Quantum brachistochrone

Tatsuhiko Koike \(^1\) \(^2\)

\(^1\)Department of Physics and Quantum Computing Center, Keio University, Hiyoshi 3-14-1, Kohoku, Yokohama 223-8522, Japan
\(^2\)Research and Education Center for Natural Sciences, Keio University, Hiyoshi 4-1-1, Kohoku, Yokohama 223-8521, Japan

Quantum brachistochrone (QB) is a quantum analogue of classical brachistochrone (shortest path). It is a solution to the following problem: How can we perform a desired quantum operation (or obtain a desired final quantum state) most quickly, by a time-dependent Hamiltonian subject to given constraints? Finding QB is a fundamental problem in quantum mechanics in its own right. Moreover, it will be useful in the study of quantum information and quantum engineering, such as quantum speed limits and implementations of quantum computers.

A general framework for finding QBs, called QB formalism, has been developed. It is based on Pontryagin’s maximum principle. We review the basics of the QB formalism, give simple examples, and briefly discuss some related studies.

This article is part of the theme issue ‘Shortcuts to adiabaticity: theoretical, experimental and interdisciplinary perspectives’.

1. Introduction

In quantum mechanics, one can change a given state to another by applying a Hamiltonian on the system. It is often desirable to know the fastest possible pathway, called the time-optimal quantum control. The examples include quantum error correction [1], quantum metrology [2], quantum cooling [3,4], quantum battery [5] and gates in quantum computers [6], because noise from the environment degrades quantum states over time. Time-optimal quantum control [7,8] has been studied for systems with fast local control [9–15] and with close-level controllable couplings [16–19], for spin chains [20–23], for the Zermelo navigation problem [24–27] and for linear networks [28]. Related interests include quantum speed limit [29–36] (see also [37]) developed from the time-energy uncertainty relation.
A promising approach to those time-optimality problems is to consider the following fundamental question in quantum mechanics: How can we perform a desired quantum operation (or obtain a desired final quantum state) most quickly, by a time-dependent Hamiltonian subject to given constraints? This is called quantum brachistochrone (QB) problem, where the name ‘quantum brachistochrone’ was inspired by classical brachistochrone [38].

A classical brachistochrone (from Greek ‘shortest time’) is the curve connecting given initial and final points in the real space so that a particle constrained on that curve travels in the shortest time $T = \int (dS/v)$ under a homogeneous gravitational field, where $dS$ is the infinitesimal distance along the curve and $v$ is the velocity of the particle. The answer is known to be a cycloid.

In [38], a QB has been defined as the curve in the quantum state space that represents the fastest time evolution between given initial and final states, where the state obeys the Schrödinger equation and the steering Hamiltonian is subject to certain constraints. Moreover, a general framework for finding QB has been presented [38]. The distance $dS$ in the quantum state space is taken to be the so-called Fubini–Study metric and the velocity $v$ is taken to be the energy fluctuation (as in [36]).

The QB formalism has been extended to time-optimal realization of unitary operations [39] and to mixed state evolution in open systems described by the Lindblad master equation [40]. A modern formulation of QB based on Pontryagin’s maximum principle (MP) (e.g. [41]) has been developed and a general theory on second-order variations are given [42].

QB question is interesting in its own right. In addition, the QB formalism provides a method of finding the time necessary to achieve given quantum operation or quantum information processing. A close relation between time complexity and gate complexity has been suggested by numerical analysis of QBs [43]. Simple systems modelling quantum information device have been analysed by the QB formalism [21–23]. The QB formalism also leads to a wider perspective to shortcuts to adiabaticity (STA) [44–58] (see also [59]). It is expected that the QB formalism is useful in the study of other subjects related to time optimality.

It is worth noting that the concept of optimality depends highly on the set-up that one considers. Although there are many ‘time-optimal’ quantum schemes, some of them may have unclear conditions and some may be merely time-efficient. An advantage of the QB formalism, apart from its simplicity and generality, is the clarity of the meaning of time optimality. It is defined completely by, and only by, the constraint on the Hamiltonian (and the Lindblad operators). Therefore, the time optimality in the QB formalism is operational and is not based on any ansatzes or geometric assumptions.

There have been studies [16,19,60–68] in which the MP is applied to time-optimal quantum control, where the MP is applied on individual quantum control problems which are cast into a standard form in control theory with real variables. By contrast, the QB formalism directly treats the general time-optimal quantum control problem on the basis of MP. We also refer the reader to a recent introduction to the applications of MP on quantum control [69].

We try to present the basics of the QB formalism in a manner as simple as possible, especially for those who are familiar with control systems. In §2, we review the QB formalism for unitary operations. In §3, we briefly present the QB formalism in other set-ups: transitions of a quantum state to another in closed and open systems. Second-order variations of the time functional is discussed in §4. The formalism is applied to simple systems in §5. Numerical methods for finding QBs is described in §6. Other applications of QBs are briefly discussed in §7. Section 8 is the conclusion.

We use a unit system in which $\hbar = 1$.

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1 There are various equivalent ways to formulate the QB problem. The original formulation ([38,39] etc.) may be easily accessed by those who are familiar with general relativity or differential geometry.
2. Quantum brachistochrone

(a) Quantum brachistochrone for realization of unitary operations

We review the QB formalism for the realization of unitary operations [39,42]. The QB problem can also be formulated in similar manners for the control of a pure state governed by the Schrödinger equation [38] and for the control of a mixed state governed by the Lindblad master equation [40], which are given in the next section.

Let $H$ be the Hilbert space of dimension $N$ that describes the quantum system under consideration. We assume that $N$ is finite. Let $\mathcal{A}$ be the set of available (or feasible) Hamiltonians, namely, a subset of the set of all Hermitian operators on $H$. Let $U(H)$ be the set of unitary operators. Let $U_f \in U(H)$ be a unitary operation on $H$ that one wants to realize. The QB problem is specified by a pair $(U_f, A)$. The question is how to realize a unitary operation $U_f \in U(H)$ in a least time $T > 0$, when $H(t)$ is subject to a condition $H(t) \in \mathcal{A}$. We call the solution $(H(t), T)$ the QB, or simply, brachistochrone.

In the QB problem, we want to minimize the functional

$$ S[U, H] = \int_0^T dt, $$

(2.1)

under the following conditions:

$$ i \frac{dU(t)}{dt} = H(t)U(t), $$

(2.2)

$$ U(0) = 1 \text{ (identity operator)} , \quad U(T) = U_f $$

(2.3)

and

$$ H(t) \in \mathcal{A}. $$

(2.4)

Equation (2.2) is the Schrödinger equation satisfied by the control $H(t)$ and the time evolution operator $U(t)$. Note that in QB formalism, the Schrödinger equation appears as a constraint equation. The other conditions, (2.3) and (2.4), are the boundary condition for the unitary $U(t)$ and the constraint for the Hamiltonian $H(t)$, respectively.

To formulate the QB problem, we introduce Pontryagin’s MP, which is a modern variational calculus for optimal control. Consider the problem of minimizing the functional

$$ S = \int_0^T f^0(x(t), u(t)) dt $$

(2.5)

by suitably choosing the time dependence of control variables $u(t) = (u^1(t), u^2(t), \ldots, u^m(t)) \in \mathcal{A}_u$ and the final time $T$, where the dynamical variables $(x^1(t), \ldots, x^n(t))$ obey equations of motion

$$ \frac{dx^a(t)}{dt} = f^a(x(t), u(t)), \quad a = 1, \ldots, n. $$

(2.6)

and satisfy given initial and final conditions. For formal simplicity, we introduce a variable $x^0(t)$ such that equation (2.6) holds for $a = 0$ as well and understand that the argument $x$ in $f^a(x, u)$ as $x = (x^0, \ldots, x^n)$ though $f^a$ do not depend on $x^0$ explicitly. Note that the functional (2.5) can be written as $S = x^0(T) - x^0(0)$. We assume that functions $f^a$ are continuous.

