Exact solutions of the isoholonomic problem and the optimal control problem in holonomic quantum computation

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Abstract

The isoholonomic problem in a homogeneous bundle is formulated and solved exactly. The problem takes a form of a boundary value problem of a variational equation. The solution is applied to the optimal control problem in holonomic quantum computer. We provide a prescription to construct an optimal controller for an arbitrary unitary gate and apply it to a \(k\)-dimensional unitary gate which operates on an \(N\)-dimensional Hilbert space with \(N \geq 2k\). Our construction is applied to several important unitary gates such as the Hadamard gate, the CNOT gate, and the two-qubit discrete Fourier transformation gate. Controllers for these gates are explicitly constructed.

Keywords: holonomy, isoholonomic problem, homogeneous bundle, holonomic quantum computation, optimal control, horizontal extremal curve

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1 Introduction

In this paper we solve the isoholonomic problem in a homogeneous bundle and apply this result to the optimal control problem in holonomic quantum computation. In other words, this paper has two purposes; first, we solve a mathematical problem which has been unsolved for more than a decade since it was initially proposed by Montgomery [1]. Second, we provide a scheme to construct explicitly an optimal controller for arbitrary unitary gate in holonomic quantum computation [2, 3].

The isoholonomic problem is one of generalizations of the isoperimetric problem. The isoperimetric problem, also known as Dido’s problem, is originally proposed in the context of plane geometry; what is the shape of a domain with the largest area surrounded by a string of a fixed length? The solution is a circle. The isoperimetric problem has a long history and various generalizations thereof have been proposed.

The isoholonomic problem is formulated as follows. Assume that we have a principal fiber bundle \((P, M, \pi, G)\) with a connection. The base space \(M\) is assumed to be a Riemannian manifold. The isoholonomic problem asks to find the shortest possible piecewise smooth loop in \(M\) with a given base point \(x_0 \in M\), that produces a given element \(g_0\) of the structure group \(G\) as its associated holonomy.

Holonomic structures naturally appear in a mechanical system and have been studied from various interests [4]-[8]. Montgomery faced this problem when physical chemists attempted to observe the non-Abelian Berry phase (the Wilczek-Zee holonomy) [9]-[12] by nuclear magnetic resonance (NMR) experiment. Montgomery [1] presented various formulations of the problem, clarified their relations, and gave partial answers. However, even in such an idealized case like a homogeneous bundle, it was difficult to obtain a complete solution to the problem, which remained as an open problem to date.

A decade later after Montgomery’s work, the notion of holonomic quantum computation was proposed by Zanardi, Rasetti and Pachos [2, 3], in which the Wilczek-Zee holonomy is utilized to implement unitary gates necessary to execute a quantum algorithm. Since then, a large number of researchers [13]-[16] have been interested in finding control parameters that implement a desired gate. Optimization of the control has been an active area of research in view of the decoherence issue. The problem to find the optimal control is nothing but a typical isoholonomic problem and its solution for an arbitrary gate must be urgently provided.

Let us briefly review the idea of quantum computation. Quantum computation, roughly speaking, consists of three ingredients: (1) an \(n\)-qubit register to store information, (2) a unitary matrix \(U \in U(2^n)\) which implements a quantum algorithm, and (3) measurements to extract information from the register. In an ordinary implementation of a quantum algorithm, we take a system whose Hamiltonian \(H(\lambda)\) depends on external control parameters \(\lambda = (\lambda^1, \ldots, \lambda^m)\). We then properly arrange the parameter
sequence $\lambda(t)$ as a function of time $t$ so that the desired unitary matrix $U$ is generated as a time-evolution operator

$$U = \mathcal{T} \exp \left[ -\frac{i}{\hbar} \int_0^T H(\lambda(t)) dt \right],$$

where $\mathcal{T}$ stands for the time-ordered product.

Holonomic quantum computing \cite{2}, in contrast, makes use of the holonomy associated with a loop $\lambda(t)$ in the parameter space. It has been demonstrated \cite{17} that an arbitrary unitary matrix can be implemented as a holonomy by choosing an appropriate loop in the parameter space. In fact, there are infinitely many loops that produce a given unitary matrix. Here we consider the isoholonomic problem, namely, to find the shortest possible loop in the parameter space that yields the given holonomy. This problem has been already analyzed previously in Ref. [18], where various penalty functions useful for numerical search for the optimal loop have been employed. Our strategy here is purely geometrical in nature and no intense numerical computations are required. In the previous work \cite{19} we found exact optimal loops to produce several unitary gates. In the present paper we extend the method of optimal loop construction to implement arbitrary gates.

