications. The general applicability of MP-QB also allows us to obtain the results that follow.

Second, we have derived a necessary condition beyond MP that singular controls become time optimal, applying the GLC condition. Singular controls are those for which the maximum condition becomes trivial so that we cannot determine the optimal control protocol. The GLC condition resolves this difficulty, at least partially, by restricting the form of the optimal singular Hamiltonians.

Third, using MP-QB and the GLC condition, we have discussed the general structure of the time-optimal quantum control, focusing on the drift fields, the singular controls, and the reduction of inequality constraints to equality ones. We have shown the following.

(a) If the constraint $A$ is lollipop type, all time-optimal controls are regular.

(b) All regular time-optimal controls lie on the boundary of $A$ in the control plane. When $A$ is planar, this implies that at least one equality is attained among the inequality constraints.

(c) If the constraint $A$ is planar and lotus leaf type with $H_E \in |C, C|$, all (regular and singular) time-optimal controls lie on the boundary of $A$ in the control plane, so that an equality is attained.

These results are summarized in table 1, which also serves as a prescription. Give the type of constraint for $H(t)$ that one is dealing with, and obtain which types of controls have possibility of being time optimal. For planar constraints, the regular optimal controls attain an equality. In the case that all inequalities reduce to equalities, one can identify the time-optimal protocol by the QB equation (14) as in the previous studies [36]. In other cases and for non-planar constraints, one must solve MP-QB (i.e., equations (14), (15) and (17)). If there is possibility of singular controls being time optimal, one must carry out the GLC test (i.e., steps (a)–(e) in section 5.2).

Finally, we have demonstrated how our framework, the GLC condition and the results above work by some examples.
We naively expect that the regular controls take the full advantage of the control Hamiltonian $H_c(t)$, while the singular controls essentially let the system evolve by the drift $H_d$. In fact, the examples in the last section have singular controls with $H_c(t) = 0$. The expectation is best seen in the systems with typical constraints: the regular controls must have the maximal norm of the control Hamiltonian $H_d$; singular controls exist only when the drift field $H_d$ is not in $C$ or $[C, C]$, which imply that $H_c(t)$ cannot help generate unitary operator $e^{-iH_d t}$ up to the second-order of infinitesimal time interval $\delta t$. This follows from the Baker–Campbell–Hausdorff formula. For example, we assume $H(t) = H_d + K_1$ for $t \in [0, \delta t]$ and $H(t) = H_d + K_2$ for $t \in [\delta t, 2\delta t]$, where $K_1, K_2 \in C$ and $H_d \notin [C, [C, C]]$. Then, we have the resulting unitary operator $U(2\delta t)$ as

$$U(2\delta t) = e^{-i\delta t(H_d + K_2)} e^{-i\delta t(H_d + K_1)} = \exp \left[ -2i\delta tH_d + \delta t(K_1 + K_2) + \frac{\delta t^2}{2} [H_d + K_2, H_d + K_1] + O(\delta t^3) \right],$$  

where $H_d \notin [C, [C, C]]$ ensures that the second and third terms in the argument of the exponential cannot produce a term proportional to $H_d$. Even for the planar constraints $A$, the situation is similar, except that the regular optimal controls must be on the boundary of $A$. Whether such an interpretation is possible in general is open.

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**Appendix A. The algebraic condition (10) in the previous studies**

Although the algebraic condition (10) did not appear in the previous studies [34–36, 40, 41], the treatments were compatible with (10). The Hamiltonians treated in the previous studies have the form $H(t) = H_d + H_c(t)$ with constraints $\text{tr}[H_c^2] = \Omega$ and $H_c \in C$, where $\Omega > 0$ and $C$ is a certain subspace of $\mathfrak{su}(N)$. Then, equation (8) has the form $F(t) = \lambda(t) H_c(t) + F'(t)$. When $H_d = 0$, the condition (10) is equivalent to $\lambda \neq 0$, which was implicitly assumed in the previous studies. The condition (10) justifies this assumption. When $H_d \neq 0$, the solutions with $\lambda = 0$ exist in general. These are the singular controls discussed in sections 3 and 6 in the present paper.