In the method of MP, one introduces Lagrange multiplier variables, or ‘momenta,’ $p(t) := (p_0(t), p_1(t), \ldots, p_n(t))$ and the MP ‘Hamiltonian’

$$ H_{MP}(x, p, u) := \sum_{a=0}^n p_a f^a(x, u), $$

(2.7)

so that the equations of motion (2.6) are cast in a Hamiltonian form,

$$ \frac{dx^a(t)}{dt} = \frac{\partial H_{MP}}{\partial p_a}(x(t), p(t), u(t)) = f^a(x(t), u(t)). $$

(2.8)
and
\[ \frac{dp_a(t)}{dt} = -\frac{\partial H_{\text{MP}}}{\partial x^a}(x(t), p(t), u(t)), \quad a = 0, 1, \ldots, n. \] (2.9)

The MP states (e.g. [41]) that a necessary condition that \( u(t) \) and \( T \) minimize the functional (2.5) is that
\[ H_{\text{MP}}(x(t), p(t), u(t)) \geq H_{\text{MP}}(x(t), p(t), v) \] (2.10)
holds for each feasible control \( v \in A_u \) for each time \( t \), namely, \( u(t) \in A_u \) maximizes \( H_{\text{MP}}(x(t), p(t), \bullet) \) for each \( t \). This condition is called the MP. Moreover, it can be shown that the maximum value of (2.10) must be zero,
\[ H_{\text{MP}}(x(t), p(t), u(t)) = 0, \] (2.11)
for each \( t \), and
\[ p_0 = \text{constant} \leq 0. \] (2.12)

The condition (2.11) holds when one can vary \( T \) in the functional (2.5).

We now formulate the QB problem by a close comparison with the general formulation of the MP, while a direct derivation, without assuming the knowledge of MP, can be found in [42]. The dynamical variables \( (x^1(t), \ldots, x^n(t)) \) correspond to the unitary \( U(t) \) in the QB problem (for the unitary operator realization). The control variable \( u(t) \) corresponds to the Hamiltonian \( H(t) \in A \). It does not matter whether \( H(t) \) is concretely parametrized by some variables \( u(t) \) or rather the condition \( H(t) \in A \) is implicitly expressed by some (in)equalities involving \( H(t) \). The Lagrange multiplier variables \( p(t) \) dual to \( x(t) \) should correspond to a new operator \( G(t) \) on \( \mathcal{H} \). Because we deal with the time optimality problem, the function \( f^0 \) in (2.5) should be \( f^0 = 1 \). The MP Hamiltonian for the QB problem is
\[ H_{\text{MP}} = p_0(t) - i \text{Tr}[G(t)H(t)U(t)]. \] (2.13)

Equations (2.8) and (2.9) now become
\[ \frac{dx^0(t)}{dt} = \frac{\partial H_{\text{MP}}}{\partial p_0} = 1, \quad \frac{dU(t)}{dt} = \frac{\partial H_{\text{MP}}}{\partial G} = -iH(t)U(t) \] (2.14)
and
\[ \frac{dp_0(t)}{dt} = -\frac{\partial H_{\text{MP}}}{\partial x^0} = 0, \quad \frac{dG(t)}{dt} = -\frac{\partial H_{\text{MP}}}{\partial U} = iG(t)H(t). \] (2.15)

The first equations in (2.14) and (2.15) merely state that \( x^0(t) = t \) and that \( p_0 \) is constant, respectively. The second of (2.14) is the Schrödinger equation (2.2). The MP (2.10) reads
\[ H_{\text{MP}}(x^0(t), U(t), p_0(t), G(t), H(t)) \geq H_{\text{MP}}(x^0(t), U(t), p_0(t), G(t), K), \] (2.16)
for each \( K \in A \). We also have \( H_{\text{MP}}(x^0(t), U(t), p_0(t), G(t), H(t)) = 0 \) and \( p_0 \) is a non-positive constant.

Letting \( G(t) = iU(t)F(t) \), we can rewrite (2.15) as
\[ \frac{dF(t)}{dt} = [H(t), F(t)]. \] (2.17)

where \([A, B] := AB - BA\) and we have used the Schrödinger equation (2.14). Equation (2.17) is called the QB equation. The operator \( F(t) \) can be considered Hermitian. In fact, if \( F(t) \) had an anti-Hermitian part, it would not affect \( \partial H_{\text{MP}}/\partial G \) in (2.14) because \( H \) is Hermitian.\(^2\) Another way of saying this is that, because of (2.17), the anti-Hermitian part of the auxiliary variable \( F(t) \), if any,

\(^2\)This may be seen clearer if one thinks of \( \partial H_{\text{MP}}/\partial G \) as \( \partial H_{\text{MP}}/\partial F \) \( U(t) = (\partial \text{Tr}[F(t)H(t)])/\partial F \) \( U(t) \).
would not evolve and would be completely decoupled from the other variables, not affecting the QB. The MP Hamiltonian (2.13) reads

\[ H_{\text{MP}} = p_0 + \text{Tr}[F(t)H(t)], \]  

(2.18)

where \( p_0 \) is a constant, which follows from (2.15). Then the MP (2.10) is that, for each \( t \), \( H(t) \) is the maximizer of \( \text{Tr}[F(t)K] \):

\[ H(t) = \arg\max_{K \in \mathcal{A}} \text{Tr}[F(t)K]. \]  

(2.19)

The additional necessary conditions, (2.11) and (2.12), read

\[ \text{Tr}[F(t)H(t)] = -p_0 \text{ (constant)} \geq 0. \]  

(2.20)

The QB formalism is summarized as follows. If the Hamiltonian \( H(t) \in \mathcal{A} \) realizes the unitary \( U_f \) in the shortest time \( T \), namely, if \( (H(t), T) \) is the solution to the QB problem \((U_f, \mathcal{A})\), then there are a unitary operator \( U(t) \) and a Hermitian operator \( F(t) \) that satisfy the following:

- the Schrödinger equation (2.2):
  \[ i \frac{dU(t)}{dt} = H(t)U(t), \]
- the boundary condition (2.3):
  \[ U(0) = 1, \; U(T) = U_f, \]
- the QB equation 2.17:
  \[ i \frac{dF(t)}{dt} = [H(t), F(t)], \]
- the MP (2.19):
  \[ H(t) = \arg\max_{K \in \mathcal{A}} \text{Tr}[F(t)K]. \]
- the algebraic condition (2.20):
  \[ \text{Tr}[F(t)H(t)] = -p_0 \text{ (constant)} \geq 0. \]

These are necessary conditions for globally time-optimal controls \((H(t), F(t), T)\).

Some remarks are in order. First, the control in the case \( p_0 = 0 \) is called an abnormal control and usually not considered. In the other case, \( p_0 < 0 \), one can choose \( p_0 = -1 \) by a rescaling of \( F(t) \). Then equation (2.20) becomes

\[ \text{Tr}[F(t)H(t)] = 1. \]  

(2.21)

Second, if the Hamiltonian \( H(t) \) is concretely parametrized by \( u(t) = (u^1(t), \ldots, u^l(t)) \) such as \( H(t) = H[u(t)] \), then the condition \( H[u(t)] \in \mathcal{A} \) is given by \( u(t) \in \mathcal{A}_u \) with \( \mathcal{A}_u \) being some domain in \( \mathbb{R}^l \). In that case, the MP (2.19) simply becomes

\[ u(t) = \arg\max_{v \in \mathcal{A}_u} \text{Tr}[F(t)H[v]]. \]  

(2.22)

Third, the QB equation (2.17) implies a useful general formula

\[ \text{Tr}[F(t)^k] = \text{constant} \]  

(2.23)

for any positive integer \( k \) [Apply the QB equation on \( d(\text{Tr}[F(t)^k])/dt \)]. Finally, the overall phase of \( U_f \) in the QB problem is often irrelevant since it does not affect the physical quantities of the resulting system. The simplest way to treat such a QB problem is to require that \( U_f \) be SU\((ht)\), unit trace unitaries, instead of \( U(H) \) and that Hamiltonian \( H(t) \) be traceless.