This paper is organized as follows. In Section 2 we briefly review the Wilczek-Zee holonomy to make this paper self-contained and to establish notation conventions. In Section 3 we introduce the geometrical setting for the problem and use it to formulate the isoholonomic problem in a variational form. We derive the associated Euler-Lagrange equation and solve it explicitly. The solution thus obtained (3.37), which we call the horizontal extremal curve, is one of the main results in the first half of the paper. The remaining problem is to adjust the solution to satisfy the boundary conditions, namely the closed loop condition (4.1) and the holonomy condition (4.2). This problem is solved in Section 4 explicitly and we obtain a set of equations (4.19)-(4.22), which we call the constructing equations of the controller. These are the main results of this paper and are machinery to construct a controller for an arbitrary unitary gate. In Section 5 this machinery is applied to several well-known important unitary gates to demonstrate its power. Section 6 is devoted to summary and discussions.

2 Wilczek-Zee holonomy as a unitary gate

2.1 Wilczek-Zee holonomy

Here we briefly review the Wilczek-Zee (WZ) holonomy \cite{10} associated with an adiabatic change of the control parameters along a loop in the control manifold. We consider a quantum system that has a finite number $N$ of states. Let $\{H(\lambda)\}$ be a family of Hamiltonians parametrized smoothly by $\lambda = (\lambda^1, \ldots, \lambda^m) \in M$, where the set of control parameters $M$ is called a control manifold. Eigenvalues and eigenstates of $H(\lambda)$ are
labeled as

\[ H(\lambda)|l, \alpha; \lambda\rangle = \varepsilon_l(\lambda)|l, \alpha; \lambda\rangle \quad (l = 1, \ldots, L; \alpha = 1, \ldots, k_l), \quad (2.1) \]

where the \( l \)-th eigenvalue \( \varepsilon_l(\lambda) \) is \( k_l \)-fold degenerate. Assume that no level crossings take place, namely, \( \varepsilon_l(\lambda) \neq \varepsilon_{l'}(\lambda) \) for arbitrary \( \lambda \) if \( l \neq l' \). Then it follows that \( \sum_{l=1}^{L} k_l = N \).

The eigenvectors satisfy the orthonormal condition,

\[ \langle l, \alpha; \lambda | l', \beta; \lambda \rangle = \delta_{l l'} \delta_{\alpha \beta}. \]

It is important to note that there is \( U(k_l) \) gauge freedom in the choice of \( \{ |l, \alpha; \lambda\rangle | \alpha = 1, \ldots, k_l \} \) at each \( \lambda \) and \( l \). Namely, we may redefine the eigenvectors by any unitary matrix \( h \in U(k_l) \) as

\[ |l, \alpha; \lambda\rangle \mapsto \sum_{\beta=1}^{k_l} |l, \beta; \lambda\rangle h_{\beta \alpha}(\lambda) \quad (2.2) \]

without violating the orthonormal condition.

We adiabatically change the parameters \( \lambda(t) \) as a function of time \( t \) along a closed loop in the control manifold so that \( \lambda(T) = \lambda(0) \). It is assumed that the adiabaticity is satisfied, namely,

\[ \{ \varepsilon_l(\lambda(t)) - \varepsilon_{l'}(\lambda(t)) \}_T \gg 2\pi \hbar \quad (2.3) \]

is satisfied for \( l \neq l' \) during \( 0 \leq t \leq T \). In other words, we change the parameters so slowly that no resonant transitions take place between different energy levels \([20]\).

We will concentrate exclusively on the ground state of the system and drop the index \( l \) (= 1) in the following. Accordingly, the basis vectors that span the ground state eigenspace are written as \( |\alpha; \lambda\rangle, (\alpha = 1, \ldots, k) \) and arranged in an \( N \times k \) matrix form as

\[ V(\lambda) = \left( |1; \lambda\rangle, |2; \lambda\rangle, \ldots, |k; \lambda\rangle \right), \quad (2.4) \]

which is called an orthonormal \( k \)-frame at \( \lambda \in M \). The system evolves, with a given \( \lambda(t) \), according to the Schrödinger equation

\[ i\hbar \frac{d}{dt} |\psi_\alpha(t)\rangle = H(\lambda(t))|\psi_\alpha(t)\rangle. \quad (2.5) \]