**Appendix B. Generalization of a result from QB**

The result in section 3.2 on the Zermelo navigation has a generalization. Suppose that the Hamiltonian $H(t) = H_d + H_c(t)$, where $H_d$ is constant, obeys the constraints $\tilde{f}(H_c) = 0$. If all the constraints $\tilde{f}(H_c) = 0$ are invariant under transition to the interaction picture by $H_d$, the QB equation reduces to that of a drift-free problem. When $\tilde{f}(H_c) = \tilde{f}'(H_{c,3})$, we have

$$S \left[ H_d + H_c, U, F, \{ \lambda' \}; \tilde{f}' \right] = S \left[ H_{c,3}, U, F, \{ \lambda' \}; \tilde{f}' \right], \quad (B.1)$$

where the action functional $S \left[ H, U, F, \{ \lambda' \}; \tilde{f}' \right]$ is given by (5) and (6). Note that the right hand side of (B.1) is an action for a drift-free problem with $H(t) = H_{c,3}(t)$. Thus, the formula (8) for $F$ and the QB equation (9) in the original problem is equivalent to those in the drift-free problem with constraints $\tilde{f}'(H_{c,3}) = 0$. The solution to the original problem is written as

$$H(t) = H_d + e^{-iH_d t} H_{c,3}(t) e^{iH_d t}, \quad U(t) = e^{-iH_d t} e^{-i\int_0^t \tilde{f}'(H_{c,3}(s))}, \quad (B.2)$$

where $\mathcal{T}$ denotes the time-ordered product. We remark that, as for the algebraic equation, we must use the original one (10) because the condition (7) was for the fixed target unitary operator $U_f$.

**Appendix C. Construction of tent and its convexity**

We construct the tent $\tilde{\mathcal{R}}_{(T,U(T))}$ of $\mathcal{R}$ at $(T, U(T)) \in \mathcal{M}$ appeared in section 4.3 and show its convexity.

First, the needle variations form a space that is closed under addition and nonnegative scalar multiplication, which are essentially operations on their intervals. A simple needle variation $M(\tau; \delta \tau; K)$ is
defined in (20). The sum \( M(\tau_1; \delta \tau_1; K_1) + M(\tau_2; \delta \tau_2; K_2) \) of needle variations is defined simply by the composition of these operations if \( \tau_1 \neq \tau_2 \). If \( \tau_1 = \tau_2 =: \tau \), the sum is given by arranging them 'side by side,' namely, the resulting \( H'(t) \) is given by

\[
H'(t) = \begin{cases} 
K_1, & \tau - \delta \tau_1 < t \leq \tau - \delta \tau_2, \\
K_2, & \tau - \delta \tau_2 < t \leq \tau, \\
H(t), & \text{otherwise.}
\end{cases}
\]

(C.1)

The sum of the sums of simple needle variations, etc., are defined similarly. The space of needle variations thus constructed is closed under 'addition,' which is not commutative. A nonnegative scalar multiplication is defined by scalar multiplications on all the intervals, e.g., \( \lambda (M(\tau_1; \delta \tau_1; K_1) + M(\tau_2; \delta \tau_2; K_2)) = M(\tau_1; \lambda \delta \tau_1; K_1) + M(\tau_2; \lambda \delta \tau_2; K_2) \). Under these operations, the space of needle variations is closed. With variations of \( \delta \tau \) defined in section 4.3 being included, the space of variations is still closed.

Second, although the 'addition' of needle variations of \( H(t) \) are non-commutative, that of the resulting variations of \( U(T) \) are commutative. This can be seen by the fact that the variation of \( U(T) \) caused by \( M(\tau; \delta \tau_1; K_1) + M(\tau; \delta \tau_2; K_2) \) is

\[
\delta U(T) = -iU(T, \tau) \left[ \delta \tau_1(K_1 - H(\tau)) + \delta \tau_2(K_2 - H(\tau)) \right] U(\tau).
\]

(C.2)

Thus, the first-order variations \( \delta \left[ U(T) \right] \) caused by the needle variations and the final time variation form a convex-linear space. This convex cone is the tent \( \tilde{R}(T, U(T)) \).