The brachistochrone is often identical to that of the problem with equality constraints [42] in the next subsection. In the simplest case that Hamiltonian has no constraints, apart from the normalization, the brachistochrone is a geodesic on the space of unitary operators [39]. Simple non-trivial examples of brachistochrone are found in [20–23,39]. Numerical examples of brachistochrone are found in [43,70].
(b) Equality constraints

In the special case when the constraint $H \in A$ is given by equalities $f^c(H) = 0$ ($c$ is an index), where $f^c$ are differentiable functions, the MP (2.19) becomes simpler. The optimal $H(t)$ minimizes

$$- \text{Tr}[F(t)H(t)] + \sum_c \lambda_c(t)f^c(H(t)), \tag{2.24}$$

where $\lambda_c(t)$ are Lagrange multipliers. The condition that variations of (2.24) with respect to $H(t)$ must vanish leads to the equation,

$$F(t) = \sum_c \lambda_c(t) \frac{\partial f^c(H(t))}{\partial H}. \tag{2.25}$$

Thus, the MP (2.19) is replaced by the equality (2.25). Therefore, one obtains the solutions to the QB by solving (2.2), (2.3), (2.17), (2.20) and (2.25). Note that the whole problem can be formulated by a simple variational principle of the action integral \[40,42\],

$$S[U, H, F, \lambda, T] = \int_0^T (1 + L_S + L_C) \text{d}t \quad \text{and} \quad L_S = \text{Tr}[F(t)\left(\frac{\text{d}U(t)}{\text{d}t}U(t) - H(t)\right)], \quad L_C = \sum_d \lambda_d(t)f^d(H(t)). \tag{2.26}$$

In the case that one adopts a concrete parametrization $H[u(t)]$ for the Hamiltonian, the condition $H(t) \in A$ is written as $u(t) \in A_u$ with some $A_u$. When the condition $u(t) \in A_u$ is expressed by equalities $g^d(u(t)) = 0$ ($d$ is an index), the MP (2.19) becomes the minimization of

$$- \text{Tr}[F(t)H[u(t)]] + N \sum_d \lambda_d(t)g^d(u(t)), \tag{2.27}$$

where $\lambda_d(t)$ are Lagrange multipliers, so that one has

$$\frac{1}{N} \text{Tr}\left[F(t)\frac{\partial H}{\partial u^d}[u(t)]\right] = \sum_d \lambda_d(t) \frac{\partial g^d(u(t))}{\partial u^d}. \tag{2.28}$$

Thus, one obtains the QB by solving (2.2), (2.3), (2.17), (2.20) and (2.28). The whole problem can be formulated by variational principle for

$$S[U, u, F, \lambda, T] = \int_0^T (1 + L_S + L_C) \text{d}t \quad \text{and} \quad L_S = \text{Tr}[F(t)\left(\frac{\text{d}U(t)}{\text{d}t}U^t(t) - H[u(t)]\right)], \quad L_C = N \sum_d \lambda_d(t)g^d(u(t)), \tag{2.29}$$

where ($d = 1, 2, \ldots$) guarantee $u(t) \in A_u$.

3. Other set-ups

(a) Quantum brachistochrone for pure state evolution

(i) The formulation

The QB problem for state evolution can be formulated in quite a similar manner \[38,42\]. The problem is to find $H(t)$ that evolves a given initial state $|\psi_i\rangle$ to a given final state $|\psi_f\rangle$ in the

\[3\text{Inclusion of } N = \text{dim } \mathcal{H} \text{ in (2.27) is a ‘matter of taste’ because it can be absorbed by a redefinition of } \lambda_d(t).\]
shortest time $T$. The state $|\psi(t)\rangle$ must satisfy the Schrödinger equation
\[ i \frac{d|\psi(t)\rangle}{dt} = H(t)|\psi(t)\rangle, \] (3.1)
and the boundary condition
\[ |\psi(0)\rangle = |\psi_i\rangle \quad \text{and} \quad |\psi(T)\rangle = e^{i\alpha} |\psi_f\rangle, \] (3.2)
where $\alpha \in \mathbb{R}$. The problem is specified by $(|\psi_i\rangle, |\psi_f\rangle, \mathcal{A})$.

A simple way to formulate the QB problem is to introduce the density operator $P(t) := |\psi(t)\rangle \langle \psi(t)|$. The canonical variables are $(x^0(t), P(t), p_0(t), G(t))$, where $G(t)$ is a Hermitian operator. The MP Hamiltonian is given by
\[ H_{MP} = p_0(t) - i \text{Tr} \left[ G(t)[H(t), P(t)] \right]. \] (3.3)
The Hamilton equations for $H_{MP}$ are equivalent to
\[ x^0(t) = t \quad \text{and} \quad p_0 = \text{constant}, \] (3.4)
\[ \frac{dP(t)}{dt} = \frac{\partial H_{MP}}{\partial G} = -i[H(t), P(t)] \] (3.5)
and
\[ \frac{dG(t)}{dt} = -i[H(t), G(t)]. \] (3.6)
Equation (3.5) is the Liouville equation, which is equivalent to the Schrödinger equation (3.1).

We can simplify the formulation by introducing a Hermitian operator $F(t) := i[G(t), P(t)]$, with which the MP Hamiltonian is written as $H_{MP} = p_0(t) + \text{Tr} [F(t)H(t)]$. The equation (3.6) becomes
\[ \frac{dF(t)}{dt} = -i[H(t), F(t)], \] (3.7)
because (3.5) and (3.6) imply $dF(t)/dt = [H(t), G(t)] + [G(t), H(t), P(t)]$, which equals $[H(t), [G(t), P(t)]]$ by the Jacobi identity. Equation (3.7) is the QB equation, which is the same as (2.17). The MP and the algebraic condition are also the same as (2.19) and (2.20), respectively.

The final task is to express the condition that $F(t)$ is written as $-i[G(t), P(t)]$ with some Hermitian operator $G(t)$. Let $F(t) = -i[G(t), P(t)]$. Since $P(t)^2 = P(t)$, we have
\[ P(t)F(t)P(t) = 0 \quad \text{and} \quad (1 - P(t))F(t)(1 - P(t)) = 0, \] (3.8)
or equivalently,
\[ F(t) = F(t)P(t) + P(t)F(t) \]
\[ \{=(1 - P(t))F(t)P(t) + P(t)F(t)(1 - P(t))\}. \] (3.9)
Conversely, the condition (3.9) for $F(t)$ implies the existence of $G(t)$ such that $F(t) = i[G(t), P(t)]$. In fact, $G(t)$ is given by $G(t) = -i[F(t), P(t)]$. By virtue of (3.5) and (3.7), equation (3.9) holds for all $t$ if it does for some $t$.

To summarize, if $(H(t), T)$ is the solution to the QB problem $(|\psi_i\rangle, |\psi_f\rangle, \mathcal{A})$, namely, if the Hamiltonian $H(t) \in \mathcal{A}$ send $|\psi_i\rangle$ to $|\psi_f\rangle$ in the shortest time $T$, then there are $|\psi(t)\rangle$ and a Hermitian operator $F(t)$ that satisfy the following:

- The Liouville equation (3.5),
- the boundary conditions [equivalent to (3.2)]:
\[ P(0) = P_i := |\psi_i\rangle \langle \psi_i| \quad \text{and} \quad P(T) = P_f := |\psi_f\rangle \langle \psi_f|, \] (3.10)
- the same QB equation (3.7), the MP (2.19), and the algebraic condition (2.20), as in the QB for unitary realization,
- the constraint (3.9) between $P(t)$ and $F(t)$. 

The time-optimal control is characterized by \((H(t), F(t), T)\). We can take \(p_0 = -1\) for normal controls as in the case of QB for unitary operations.

If Hamiltonian has no constraints, apart from the normalization, the brachistochrone is a geodesic on the state space [38]. The simplest non-trivial brachistochrone is given in [38].

(ii) Equality constraints

When the condition \(\mathcal{H} \in \mathcal{A}\) is expressed by equalities \(f^c(\mathcal{H}) = 0\), the MP (2.19) is equivalent to the minimization of

\[- \text{Tr}[F(t)H(t)] + \sum_c \lambda_c(t) f^c(H(t)), \quad (3.11)\]

which implies the stationarity condition

\[F(t) = \sum_c \lambda_c(t) \frac{\partial f^c(H(t))}{\partial H}. \quad (3.12)\]

Thus, one obtains the QB by solving (3.5), (3.10), (2.17), (2.20) and (3.12). The whole problem can also be formulated by a simple variational principle [38, 42],

\[
S[|\psi\rangle, H, F, \lambda, T] = \int_0^T (1 + L_S + L_C) \, dt
\]

and

\[
L_S = \text{Tr} \left[ F(t) \left( \frac{dP(t)}{dt} + i[H(t), P(t)] \right) \right], \quad L_C = \sum_c \lambda_c(t) f^c(H(t)),
\]

where \(P(t) = |\psi(t)\rangle \langle \psi(t)|\).