Suppose the initial condition is \( \lambda(0) = \lambda_0 \) and \( |\psi_\alpha(0)\rangle = |\alpha; \lambda_0\rangle \). The adiabatic theorem \([20] \) tells us that the state \( |\psi_\alpha(t)\rangle \) remains in the ground state eigenspace during the time-evolution. Therefore \( |\psi_\alpha(t)\rangle \) is expanded as

\[ |\psi_\alpha(t)\rangle = \sum_{\beta=1}^{k} |\beta; \lambda(t)\rangle c_{\beta \alpha}(t). \quad (2.6) \]

By substituting (2.6) into (2.5), we find

\[ \frac{d}{dt} c_{\beta \alpha}(t) = -\frac{i}{\hbar} \varepsilon(\gamma(t)) c_{\beta \alpha}(t) - \sum_{\gamma=1}^{k} \langle \beta; \lambda(t) | \frac{d}{dt} | \gamma; \lambda(t) \rangle c_{\gamma \alpha}(t), \quad (2.7) \]
whose formal solution is
\[ c_{\beta\alpha}(t) = \exp \left( -\frac{i}{\hbar} \int_0^t \varepsilon(s) ds \right) \mathcal{T} \exp \left( -\int_0^t \mathcal{A}(s) ds \right) \]
with the matrix-valued function
\[ \mathcal{A}_{\beta\alpha}(t) = \left\langle \beta; \lambda(t) \mid \frac{d}{dt} \right| \alpha; \lambda(t) \right\rangle = \sum_{\mu=1}^k \left\langle \beta; \lambda \mid \frac{\partial}{\partial \lambda^\mu} \right| \alpha; \lambda \right\rangle d\lambda^\mu. \]

It is easily verified that \( \mathcal{A}^*_{\beta\alpha} = -\mathcal{A}_{\alpha\beta} \) since \( \{ |\alpha; \lambda(t)\rangle \} \) is orthonormal. We introduce a \( u(k) \)-valued one-form
\[ \mathcal{A}_{\beta\alpha}(\lambda) = \sum_{\mu=1}^k \left\langle \beta; \lambda \mid \frac{\partial}{\partial \lambda^\mu} \right| \alpha; \lambda \right\rangle d\lambda^\mu, \]
which is called the Wilczek-Zee (WZ) connection. Then the unitary matrix appearing in (2.8) is rewritten as
\[ \Gamma(t) = \mathcal{P} \exp \left( -\int_{\lambda(0)}^{\lambda(t)} \mathcal{A} \right), \]
where \( \mathcal{P} \) stands for the path-ordered product. As noted in (2.2) the frame (2.4) can be redefined by a family of unitary matrices \( h(\lambda) \in U(k) \). The WZ connection transforms under the change of frame as
\[ \mathcal{A} \mapsto \mathcal{A}' = h^* \mathcal{A} h + h^* dh. \]
This is nothing but the gauge transformation rule of a non-Abelian gauge potential [21].

We assumed that the control parameter \( \lambda(t) \) comes back to the initial point \( \lambda(T) = \lambda(0) = \lambda_0 \). However, the state \( |\psi_{\alpha}(T)\rangle \) fails to assume the initial state and is subject to a unitary rotation as
\[ |\psi_{\alpha}(T)\rangle = \exp \left( -\frac{i}{\hbar} \int_0^T \varepsilon(s) ds \right) \sum_{\beta=1}^k |\psi_{\beta}(0)\rangle \Gamma_{\beta\alpha}(T). \]
The unitary matrix
\[ \Gamma[\lambda] := \Gamma(T) = \mathcal{P} \exp \left( -\oint_{\lambda} \mathcal{A} \right) \in U(k) \]
is called the holonomy matrix associated with the loop \( \lambda(t) \). It is important to realize that \( \Gamma[\lambda] \) is independent of the parametrization of the loop \( \lambda(t) \), namely, it is independent of how fast the loop \( \lambda \) is traversed, so long as the adiabaticity is observed, and that it depends only on the geometrical image of \( \lambda \) in \( M \).

\[ ^a \text{We denote the Lie algebra of the Lie group } U(k) \text{ by } u(k), \text{ which is the set of } k \text{-dimensional skew-Hermite matrices.} \]
2.2 Quantum computation with holonomy