### Appendix D. Invariance of the GLC condition under coordinate transformation

Although the matrices \( Q^{(m)} \) depend on the parametrization of the Hamiltonian, the conditions \( Q^{(M)} = 0 \), \( Q^{(M')} \geq 0 \), and \( Q^{(M')} \leq 0 \) (the latter two mean positive and negative semidefiniteness) do not, where \( M \) is the smallest integer with \( Q^{(M')} \neq 0 \). Let \( u = \{ u^j(t) \} \) and \( v = \{ v^j(t) \} \) be parametrizations of the same Hamiltonian \( H(t) \). We have

\[
\frac{\partial}{\partial u^j} = \sum_{i=1}^{l} \frac{\partial v^i}{\partial u^j} \frac{\partial}{\partial v^i} \tag{D.1}
\]

where the Jacobian matrix \( \frac{\partial v^i}{\partial u^j} \) is invertible. Let us derive the relation between \( Q^{(M)}(u) \) and \( Q^{(M')}(v) \), where \( M \) and \( M' \) are the smallest integers for which \( Q^{(M)}(u) \) and \( Q^{(M')}(v) \), respectively, have at least one nonzero element. We assume \( M \leq M' \) without loss of generality. Direct application of (D.1) to (31) leads to

\[
Q^{(M)}_{ij}(u) = \sum_{p,q=1}^{l} \frac{\partial v^p}{\partial u^j} \frac{\partial}{\partial v^p} \left( \left( \frac{d}{dt} \right)^{M} \left( \frac{d}{dt} \right) \frac{\partial}{\partial v^q} H_{MP} \right)
\]

\[
= \sum_{n=0}^{M} \binom{M}{n} \sum_{p,q=1}^{l} \frac{\partial v^p}{\partial u^j} \frac{\partial}{\partial v^p} \left[ \left( \frac{d}{dt} \right)^{n} \left( \frac{d}{dt} \right) \frac{\partial}{\partial v^q} H_{MP} \right]. \tag{D.2}
\]

However, the terms with \( n > 0 \) vanish because \( Q^{(m)}(v) = 0 \) for \( m < M' \) and because

\[
\left( \frac{d}{dt} \right)^{m} \left( \frac{d}{dt} H_{MP} \right) = 0, \quad m \geq 0, \tag{D.3}
\]

which is equivalent to the \( m \)th time derivative of the singularity condition (29). We therefore obtain

\[
Q^{(M)}_{ij}(u) = \frac{\partial v^k}{\partial u^j} Q^{(M)}_{kl}(v) \frac{\partial v^l}{\partial u^i}. \tag{D.4}
\]

Since the matrix \( \frac{\partial v^l}{\partial u^i} \) is invertible, we have \( Q^{(M)}(u) = 0 \Leftrightarrow Q^{(M)}(v) = 0, Q^{(M)}(u) \geq 0 \Leftrightarrow Q^{(M)}(v) \geq 0 \), and \( Q^{(M)}(u) \leq 0 \Leftrightarrow Q^{(M)}(v) \leq 0 \).

### Appendix E. Recurrence relation of the matrix \( Q^{(m)} \)

We shall demonstrate the calculation of the matrix \( Q^{(m)} \) in our formulation in section 5.

From (31), we obtain the recurrence relation for general \( m > 0 \) as

\[
Q^{(m)}_{ij} = \frac{\partial}{\partial u^j} \left[ \frac{d}{dt} \left( \frac{d}{dt} \right)^{m-1} \frac{\partial}{\partial u^i} H_{MP} \right].
\]
The operators on \( H_{\text{sym}} \) are traceless themselves. In the Gell–Mann matrices \( \lambda_i \), they are
\[
\tilde{\Sigma}^x = \lambda_4 = \frac{1}{2} \lambda_3 + \frac{1}{2\sqrt{3}} \lambda_8, \quad \tilde{\Sigma}^y = \lambda_3 = \frac{1}{\sqrt{3}} \lambda_8, \quad S^z = \frac{1}{2} (\lambda_1 + \lambda_8),
\]
\[
S^x = \frac{1}{2} (\lambda_2 + \lambda_7), \quad S^y = \frac{1}{2} (\lambda_3 + \sqrt{3} \lambda_8).
\]