In the case that the Hamiltonian is concretely parametrized by \(u(t) = (u^1(t), \ldots, u^D(t))\) and that \(H(t) \in \mathcal{A}\) is equivalent to \(g^d(u(t)) = 0, d = 1, 2, \ldots\), the MP (2.19) becomes the minimization of

\[- \text{Tr}[F(t)H[u(t)]] + N \sum_d \lambda_d(t) g^d(u(t)), \quad (3.14)\]

which implies

\[
\frac{1}{N} \text{Tr} \left[ F(t) \frac{\partial H}{\partial u^d}(u(t)) \right] = \sum_d \lambda_d(t) \frac{\partial g^d(u(t))}{\partial u^d}. \quad (3.15) \]

Thus, one obtains the QB by solving (3.5), (3.10), (2.17), (2.20) and (3.15). The whole problem can also be formulated by a variational principle,

\[
S[|\psi\rangle, u, F, \lambda, T] = \int_0^T (1 + L_S + L_C) \, dt
\]

and

\[
L_S = \text{Tr} \left[ F(t) \left( \frac{dP(t)}{dt} + i[H[u(t)], P(t)] \right) \right], \quad L_C = N \sum_d \lambda_d(t) g^d(u(t)), \quad (3.16)
\]

where \(P(t) = |\psi(t)\rangle \langle \psi(t)|\).

(b) Quantum brachistochrone for mixed state evolution

The QB problem for mixed state evolution [40] can be formulated in a similar manner if the state obeys the master equation of the Lindblad form. The Lindblad equation is justified for a restricted class of open systems, e.g. those weakly interacting with a large reservoir which relaxes quickly and does not keep memory of them. The Lindblad equation is often used, for example, to model an atom interacting with electromagnetic radiation.

The mixed state of a physical system is expressed by a density operator \(\rho\), on a Hilbert space \(\mathcal{H}\), which is positive definite and has a unit trace. We assume that the state \(\rho(t)\) satisfies the Lindblad
The integer \( j \) in (3.17) runs from 1 to at most \((\dim \mathcal{H})^2 - 1\). Without loss of generality, one can choose \( L = \{L_j\} \) so that \( L_j \) are mutually orthogonal with respect to the Hilbert–Schmidt inner product \( \text{Tr} A^\dagger B \) and that each \( L_j \) is traceless. We will often omit the subscripts of \( \mathcal{L}_{H(t),L(t)} \) when there is no ambiguity.

The problem is to find \( H(t) \) and \( \{L_j(t)\} \), in a given set \( \mathcal{A} \) of available \( \{H, \{L_j\}\} \), that evolves a given initial state \( \rho_j \) to a given final state \( \rho_f \) in the shortest time \( T \). The problem is specified by \( (\rho_j, \rho_f, \mathcal{A}) \).

The canonical variables are \((x^0(t), \rho(t), p_0(t), G(t))\), where \( G(t) \) is a Hermitian operator. The MP Hamiltonian is given by

\[
H_{MP} = p_0(t) + \text{Tr}[G(t)\mathcal{L}(\rho(t))].
\] (3.19)

The Hamilton equations for \( H_{MP} \) are equivalent to

\[
x^0(t) = t \quad \text{and} \quad p_0 = \text{constant},
\] (3.20)

\[
\frac{d\rho(t)}{dt} = \frac{\partial H_{MP}}{\partial G} = \mathcal{L}(\rho(t))
\] (3.21)

and

\[
\frac{dG(t)}{dt} = -\frac{\partial H_{MP}}{\partial \rho} = -\mathcal{L}^\dagger(G(t)),
\] (3.22)

where the superoperator \( \mathcal{L}^\dagger \) is defined by \( \text{Tr}[A^\dagger \mathcal{L}(B)] = \text{Tr}[\mathcal{L}^\dagger(A)B] \) and \( \tilde{A} \) is the traceless part of \( A \). Equation (3.21) is the Lindblad equation (3.17). In (3.22), the reason for the traceless part being taken is that the variations are taken by a variable \( \rho \) with a constant trace.

The MP (2.10) is the condition that, for each \( t \), the function

\[
\text{Tr}[G(t)\mathcal{L}_{K,M}(\rho(t))] \quad (K,M) \in \mathcal{A},
\] (3.23)

is maximized at \((K,\{M_j\}) = (H(t),\{L_j(t)\})\). We also have the algebraic condition

\[
\text{Tr}[G(t)\mathcal{L}_{H(t),L(t)}(\rho(t))] = -p_0 \geq 0.
\] (3.24)

We can take \( p_0 = -1 \) for normal controls as in the case of QB for unitaries.

### 4. Second-order variations

#### (a) Generalized Legendre–Clebsch condition

We have described the QB framework in §2 (and those of other set-ups in §3). One can obtain the time-optimal control \((H(t), T)\) for the QB problem \((U_f, \mathcal{A})\) by solving the QB equation (2.17) and the MP (2.19), together with (2.2), (2.3) and (2.20).

In this section, we discuss the control with \( F(t) \) being such that \( \text{Tr}[F(t)\bullet] \), as a function on \( \mathcal{A} \), satisfies

\[
\text{Tr}[F(t)\bullet] = \text{constant},
\] (4.1)

at fixed \( t \). This situation causes a problem in the search of time-optimal control because for such \( F(t) \) all \( H(t) \) satisfy the MP (2.19) and remain to be candidates for the time-optimal control. The controls \((H(t), F(t))\) satisfying (4.1) are called singular. It is desired that we have criteria that distinguishes optimal and non-optimal singular controls; otherwise, we need to compare the total time duration \( T \) for all singular controls.
Such a criterion, a necessary condition for optimality, is obtained by considering the second-order variations for \((H(t), F(t))\). In the general theory of MP, it is called the generalized Legendre-Clebsch (GLC) condition \([71,72]\). There, by taking the variations of \(u(t)\) in certain special forms and by extensively using the equation of motion (2.8) and (2.9), one makes the second-order variations of \(H_{MP}\) to a simple quadratic functional of \(u(t)\). The GLC condition is applied the QB in \([42]\).

Let \(H(t) \in \mathcal{A}\) be parametrized as \(H[u(t)], u(t) \in \mathcal{A}_u \subseteq \mathbb{R}^l\). We define an \(l \times l\) matrix \(Q^{(m)}\), \(m = 0, 1, 2, \ldots\), whose \((i, j)\) element is given by

\[
Q^{(m)}_{ij} := \frac{\partial}{\partial u_i} \left( \frac{d}{dt} \right)^m \frac{\partial}{\partial u_j} \text{Tr} \left[ H[u(t)]F(t) \right].
\]  

(4.2)

The matrix \(Q^{(m)}\) is known to be symmetric for even \(m\) and antisymmetric for odd \(m\). Let \(M\) be the smallest \(m\) with a non-vanishing \(Q^{(m)}\). It can be shown that, if \((H[u(t)], F(t))\) is optimal, then \(M\) is even and \((-1)^{M/2}Q^{(M)}\) is negative semidefinite. For a regular (i.e. non-singular) control, the MP implies the negative semidefiniteness of \(Q^{(0)}_{ij}\), which corresponds to the case \(M = 0\). When the control is singular, \(Q^{(0)} = 0\) and \(M > 0\) follow.

When \(Q^{(k)} = 0\) hold for \(k = 0, 1, \ldots, m - 1\), equation (4.2) can be written as

\[
Q^{(m)}_{ij} = -i \text{Tr} \left[ [h_i(t), F(t)]R^{(m-1)}_{ij} \right],
\]  

(4.3)

where \(h_i(t) := \partial H/\partial u^i\) and \(R^{(m)}_{ij}\) is defined by

\[
R^{(m)}_{ij} = \frac{d}{dt} R^{(m-1)}_{ij} - i[R^{(m-1)}_{ij}, H(t)] \quad \text{and} \quad R^{(0)}_{ij} = h_j(t).
\]  

(4.4)

We can restrict singular quantum controls that are potentially time-optimal by imposing additional necessary conditions through the following GLC test.