In quantum computation one implements a quantum algorithm by a product of various unitary gates. It is a natural idea to use the WZ holonomy to produce unitary gates necessary for quantum computation. Zanardi and Rasetti [2] were the first who proposed this holonomic quantum computation (HQC). To implement an $n$-qubit resistor we take a quantum system whose ground state is $k$-fold degenerate where $k = 2^n$. We call the $N$-dimensional Hilbert space a working space and call the $k$-dimensional subspace a qubit space. Then by changing the control parameter adiabatically we will obtain any unitary gate as a resultant holonomy (2.14). Of course we need to design an appropriate control loop $\lambda$ to implement a particular unitary gate. It is easy, in principle, to compute the holonomy for a given loop. In contrast, to find a loop $\lambda$ which produces a specified unitary matrix $\Gamma$ as its holonomy is far from trivial. Moreover, to build a working quantum computer it is strongly desired to reduce the time required to manipulate the computer since a sequence of operations should be carried out before decoherence extinguishes quantum information from the system. At the same time, the control parameter must be changed as slowly as possible to keep adiabaticity intact. Therefore our task is to find a control loop as short as possible to fulfill these seemingly opposed conditions. This is a typical example of the so-called isoholonomic problem, which is first formulated by Montgomery [1]. In the next section we introduce a geometric setting in a form suitable for our expositions.

3 Formulation of the problem and its solution

3.1 Geometrical setting

The WZ connection is identified with the canonical connection [22] of the homogenous bundle, as pointed out by Fujii [23]. While precise definitions of these terms can be found in books [21, 22], we outline the geometrical setting of the problem here to make this paper self-contained.

Suppose that the system has a family of Hamiltonians acting on the Hilbert space $\mathbb{C}^N$ and that the ground state of each Hamiltonian is $k$-fold degenerate ($k < N$). The most natural mathematical setting to describe this system is the principal bundle $(S_{N,k}(\mathbb{C}), G_{N,k}(\mathbb{C}), \pi, U(k))$, which consists of the Stiefel manifold $S_{N,k}(\mathbb{C})$, the Grassmann manifolds $G_{N,k}(\mathbb{C})$, the projection map $\pi : S_{N,k}(\mathbb{C}) \to G_{N,k}(\mathbb{C})$, and the unitary group $U(k)$ as explained below.

The Stiefel manifold is the set of orthonormal $k$-frames in $\mathbb{C}^N$,

$$S_{N,k}(\mathbb{C}) = \{ V \in M(N, k; \mathbb{C}) \mid V^\dagger V = I_k \},$$

(3.1)

where $M(N, k; \mathbb{C})$ is the set of $N \times k$ complex matrices and $I_k$ is the $k$-dimensional unit
matrix. The unitary group $U(k)$ acts on $S_{N,k}(\mathbb{C})$ from the right
\[ S_{N,k}(\mathbb{C}) \times U(k) \to S_{N,k}(\mathbb{C}), \quad (V,h) \mapsto Vh \] (3.2)
by means of matrix product. It should be noted that this action is free. In other words, $h = I_k$ if there exists a point $V \in S_{N,k}(\mathbb{C})$ such that $Vh = V$.

The Grassmann manifold is defined as the set of $k$-dimensional hyperplanes in $\mathbb{C}^N$,
\[ G_{N,k}(\mathbb{C}) = \{ P \in M(N, N; \mathbb{C}) \mid P^2 = P, \ P^\dagger = P, \ \text{tr}P = k \}, \] (3.3)
where $P$ is a projection operator to a hyperplane in $\mathbb{C}^N$ and the condition $\text{tr}P = k$ guarantees that the hyperplane is indeed $k$-dimensional.

The projection map $\pi : S_{N,k}(\mathbb{C}) \to G_{N,k}(\mathbb{C})$ is defined as
\[ \pi : V \mapsto P := VV^\dagger. \] (3.4)
It is easily proved that the map $\pi$ is surjective. Namely, for any $P \in G_{N,k}(\mathbb{C})$, there is $V \in S_{N,k}(\mathbb{C})$ such that $\pi(V) = P$. The right action of $h \in U(k)$ sends a point $V \in S_{N,k}(\mathbb{C})$ to a point $Vh$ on the same fiber since
\[ \pi(Vh) = (Vh)(Vh)^\dagger = Vhh^\dagger V^\dagger = VV^\dagger = \pi(V). \] (3.5)
Thus the Stiefel manifold $S_{N,k}(\mathbb{C})$ becomes a principal bundle over $G_{N,k}(\mathbb{C})$ with the structure group $U(k)$.