**Appendix G. Non-optimality of boundary singular controls in example 3**

We show that the boundary singular controls in example 3 (section 7.3), which satisfy
\[
J^2 + (b^1)^2 + (b^2)^2 + (b^3)^2 = \Omega^2,
\]
are non-optimal. We will reduce the number of control variables and apply the GLC condition.
The singularity condition (29) and its time derivative (30) imply (45), (46) and the following:

\[ b^4 f^2 - b^2 f' = 0, \]  
\[ Jf^2 = 0, \]  
\[ f^4 (J - \omega_0) = 0. \]  

The second time derivative of (29) implies

\[ b^4 f^4 + b^2 f'^2 + \sqrt{2} b^2 f'^4 = 0. \]  

The algebraic condition (17) leads to \( f^4 \neq 0 \) (equation (46)). These hold for both interior and boundary singular controls.

Let us perform the GLC test. We shall show by contradiction that singular optimal controls must have \( b^4 = 0 \) for \( i = 1, 2, 3 \) and then examine the optimality of such controls. First, we assume \( b^4 \neq 0 \). We regard the Hamiltonian (42) as a function of \((b^4, b^2, J)\),

\[ H(t) = \omega_0 \Sigma + f \Sigma + \sum_{i=1}^3 b^4(t) S^i + b^2(b^2, b^2, J; t) S^i, \]  

where \( b^4(b^4, b^2, J; t) = \pm \sqrt{\Omega^2 - f^2 - (b^2)^2 - (b^2)^2} \). We have

\[ h_i := \frac{\partial H}{\partial b^i} = S^i - \frac{b^i}{b^2} S^2; \quad (i = 1, 2), \quad h_3 := \frac{\partial H}{\partial J} = \tilde{\Sigma} - \frac{1}{b^2} S^2. \]  

The \( 3 \times 3 \) matrix \( Q^{(1)} \) given in (32) has nonzero components

\[ Q_{13}^{(1)} = -Q_{31}^{(1)} = -4\sqrt{2} f^2, \quad Q_{32}^{(1)} = -Q_{23}^{(1)} = 4\sqrt{2} f^4. \]  

The GLC condition \( Q^{(1)} = 0 \) implies \( f^2 = 0 \). These together with (G.5) and \( f^4 \neq 0 \) imply \( b^4 = 0 \), contradicting the assumption \( b^4 \neq 0 \). We thus have \( b^4 = 0 \). Next, we assume \( b^4 \neq 0 \) under \( b^4 = 0 \). Thanks to (G.2) and (G.5), we obtain \( f^4 = 0 \). However, \( df^2/dt = -i \text{tr} [J_{\lambda} [H, F]] = 0 \) implies \( b^4 = 0 \), a contradiction. We thus have \( b^4 = 0 \). Finally, we assume \( b^4 \neq 0 \) under \( b^4 = 0 \). Equation (G.2) implies \( f^3 = 0 \). However, \( df^4/dt = -i \text{tr} [J_{\lambda} [H, F]] = 0 \) implies \( b^4 = 0 \), a contradiction. Therefore, the singular optimal control must have \( b^4 = 0 \) for \( (i = 1, 2, 3) \).

The only remaining possibility is \((J, b^4) = (\pm \Omega, 0)\). Near there, we regard \( J \) and the Hamiltonian (42) as functions of \((b^4, b^2, J)\). We have

\[ h_i := \frac{\partial H}{\partial b^i} = S^i, \]  

thanks to the conditions \( |J| = \Omega \) and \( b^4 = 0 \). Since the operators \( h_i \) are the same as those of the interior control, we have \( Q^{(1)} = 0 \) and \( Q^{(2)} \) as the first \( 3 \times 3 \) matrix of (49). Thus, we obtain the same conclusion (50), which contradicts \(|J| = \Omega > \omega_0\). As a result, all singular controls on the boundary are non-optimal.

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