\(\text{(o)}\) Let \(m = 0\). We have \(Q^{(m)} = 0\).

\(\text{(i)}\) Increase \(m\) by one and calculate \(Q^{(m)}\) by equations (4.3) and (4.4).

\(\text{(ii)}\) If \(Q^{(m)}\) vanishes, after applying the previously obtained equalities, go to (i).

\(\text{(iii)}\) If \(m\) is odd, impose a condition \(Q^{(m)} = 0\) and go to (i).

\(\text{(iv)}\) Impose negative semidefiniteness on \((-1)^{m/2}Q^{(m)}\) and halt.

In the special case that \(H[u(t)]\) is first order in \(u(t)\) such as

\[
H(t) = H_d + \sum_{j=1}^l u^j(t) h_j,
\]  

(4.5)

where \(H_d\) is a constant operator, then \(h_j\) in equations (4.3) and (4.4) become fixed operators. The first few \(Q^{(m)}\) in (4.3) read

\[
\begin{align*}
Q^{(1)}_{ij} &= -i \text{Tr} \left[ [h_j, h_i] F(t) \right], \\
Q^{(2)}_{ij} &= \text{Tr} \left[ [[H(t), h_i], h_j] F(t) \right] \\
Q^{(3)}_{ij} &= i \text{Tr} \left[ [[H(t), [H(t), h_j]], h_i] F(t) \right] + \text{Tr} \left[ \left[ \frac{dH(t)}{dt}, h_j \right], h_i \right] F(t).
\end{align*}
\]

(4.6)

\(\text{(b)}\) Application

The GLC condition can be applied to restrict the candidates of the time-optimal controls in advance according to the type of constraints \(\mathcal{A}\) for the Hamiltonians. Here, we simply list basic results. For details and more general statements, see \([42]\).
In the QB formalism of §2, suppose that $H(t) \in A$ is expressed by

$$H(t) = H_d + H_c[u(t)], \quad H_c[u(t)] = \sum_{i=1}^l u_i(t)A_i, \quad g^d(u(t)) \leq 0 \text{ (d is an index)},$$

(4.7)

where $H_d$, called the drift, is a fixed Hermitian operator and $A_i$ are linearly independent Hermitian operators. Such a constraint $A$ is called planar and $C := \text{span} \{A_1, \ldots, A_l\}$ is called the control subspace. The following can be shown.

(i) All regular QBs $(H(t), F(t))$ attain the equality $g^d(u(t)) = 0$ for at least one $d$.

(ii) If $H_d \in C$, all QBs $(H(t), F(t))$ are regular.

(iii) If $H_d \notin C$ and $H_d \in [C, C]$, all QBs $(H(t), F(t))$, not only regular ones but also singular ones, attain the equality $g^d(u(t)) = 0$ for at least one $d$.

5. Simple examples

We give some simplest examples. Other examples related to quantum information processing are found in [20,22,23,42,43,70].

(a) General Hamiltonian

Let us consider the QBs for the state change problem $(|\psi_i\rangle, |\psi_f\rangle, A)$ in §3a, which is governed by the QB equation (3.7), the MP (2.19), together with (3.5), (3.10), (2.20) and (3.9). Since we are not interested in the overall phase of $|\psi(t)\rangle$, we assume that the Hamiltonian $H(t)$ is traceless, namely, $H(t) \in \text{su}(N)$, where $\text{su}(N)$ is the Lie algebra of $\text{SU}(N)$.

A simplest example is the case the set $A$ of available Hamiltonians consists of arbitrary ones except for a normalization constraint,

$$A = \{H \in \text{su}(N); 2f^0(H) := \text{Tr} H^2 - \mathcal{E}^2 \leq 0\}. \quad (5.1)$$

We remark that $\text{Tr} H^2$ is the Hilbert–Schmidt norm squared $||H||^2_{HS}$, where $||A||_{HS} := \sqrt{\langle A, A \rangle_{HS}}$ and $\langle A, B \rangle_{HS} := \text{Tr}[A^\dagger B]$ is the Hilbert–Schmidt inner product. Note that without any bound the process time $T$ could be made arbitrarily small. Physically, the bound in (5.1) is an expression that only a finite energy bandwidth is available during the process.

It is easily seen that the time-optimal control $H(t)$ always attains the equality in (5.1),

$$\text{Tr} H^2 = \mathcal{E}^2 \quad (5.2)$$

because otherwise $a(t)H(t)$, with $a(t) \geq 1$ always and $a(t) > 1$ at some $t$, would give a faster control (or alternatively, this can be shown by the results in §4b).

Thus the MP (2.19) can be replaced by the expression for $F$, (3.12), which now reads

$$F(t) = \lambda_0(t)H(t). \quad (5.3)$$

We see that $\lambda_0(t)$ is constant as follows. The QB equation implies equation (2.23). Equation (5.2) therefore implies $\text{Tr}[F(t)^2] = \lambda_0(t)^2\mathcal{E}^2$ is constant and so is $\lambda_0(t)$. The value of $\lambda_0$ is found by (2.20).

The QB equations (3.7) and (5.3) implies $dH(t)/dt = 0$ so that $H(t)$ is constant. The constraint (3.9) implies

$$H = (1 - P_s)HP_s + P_sH(1 - P_s) \quad (* = i, f). \quad (5.4)$$

For a vector $|\chi\rangle$ which is orthogonal to both $|\psi_i\rangle$ and $|\psi_f\rangle$, the vector $H|\chi\rangle = P_fH|\chi\rangle = P_fH|\chi\rangle$ is proportional to both $|\psi_i\rangle$ and $|\psi_f\rangle$, so that $H|\chi\rangle = 0$. Thus, the optimal Hamiltonian is

$$H = \frac{\mathcal{E}}{\sqrt{2}} \left( |\psi_f\rangle\langle \psi_i| - |\psi_i\rangle\langle \psi_f| \right), \quad (5.5)$$

where the state $|\psi_f\rangle$ is in span $\{|\psi_i\rangle, |\psi_f\rangle\}$ and is normal to $|\psi_i\rangle$. For later convenience, we choose the phase of $|\psi_f\rangle$ so that the phase of $\langle \psi_f|\psi_i\rangle$ equals that of $\langle \psi_f|\psi_i\rangle$ [namely, $\langle \psi_f| = (1 - P_s)P_f|\psi_i\rangle$]

\[ \]
divided by its norm]. The Hamiltonian $H$ generates a rotation in span $\{|\psi_i\rangle, |\psi_f\rangle\}$. The optimal state evolution $|\psi(t)\rangle = e^{-iHt}|\psi_i\rangle$ is given by

$$|\psi(t)\rangle = |\psi_i\rangle \cos \frac{\mathcal{E}t}{\sqrt{2}} + |\psi_f\rangle \sin \frac{\mathcal{E}t}{\sqrt{2}}.$$  

(5.6)

The evolution (5.6) is a geodesic [38] on the state space consisting of the ‘rays’ in $\mathcal{H}$, i.e. the projective space $\mathbb{C}P^{N-1}$, endowed with the Fubini–Study metric

$$ds^2 = (d\psi_i)(1 - |\psi\rangle\langle\psi|)d\psi_i.$$  

(5.7)

Although this fact can be verified by deriving the geodesic equation for (5.7), an intuitive understanding would be that the curve (5.6) on $\mathbb{C}P^{N-1}$ corresponds to a great circle on a sphere.

The optimal time $T$ is therefore [38]

$$T = \frac{\sqrt{2}}{\mathcal{E}} \arccos |\langle\psi_i|\psi_f\rangle| = \frac{\sqrt{2}}{|H|_{\text{HS}}} \arccos |\langle\psi_i|\psi_f\rangle|,$$  

(5.8)

which can be obtained by the condition $|\langle\psi_i|\psi_f\rangle| = \cos(\mathcal{E}T/\sqrt{2})$ because of $|\psi_f\rangle = |\psi_i\rangle\langle\psi_i|\psi_f\rangle + |\psi_f\rangle\langle\psi_f|\psi_f\rangle$ and equation (5.6). One can verify that the boundary condition (3.2) [or (3.10)] holds, recalling the phase chosen for $|\psi_f\rangle$.