Moreover, the group $U(N)$ acts on both $S_{N,k}(\mathbb{C})$ and $G_{N,k}(\mathbb{C})$ as
\[ U(N) \times S_{N,k}(\mathbb{C}) \to S_{N,k}(\mathbb{C}), \quad (g, V) \mapsto gV, \] (3.6)
\[ U(N) \times G_{N,k}(\mathbb{C}) \to G_{N,k}(\mathbb{C}), \quad (g, P) \mapsto gPg^\dagger \] (3.7)
by matrix product. It is easily verified that $\pi(gV) = g\pi(V)g^\dagger$. This action is transitive, namely, there is $g \in U(N)$ for any $V, V' \in S_{N,k}(\mathbb{C})$ such that $V' = gV$. There is also $g \in U(N)$ for any $P, P' \in G_{N,k}(\mathbb{C})$ such that $P' = gPg^\dagger$. The stabilizer group of each point in $S_{N,k}(\mathbb{C})$ is isomorphic to $U(N-k)$ while that of each point in $G_{N,k}(\mathbb{C})$ is isomorphic to $U(k) \times U(N-k)$. Thus, they are homogeneous spaces and the fiber bundle
\[ \pi : S_{N,k}(\mathbb{C}) \cong U(N)/U(N-k) \to G_{N,k}(\mathbb{C}) \cong U(N)/(U(k) \times U(N-k)) \] (3.8)
is call a homogeneous bundle.

The canonical connection form on $S_{N,k}(\mathbb{C})$ is defined as a $\mathfrak{u}(k)$-valued one-form
\[ A = V^\dagger dV, \] (3.9)
which is a generalization of the WZ connection $\text{2.10}$. This is characterized as the unique connection that is invariant under the action $\text{3.6}$. The associated curvature two-form is then defined as
\[ F = dA + A \wedge A = dV^\dagger \wedge dV + V^\dagger dV \wedge V^\dagger dV = dV^\dagger \wedge (I_N - VV^\dagger)dV. \] (3.10)
These manifolds are equipped with Riemannian metrics. We define a metric
\[ \|dV\|^2 = \text{tr} \left( dV^\dagger dV \right) \] (3.11)
for the Stiefel manifold and
\[ \|dP\|^2 = \text{tr} \left( dP dP \right) \] (3.12)
for the Grassmann manifold.

### 3.2 The isoholonomic problem

Here we reformulate the WZ holonomy in terms of the geometric terminology introduced above. The state vector \( \psi(t) \in \mathbb{C}^N \) evolves according to the Schrödinger equation
\[ i\hbar \frac{d}{dt} \psi(t) = H(t) \psi(t). \] (3.13)

The Hamiltonian admits a spectral decomposition
\[ H(t) = \sum_{l=1}^{L} \varepsilon_l(t) P_l(t) \] (3.14)
with projection operators \( P_l(t) \). Therefore, the set of energy eigenvalues \( (\varepsilon_1, \ldots, \varepsilon_L) \) and orthogonal projectors \( (P_1, \ldots, P_L) \) constitutes a complete set of control parameters of the system. Now we concentrate on the eigenspace associated with the lowest energy, which is assumed to be identically zero, \( \varepsilon_1 \equiv 0 \). We write \( P_1(t) \) as \( P(t) \) for simplicity. Suppose that the degree of degeneracy \( k = \text{tr} P(t) \) is constant. For each \( t \), there exists \( V(t) \in S_{N,k}(\mathbb{C}) \) such that \( P(t) = V(t)V^\dagger(t) \). By adiabatic approximation we mean substitution of \( \psi(t) \in \mathbb{C}^N \) by a reduced state vector \( \phi(t) \in \mathbb{C}^k \) as
\[ \psi(t) = V(t)\phi(t). \] (3.15)
Since \( H(t)\psi(t) = \varepsilon_1 \psi(t) = 0 \), the Schrödinger equation (3.13) becomes
\[ \frac{d\phi}{dt} + V^\dagger \frac{dV}{dt} \phi(t) = 0 \] (3.16)
and its formal solution is written as
\[ \phi(t) = \mathcal{P} \exp \left( - \int V^\dagger dV \right) \phi(0). \] (3.17)
Therefore \( \psi(t) \) is written as
\[ \psi(t) = V(t)\mathcal{P} \exp \left( - \int V^\dagger dV \right) V^\dagger(0)\psi(0). \] (3.18)
In particular, when the control parameter comes back to the initial point as \( P(T) = P(0) \), the holonomy \( \Gamma \in U(k) \) is defined via

\[
\psi(T) = V(0) \Gamma \phi(0)
\]

(3.19)

and it is given explicitly as

\[
\Gamma = V(0)^\dagger V(T) \mathcal{P} \exp \left( - \int V^\dagger dV \right).
\]

(3.20)

If the condition

\[
V^\dagger \frac{dV}{dt} = 0
\]

(3.21)

is satisfied, the curve \( V(t) \) in \( S_{N,k}(\mathbb{C}) \) is called a horizontal lift of the curve \( P(t) = \pi(V(t)) \) in \( G_{N,k}(\mathbb{C}) \). Then the holonomy (3.20) is reduced to

\[
\Gamma = V^\dagger(0)V(T) \in U(k).
\]

(3.22)

Now we are ready to state the isoholonomic problem in the present context; given a specified unitary gate \( U_{\text{gate}} \in U(k) \) and a fixed point \( P_0 \in G_{N,k}(\mathbb{C}) \), find the shortest loop \( P(t) \) in \( G_{N,k}(\mathbb{C}) \) with the base points \( P(0) = P(T) = P_0 \) whose horizontal lift \( V(t) \) in \( S_{N,k}(\mathbb{C}) \) produces a holonomy \( \Gamma \) that coincides with \( U_{\text{gate}} \). This problem was first motivated from experimental study of geometric phase and investigated in detail from a mathematician’s viewpoint by Montgomery [1].

We now formulate the isoholonomic problem as a variational problem. The length of the horizontal curve \( V(t) \) is evaluated by the functional

\[
S[V, \Omega] = \int_0^T \left\{ \text{tr} \left( \frac{dV^\dagger}{dt} \frac{dV}{dt} \right) - \text{tr} \left( \Omega V^\dagger \frac{dV}{dt} \right) \right\} dt,
\]

(3.23)

where \( \Omega(t) \in \mathfrak{u}(k) \) is a Lagrange multiplier to impose the horizontal condition (3.21) on the curve \( V(t) \). Note that the value of the functional \( S \) is equal to the length of the projected curve \( P(t) = \pi(V(t)) \),

\[
S = \int_0^T \frac{1}{2} \text{tr} \left( \frac{dP}{dt} \frac{dP}{dt} \right) dt.
\]

(3.24)

Thus the problem is formulated as follows; find a curve \( V(t) \) that attains an extremal value of the functional (3.23) and satisfies the boundary condition (3.22).

\footnote{The definition of the holonomy presented here is slightly different from the one given in the previous Letter [19]. To make a correct sense as a unitary gate the holonomy is to be defined in the present form.}
3.3 The solution: horizontal extremal curve

Our task is to find a solution of the variational problem of the functional (3.23). Now we derive the associated Euler-Lagrange equation and solve it explicitly. A variation of the curve \( V(t) \) is defined by an arbitrary smooth function \( \eta(t) \in u(N) \) such that \( \eta(0) = \eta(T) = 0 \) and an infinitesimal parameter \( \epsilon \in \mathbb{R} \) as

\[
V_\epsilon(t) = (1 + \epsilon \eta(t))V(t).
\]

By substituting \( V_\epsilon(t) \) into (3.23) and differentiating with respect to \( \epsilon \), the extremal condition yields

\[
0 = \frac{dS}{d\epsilon} \bigg|_{\epsilon=0} = \int_0^T \text{tr} \{ \eta (V\dot{V}^\dagger - \dot{V}V^\dagger - V\Omega V^\dagger) \} \, dt
\]

\[
= \left[ \text{tr} \{ \eta (V\dot{V}^\dagger - \dot{V}V^\dagger - V\Omega V^\dagger) \} \right]_{t=0}^{t=T}
- \int_0^1 \text{tr} \{ \eta \frac{d}{dt} (V\dot{V}^\dagger - \dot{V}V^\dagger - V\Omega V^\dagger) \} \, dt.
\]

Thus we obtain the Euler-Lagrange equation

\[
\frac{d}{dt} (\dot{V}V^\dagger - V\dot{V}^\dagger + V\Omega V^\dagger) = 0.
\]

We reproduce the horizontal equation \( V^\dagger \dot{V} = 0 \) from the extremal condition with respect to \( \Omega(t) \). Finally, the isoholonomic problem is reduced to the set of equations (3.21) and (3.27), which we call a horizontal extremal equation. It may be regarded as a homogeneous-space version of the Wong equation [24].