We remark that the QB is also optimal, in some sense, in the context of the quantum speed limit. The time duration $T$ for the QB, equation (5.8), attains the Bhattacharyya lower bound [30]

$$T_{\text{QSL}} := \frac{1}{\Delta E} \arccos |\langle\psi_i|\psi_f\rangle|,$$  

(5.9)

which is a non-orthogonal generalization of the Mandelstam–Tamm bound [29], for the time necessary to send $|\psi_i\rangle$ to $|\psi_f\rangle$ (up to phase), where $\Delta E$ is the energy variance of $|\psi_i\rangle$. That $T = T_{\text{QSL}}$ follows from the traces of the constraint (5.4) itself and of (5.4) multiplied by $H$, i.e. $\langle H \rangle = 0$ and $\langle H^2 \rangle = ||H||_{\text{HS}}^2/2$, which imply $\Delta E = ||H||_{\text{HS}}/\sqrt{2}$.

(b) One-qubit system

Let us discuss the following QB problem $\mathcal{A}$ for unitary operations in a one-qubit system. The available Hamiltonians $H(t) \in \mathcal{A}$ are

$$H(t) = \omega_0 \sigma^z + u^x(t)\sigma^x + u^y(t)\sigma^y$$ and $$2g^0(u(t)) := (u^x(t))^2 + (u^y(t))^2 - E^2 \leq 0.$$  

(5.10)

where $\omega_0$, $\mathcal{E}$ are positive constants and $\sigma^x$, etc. are the Pauli operators. The model was intensively studied in [68]. We outline a simplified argument thanks to the GLC condition [42]. The constraint $\mathcal{A}$ is planar in the terminology of §4b: The drift is $H_d = \omega_0 \sigma^z$ and the control subspace is $\mathcal{C} = \text{span} \{\sigma^x, \sigma^y\}$. We have $H_d \notin \mathcal{C}$ and $H_d \in [C, C]$. By a result in §4b, this implies that all QBs must attain the equality $g^0(u(t)) = 0$.

It turns out that singular controls are not optimal. The singularity condition $\text{Tr} CF(t) = 0$ implies that $F(t)$, non-zero due to the algebraic condition (2.21), is proportional to $\sigma^z$. The time derivative of $\text{Tr} CF(t) = 0$ and the QB equation imply $u^x(t) = u^y(t) = 0$, which does not satisfy the necessary condition for optimality, $g^0(u(t)) = 0$.

Let us discuss regular controls. Since optimality implies $g^0(u(t)) = 0$, we can apply the discussion in §2b. By equation (2.28), we have

$$F(t) = \lambda_0(t)(u^x(t)\sigma^x + u^y(t)\sigma^y) + f^z(t) \sigma^z,$$  

(5.11)

where $\lambda_0(t)$ is the Lagrange multiplier for $g^0(u)$ and $f^z(t)$ is an unknown component of $F(t)$. The QB equation (2.17) reads

$$(\lambda_0 u^x)^2 = 2(\mathcal{E}^2 - \omega_0 \lambda_0) u^y$$ and $$(\lambda_0 u^y)^2 = -2(\mathcal{E}^2 - \omega_0 \lambda_0) u^x, \quad f^z = 0.$$  

(5.12)
where a dot denotes the time derivative. Therefore, \( f^2 \) is a constant. Then, the formula \( \text{Tr} F^2 = \) constant (2.23) and \( g^0(u(t)) = 0 \) implies that \( \lambda_0 \) is also a constant. The solution of (5.12) is

\[
\begin{align*}
\dot{u}^x(t) &= \mathcal{E} \cos \theta(t) \quad \text{and} \quad \dot{u}^y(t) = \mathcal{E} \sin \theta(t), \quad \theta(t) := \omega t + \theta_0, \quad (5.13)
\end{align*}
\]

where \( \omega := 2(f^2/\lambda_0 - \omega_0) \) and \( \theta_0 \) is a constant. The time-optimal Hamiltonian \( H(t) \) is given by \( (5.13) \) substituted into \( (5.10) \). Observing that \( H(t) = V(t)(\omega_0 \sigma^z + \mathcal{E} \sigma^x) V^\dagger(t), \) \( V(t) := e^{-i \theta(t) \sigma^z/2}, \) we write the Schrödinger equation (2.14), \( iU = HU, \) as \( i(V^\dagger(t)U(t)) = ((\omega_0 - \omega/2)\sigma^z + \mathcal{E} \sigma^x)V^\dagger(t)U(t). \) The unitary is found to be

\[
U(t) = e^{-i \theta(t) \sigma^z/2} e^{-i((\omega_0 - \omega/2)\sigma^z + \mathcal{E} \sigma^x).} \quad (5.14)
\]

In the matrix form with respect to the eigenbasis of \( \sigma^z \), we have

\[
U(t) = \begin{pmatrix}
e^{-i \theta(t)/2} (\cos \Omega t - i \sin \Omega t \cos \varphi) & -i e^{-i \theta(t)/2} \sin \varphi \sin \Omega t \\
e^{i \theta(t)/2} \sin \varphi \sin \Omega t & e^{i \theta(t)/2} (\cos \Omega t - i \sin \Omega t \cos \varphi)
\end{pmatrix}, \quad (5.15)
\]

where \( \Omega := \sqrt{(\omega_0 - \omega/2)^2 + \sigma^2} \) and \( \varphi := \arccos((\omega_0 - \omega/2)/\Omega). \) One determines the parameters \( (\omega, \theta_0, T) \) so that \( U(T) \) equals the given target \( U_f \in SU(2). \)

6. Numerical methods

The QB problem is a two-point boundary value problem (BVP). One can obtain exact solutions for simple systems, e.g. of a few qubits (e.g. \([22,23,38-40]\)), but the problem becomes increasingly difficult as the dimensionality \( N \) of the Hilbert space \( \mathcal{H} \) and the number of control variables become large. Thus, numerical approaches are necessary. Although any method for the BVP can be applied, we review the numerical methods developed for the QB problem in this section.

We consider the QB problem for unitary operations in §2. We ignore the overall phase of \( U_f \) and restrict \( U_f \) to \( SU(\mathcal{H}) \) and \( H(t) \) to \( su(\mathcal{H}) \), the space of traceless Hermitian operators on \( \mathcal{H} \). As a model problem, we shall treat the case that the condition \( H(t) \in \mathcal{A} \) is written as

\[
H(t) \in \mathcal{C} \quad \text{and} \quad ||H(t)||_{HS} \leq \mathcal{E}, \quad (6.1)
\]

where \( \mathcal{C} \) is a subspace of \( su(\mathcal{H}) \), \( \mathcal{E} \) is a positive constant. Physically, the inequality in (6.1) represents the existence of a bound on the available energy bandwidth. The constraint \( \mathcal{A} \) of the form (6.1) is said ‘linear and homogeneous’ in \([39]\)\(^4\) and ‘typical’ in \([42]\). Such \( H(t) \) can be expressed as

\[
H[u(t)] = \sum_{a=1}^{\dim \mathcal{C}} u^a(t) A_a, \quad ||u|| \leq \mathcal{E}, \quad u^a(t) \in \mathbb{R},
\]

where \( ||u|| := \sqrt{\sum_{a=1}^{\dim \mathcal{C}} (u^a(t))^2} \), and \( \{A_a\}_{a=1,\ldots,\dim \mathcal{C}} \) is an orthonormal basis of \( su(\mathcal{H}) \) such that \( A_1, \ldots, A_{\dim \mathcal{C}} \) form a basis of \( \mathcal{C} \) and \( A_{\dim \mathcal{C} + 1}, \ldots, A_{\dim \mathcal{C} + N^2 - 1} \) form a basis of \( \mathbb{C}^\perp \), the orthogonal complement of \( \mathcal{C} \). It can be easily shown \([42,73]\) that the brachistochrone (time-optimal control) in this case attains the equality in (6.1), or equivalently, in (6.2), for all \( t \).

(a) Geodesic deformation method

There is an intriguing numerical method \([73]\) of solving the QB equation, which we call the geodesic deformation method here.\(^5\)

\(^4\)Here, we slightly generalize the term in \([39]\), where the constraint was (6.2) with the inequality sign replaced by an equal sign.