Next, we solve the equations (3.21) and (3.27). The equation (3.27) is integrated to yield

\[
\dot{V}V^\dagger - V\dot{V}^\dagger + V\Omega V^\dagger = \text{const} = X \in u(N).
\]

Conjugation of the horizontal condition (3.21) yields \( \dot{V}^\dagger V = 0 \). Then, by multiplying \( V \) on (3.28) from the right we obtain

\[
\dot{V} + V\Omega = XV.
\]

By multiplying \( V^\dagger \) on (3.29) from the left we obtain

\[
\Omega = V^\dagger XV.
\]

The equation (3.29) implies \( \dot{V} = XV - V\Omega \), and hence the time derivative of \( \Omega(t) \) becomes

\[
\dot{\Omega} = V^\dagger XV + \dot{V}^\dagger XV = V^\dagger X(VX - V\Omega) + (-V^\dagger X + \Omega V^\dagger)XV = [\Omega, \Omega] = 0.
\]

Thus, \( \Omega(t) \) is actually a constant. Thus the solution of (3.28) and (3.30) is

\[
V(t) = e^{tX} V_0 e^{-t\Omega}, \quad \Omega = V_0^\dagger XV_0.
\]
We call this solution the horizontal extremal curve. Then (3.28) becomes

\[(XV - V\Omega)V^\dagger - V(-V^\dagger X + \Omega V^\dagger) + V\Omega V^\dagger = X,\]

which is arranged as

\[X - (VV^\dagger X + XV^\dagger - VV^\dagger XVV^\dagger) = 0, \quad (3.33)\]

where we used (3.30). We may take, without loss of generality,

\[V_0 = \left( \begin{array}{c} I_k \\ 0 \end{array} \right) \in S_{N,k}(\mathbb{C}) \quad (3.34)\]

as the initial point. We can parametrize \(X \in \mathfrak{u}(N)\), which satisfies (3.30), as

\[X = \left( \begin{array}{cc} \Omega & W \\ -W^\dagger & Z \end{array} \right) \quad (3.35)\]

with \(W \in M(k, N - k; \mathbb{C})\) and \(Z \in \mathfrak{u}(N - k)\). Then the constraint equation (3.33) forces us to choose

\[Z = 0. \quad (3.36)\]

Finally, we obtained a complete set of solution (3.32) of the horizontal extremal equation (3.21) and (3.27). When we take the initial point \(V_0\) as (3.34), the solutions are parametrized by constant matrices \(\Omega \in \mathfrak{u}(k)\) and \(W \in M(k, N - k; \mathbb{C})\). For definiteness we write down the complete solution

\[V(t) = e^{tX} V_0 e^{-t\Omega}, \quad X = \left( \begin{array}{cc} \Omega & W \\ -W^\dagger & 0 \end{array} \right). \quad (3.37)\]

This is one of our main results. We call the matrix \(X\) a controller. At this time the holonomy (3.22) is expressed as

\[\Gamma = V^\dagger(0)V(T) = V_0^\dagger e^{TX} V_0 e^{-T\Omega} \in U(k). \quad (3.38)\]

These results (3.37) and (3.38) have been also given in Montgomery’s paper\(^c\). In the present paper we took a different approach from his. Here we wrote down the Euler-Lagrange equation and solved it directly.

We evaluate the length of the extremal curve for later convenience by substituting (3.37) into (3.24) as

\[S = \int_0^T \frac{1}{2} \text{tr} \left( \frac{dP}{dt} \frac{dP}{dt} \right) dt = \text{tr} \left( W^\dagger W \right) T. \quad (3.39)\]

\(^c\)In his paper Montgomery cited Bär’s theorem to complete the proof. However, Bär’s paper being a diploma thesis, it is not widely available. Therefore we took a more direct approach to justify them.
4 Solution to the inverse problem

Once the solution (3.37) of the horizontal extremal equation is obtained, the remaining problem is to find the matrices $\Omega$ and $W$ that satisfy the closed loop condition

$$V(T)V^\dagger(T) = e^{TX}V_0V_0^\dagger e^{-TX} = V_0V_0^\dagger \tag{4.1}$$

and the holonomy condition

$$V_0^\dagger V(T) = V_0^\dagger e^{TX} V_0 e^{-T\Omega} = U_{\text{gate}} \tag{4.2}$$

for a specific unitary gate $U_{\text{gate}} \in U(k)$. Montgomery \cite{1} presented this inverse problem as an open problem. In this section we give a scheme to construct systematically a series of solutions to this problem and in the next section we will apply it to implement various important unitary gates.