\(^5\)We use the term ‘geodesic deformation’ here in a wider and more naive sense than in \([73]\).
Consider a curve $U(t)$, which is determined by $H(t)$ through (2.14). Let us define the length of the curve $U(t)$ by

$$L = \int_0^T \|H(t)\|_{HS} \, dt.$$  

(6.3)

For the QB ($H(t), T$), one has $L = \mathcal{E} T$ so that the QB corresponds to the minimum length curve. The idea of the geodesic deformation method is that one does not forbid $H(t)$ to have components in the direction of $C^\perp$ but impose a penalty on it, and then gradually increase the penalty. Define a Hilbert–Schmidt-like inner product on $su$ \cite{73–76},

$$\langle A, B \rangle_q := \langle A_\parallel, B_\parallel \rangle_{HS} + q \langle A_\perp, B_\perp \rangle_{HS},$$

(6.4)

where $q > 0$ and $A := A_\parallel + A_\perp$ is the orthogonal decomposition of $A$ into $C$ and $C^\perp$, and define the corresponding norm $\|A\|_q := \sqrt{\langle A, A \rangle_q}$. Consider the QB problem with the following constraint for $H(t)$:

$$H(t) \in C \quad \text{and} \quad \|H(t)\|_q = \mathcal{E}.$$  

(6.5)

The original problem (6.1) corresponds to the case $q = \infty$. On the other hand, the case $q = 1$ is trivial because the brachistochrone $U(t)$ is a geodesic on SU($\mathcal{H}$) with the standard metric, and $H(t)$ is constant, $H(t) = ic \log U_f$, where $c$ is a positive constant for the condition $\|H(t)\|_{HS} = \mathcal{E}$ \cite{39}. Geometrically, the QB problem (6.5) for each $q < \infty$ is equivalent to finding the shortest-length geodesic curve on the Riemannian manifold SU($\mathcal{H}$) with a (non-standard) metric defined by (6.4). One expects that the geodesic converges to the QB for the original problem (6.1) when $q \to \infty$.

The procedure of the geodesic deformation method is the following. One starts with solving the QB with $q = 1$ (analytically or, e.g., by numerical diagonalization of $U_f$). If one has the solution for $q$, solve the QB for $q + \Delta q$ by the shooting method with the ‘initial guess’ being the solution for the previous $q$. Repeating this process, one finally obtains the QB for the original problem (6.1) when $q$ becomes sufficiently large.

We close the section by writing down the QB equation for (6.5) according to the results in §2b. The only constraint for $H(t)$ is

$$0 = f(H) := \frac{1}{2} (\text{Tr}[H_\parallel(t)^2 + q H_\perp(t)^2] - \mathcal{E}^2).$$

(6.6)

From (2.25), one has$^6$

$$F(t) = \lambda(t)(H_\parallel(t) + q H_\perp(t)).$$

(6.7)

It follows from (2.20), (6.6) and (6.7) that $\lambda(t)$ is a constant, which can be taken unity by the rescaling of $F(t)$ (or, equivalently, by the choice of the constant $p_0$). Then the QB equation (2.17) is

$$\frac{dH_\parallel(t)}{dt} + q \frac{dH_\perp(t)}{dt} = -i[H(t), H_\parallel(t) + q H_\perp(t)].$$

(6.8)

This can also be derived as the geodesic equation on the space with metric (6.4).

For cases with more general constraints $A$ on the Hamiltonian and for the subtleties in the method, see \cite{70,73}.

(b) Krotov-type method

In [43], numerical study of the QB is performed. There, the QB problem is first cast to a fidelity-optimality problem and a Krotov-type numerical algorithm is developed for it. Although the following description is for the model problem (6.1), the method is applicable to more general QB problems in the same manner.

$^6$Since $H_\parallel = \sum_{\sigma \in \dim C} A_{\sigma} \text{Tr}[A_{\sigma} H]$, one has $\text{Tr}[H_\parallel^2] = \sum_{\sigma \in \dim C} (\text{Tr}[A_{\sigma} H])^2$ and $\partial \text{Tr}[H_\parallel^2]/\partial H = 2 \sum_{\sigma \in \dim C} A_{\sigma} \text{Tr}[A_{\sigma} H] = 2H_\parallel$. Similar for $H_\perp$. 


Let us cast the QB problem (6.1), with inequality replaced by equality, to a fidelity-optimality problem. We consider a variational principle for \( \text{cf. (3.13)} \)

\[
S[U, u, V, \lambda] = \frac{N}{2} \mathcal{F}(U_f, U(T))^2 + \int_0^T (L_S + L_C) \, dt, \tag{6.9}
\]

\[
\mathcal{F}(A, B) = \frac{1}{N} |\text{Tr}[A^*B]| \tag{6.10}
\]

and

\[
L_S = \text{Re} \text{Tr} \left[ V^\dagger(t) \left( i \frac{dU(t)}{dt} - H[u(t)]U(t) \right) \right], \quad L_C = \frac{1}{2} \lambda(t)(||u(t)||^2 - \mathcal{E}^2), \tag{6.11}
\]

where \( H[u(t)] \) is as in (6.2), and the unitary \( V(t) \) and the real \( \lambda(t) \) are Lagrange multipliers. Here, we impose the Schrödinger equation (2.14) in a slightly different manner from §2b. The present way makes the equations for \( U(t) \) and \( V(t) \) symmetric, which is convenient for the Krotov-type method. The relation with \( F(t) \) in §2b is given by

\[
F(t) = \frac{1}{2} (U(t)V^\dagger(t) + V(t)U^\dagger(t)), \tag{6.12}
\]

up to total derivative terms in the action \( S \). We also note that the time \( T \) in (6.9) is fixed, in contrast to the case of (3.13). The problem (6.9) is to maximize the fidelity \( \mathcal{F} \) within the time \( T \). The form of the fidelity term is not unique but is so chosen that its numerical calculation is easy. The absolute value in \( \mathcal{F} \) reflects the set-up that we ignore the overall phase of \( U_f \) and \( U(t) \). For unitary \( A \) and \( B \), the fidelity \( \mathcal{F}(A, B) \) attains the maximum 1 when \( A \) equals \( B \) up to phase.

The fidelity-optimality problem is complementary to the time-optimality problem in the sense that if the control \( (H[u(t)], U(t)) \) solves the fidelity-optimal problem with the maximum fidelity \( \mathcal{F}_0 \), the same control is the fastest to achieve that fidelity \( \mathcal{F}_0 \) [43]. Thus one can obtain the QB by solving the fidelity-optimality problem (6.9) for an increasing sequence of \( T \) and see in which \( T \) one has \( \mathcal{F} \rightarrow 1 \).

The Euler–Lagrange equations for \( S \) is the following [43]: the Schrödinger equation (2.14), the dual Schrödinger equation

\[
i \frac{dV(t)}{dt} = H[u(t)]V(t), \tag{6.13}
\]

the constraint

\[
||u(t)|| = E, \tag{6.14}
\]

a boundary condition

\[
V(T) = \frac{i}{N} U_f \text{Tr}[U_f^\dagger U(T)], \tag{6.15}
\]

and an algebraic equation\( \footnote{Equation (6.18) corresponds to (2.28) in the QB problem.} \)

\[
\lambda(t)u^\dagger(t) = \text{Tr}[A_a F(t)]. \tag{6.16}
\]

where the auxiliary variable \( F(t) \) is given by (6.12). The boundary conditions imposed prior to the variations is

\[
U(0) = 1. \tag{6.17}
\]

The constraint (6.14) and the algebraic equation (6.16) imply

\[
\lambda(t) = \sqrt{\sum_{a=1}^{\dim C} (\text{Tr}[A_a F(t)])^2}. \tag{6.18}
\]

Thus, if one knows \( U(t) \) and \( V(t) \) at certain time \( t \), one can algebraically obtain \( \lambda(t) \) and \( u(t) \) at the same \( t \) through (6.18) and (6.16). Note that \( U(t) \) has the initial boundary condition and \( V(t) \) has the final boundary condition, which is essential for the Krotov-type scheme.

We shall describe the Krotov-type scheme for solving the problem (6.9). The main difference between the present scheme and the usual Krotov method (e.g. [77]) is that \( \lambda(t) \) and \( F(t) \) are
Lagrange multiplier variables in the former while they are given constants to impose penalties in the latter. We first introduce copies of $u(t)$ and $\lambda(t)$ which we denote by $\tilde{u}(t)$ and $\tilde{\lambda}(t)$. Hereafter, we call the equation (6.13), with $(u(t), \lambda(t))$ being replaced by $(\tilde{u}(t), \tilde{\lambda}(t))$, the equation (6.13), and so forth. The Krotov-type scheme is the following iteration procedure.

(i) Prepare control variable $u(t)$ (dim $C$ components), $0 \leq t \leq T$ as a seed. Set $U(0) = 1$ and evolve $U(t)$ from $t = 0$ to $t = T$ by the Schrödinger equation (2.14) with the prepared $u(t)$.

(ii) Set $V(T)$ by (6.15) and evolve $(V(t), \tilde{u}(t), \tilde{\lambda}(t))$ backward in time from $t = T$ to $t = 0$ by equations (6.18), (6.16) and (6.13), during which $U(t)$ is understood as a given function.

(iii) Set $U(0) = 1$ and evolve $(U(t), u(t), \lambda(t))$ forward in time from $t = 0$ to $t = T$ by equations (6.18), (6.16) and (2.14), during which $V(t)$ is understood as a given function.

(iv) Repeat (b) and (b) until the variables converge (e.g. $u(t)$ and $\tilde{u}(t)$ becomes close enough).

The resulting $u(t)$ is the optimal control and $F(U_f, U(T))$ is the maximum achievable fidelity.

It can be shown [43] that this Krotov-type algorithm is monotonic, namely, the value of the action functional $S$ decreases in each cycle of the algorithm, which is important in practical use. Koike & Okudaira [43] provides simulation results when the available Hamiltonians consist of one- and two-qubit interactions.

7. Other applications

(a) Experiments

The first experimental demonstration of the QB is done in diamond [70]. There, an electron spin and a nuclear spin in a nitrogen-vacancy centre form a two-qubit system. In the rotating wave approximation, the Hamiltonian is

$$H(t) = H_d + H_c(t), \quad H_d = a S_z, \quad H_c(t) = b(\cos \phi(t) S_x + \sin \phi(t) S_y),$$

(7.1)

for the one-qubit experiment and

$$H(t) = H_d + H_c(t), \quad H_d = a S_z I_z, \quad H_c(t) = b(\cos \phi(t) S_x + \sin \phi(t) S_y),$$

(7.2)

for the two-qubit experiment, where $I_z$ is the nuclear spin-$z$ operator, $S_i$ are the electron spin operators, and $a, b > 0$. The phase $\phi(t)$ of the microwave pulse is determined by the QB equation. When the QB equation is not solvable analytically, it is solved numerically by the geodesic deformation method [73] (§6). Several target unitaries are realized for several parameter ratios $a/b$ and the performance is checked by quantum process tomography. For one qubit, the brachistochrone was faster than the Euler angle rotation and the fidelity was around 0.99. For two qubits, the brachistochrone was faster than the conventional method and the fidelity was around 0.99. Thus, the time-optimal universal one- and two-qubit control is achieved. The authors remark that the time-optimal control is favourable for high fidelity of the operation because the short time duration reduces the dephasing effect and the small strength of the control field reduces the noise.

(b) Time complexity and gate complexity

The physical time necessary for a quantum computation, described by a unitary operator $U$, is called time complexity $T(U)$, while ‘information-theoretic time’ which is defined as the necessary number of elementary quantum gates is called gate complexity $G(U)$. Estimation of gate complexity $G(U)$ is difficult in general since finding the optimal quantum circuit is a discrete and combinatorial problem. Time complexity $T(U)$, which can be estimated by the QB method, may be a good tool to estimate gate complexity. Gate complexity $G(U)$ can be bounded from below by time complexity $T(U)$ with suitable choice of available Hamiltonians, e.g. consisting of interactions up to two qubits only; intuitively, there is a curve in the space of unitary operators...
that is shorter than the segmented line representing the gate-optimal circuit. On the other hand, it is seen by counting the degrees of freedom that gate complexity $G(U)$ is not bounded from above by time complexity $T(U)$ in general. It is possible, however, to bound gate complexity $G(U, \varepsilon)$ of a unitary operation $U$ by (a polynomial of) time complexity $T(U)$ if one allows errors less than $\varepsilon$ [74]. Based on these facts, a question has been posed [43] to what extent holds the following: The gate complexity $G(U)$ of a unitary operation $U$ is polynomial (or exponential) in the input size if and only if the time complexity $T(U)$ is polynomial (or exponential, respectively). In [43], the gate complexity $G(U)$ is defined so that the elementary gates are one- and two-qubit unitary operations. The time complexity $T(U)$ is defined so that the time-dependent Hamiltonian $H(t)$ allows only one- and two-qubit interactions, namely,

$$H(t) = \sum_{1 \leq i < j \leq n} \sum_{\alpha=x,y,z} h_{ij}^{\alpha\beta}(t) \sigma_i^{\alpha} \sigma_j^{\beta} + \sum_{1 \leq i \leq n} \sum_{\alpha=x,y,z} h_i^{\alpha}(t) \sigma_i^{\alpha}, \quad ||H(t)||_{HS} \leq \mathcal{E}. \quad (7.3)$$

where $\sigma_i^\alpha$ denotes the $\alpha$-component Pauli operator on the qubit $i$, and $h_{ij}^{\alpha\beta}(t)$ and $h_i^{\alpha}(t)$ are control parameters. It is demonstrated by numerical examples that for a target unitary $U_f$ with known polynomial-gate algorithm has polynomial time complexity and for $U_f$ without symmetry, which is likely to have exponential gate complexity, has exponential time complexity.

(c) Simple systems

In [20–23], a model problem of three spins is considered. The spins in the end are indirectly coupled through the middle one on which a controllable magnetic field is applied. The available Hamiltonians $H(t) \in A$ is specified by

$$H(t) = J_{12}\sigma_1^x\sigma_2^x + J_{23}\sigma_2^x\sigma_3^x + B(t) \cdot \sigma_2, \quad ||B(t)|| \leq \mathcal{E}, \quad (7.4)$$

where $J_{12}$ and $J_{23}$ are fixed coupling constants, and $B(t)$ is a controllable magnetic field on the middle qubit. QBs are considered for various target unitaries and realizations faster than previously known time-efficient schemes are provided. Transfer of coherence and entanglement of the brachistochrone are also discussed.

In the simplest system where the Hamiltonian is essentially unconstrained so that the QB trivially becomes the geodesic [38] and admits a simple geometric construction [78], the relations between the QB and bipartite and tripartite entanglements and correlations are intensively studied [79–84]. In a two-level system, relations between the QSL and the time-optimal controls with constraints are explored [85].

The Zermelo navigation problem [24–27] is the time optimality problem where the constraint for the Hamiltonian, $H(t) \in A$, is written as

$$H(t) = H_d + H_c(t), \quad ||H_c(t)||_{HS} \leq \mathcal{E}. \quad (7.5)$$

The symmetry of the problem allows a neat geometric approach [25,26], while in the context of QB formalism the problem is easily solved by moving to the interaction picture in the QB equations [42].

(d) Shortcut to adiabaticity

STA [44–58] (see also [59]) are accelerated paths for slow adiabatic changes of quantum states. STA may, for example, speed up quantum annealing [86] and adiabatic quantum computation [87]. The QB formalism, by its generality and simplicity, provides a unified understanding of various methods of STA [44–48]. It has been shown that the assisted adiabatic passage [49,50], transitionless quantum driving [51] and STA [52,53] can be derived from the QB equation and are essentially equivalent. The QB formalism is also useful in studying the stability of STA [44–48].
**Non-Hermitian quantum brachistochrone**

QB systems have been extensively studied in the context of quantum mechanics with non-Hermitian, parity-time-reversal-symmetric ($PT$-symmetric) Hamiltonians [88]. It is claimed in non-Hermitian QB problems [89–91] that transformation of states can be carried out faster than in Hermitian quantum mechanics, or even arbitrarily fast. These problems including non-Hermitian quantum mechanics itself are under active discussion.

### 8. Conclusion

We have briefly review the basic formalism, the numerical techniques, the experimental results and the related topics of the QB. We hope that the QB method serves in further theoretical and experimental advances.

**Data accessibility.** This article has no additional data.

**Conflict of interest declaration.** I declare I have no competing interests.

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