4.1 Equivalence class

There is a class of equivalent solutions with a given initial condition $V_0$ and a given final condition $V(T) = V_0U_{\text{gate}}$. Here we clarify the equivalence relation among solutions $\{V(t)\}$ that have the form (3.37) and satisfy (4.1) and (4.2).

We say that two solutions $V(t)$ and $V'(t)$ are equivalent if there are elements $g \in U(N)$ and $h \in U(k)$ such that $V(t)$ and

$$V'(t) = gV(t)h^\dagger. \tag{4.3}$$

satisfy the same boundary conditions

$$gV_0h^\dagger = V_0 \tag{4.4}$$

and

$$hU_{\text{gate}}h^\dagger = U_{\text{gate}}. \tag{4.5}$$

For the initial point (3.34), the condition (4.4) states that $g \in U(N)$ must have a block-diagonal form

$$g = \begin{pmatrix} h_1 & 0 \\ 0 & h_2 \end{pmatrix}, \quad h = h_1 \in U(k), \quad h_2 \in U(N-k). \tag{4.6}$$

The controller $X'$ of $V'(t)$ are then found from

$$V'(t) = gV(t)h^\dagger = ge^{TX}g^\dagger V_0h^\dagger e^{-th}\Omega h^\dagger = e^{tgXg^\dagger}V_0h^\dagger e^{-th}\Omega h^\dagger = e^{tgXg^\dagger}V_0 e^{-th}\Omega h^\dagger. \tag{4.7}$$

In summary, two controllers $X$ and $X'$ are equivalent if and only if there are unitary matrices $h_1 \in U(k)$ and $h_2 \in U(N-k)$ such that

$$X = \begin{pmatrix} \Omega & W \\ -W^\dagger & 0 \end{pmatrix}, \quad X' = \begin{pmatrix} h_1\Omega h_1^\dagger & h_1W h_2^\dagger \\ -h_2W^\dagger h_1 & 0 \end{pmatrix}, \quad h_1U_{\text{gate}}h_1^\dagger = U_{\text{gate}}. \tag{4.8}$$
4.2 \textit{U}(1) holonomy

Here we calculate the holonomy for the case \(N = 2\) and \(k = 1\). In this case the homogeneous bundle \(\pi : S_{2,1}(\mathbb{C}) \rightarrow G_{2,1}(\mathbb{C})\) is the Hopf bundle \(\pi : S^3 \rightarrow S^2\) with the structure group \(U(1)\) and the WZ holonomy reduces to the Berry phase. In the subsequent subsection we will generalize this result to a non-Abelian holonomy. We normalize the cycle time as \(T = 1\) in the following. Using real numbers \(w_1, w_2, w_3 \in \mathbb{R}\) we parametrize the controller as

\[
X = \begin{pmatrix}
2iw_3 & iw_1 + w_2 \\
 iw_1 - w_2 & 0
\end{pmatrix} = iw_3 I + iw_1 \sigma_1 + iw_2 \sigma_2 + iw_3 \sigma_3,
\]

(4.9)

where \(\{\sigma_j\}\) are the Pauli matrices. Its exponentiation is

\[
e^{tX} = e^{itw_3} (I \cos \rho t + i \mathbf{n} \cdot \mathbf{\sigma} \sin \rho t),
\]

(4.10)

where \(\rho\) and \(\mathbf{n}\) are defined as

\[
\rho := \|\mathbf{w}\| = \sqrt{(w_1)^2 + (w_2)^2 + (w_3)^2}, \quad \mathbf{w} = \|\mathbf{w}\| \mathbf{n}.
\]

(4.11)

The associated horizontal extremal curve (3.32) then becomes

\[
V(t) = e^{tX} V_0 e^{-t\Omega} = e^{-itw_3} \begin{pmatrix} \cos \rho t + i n_3 \sin \rho t \\ (i n_1 - n_2) \sin \rho t \end{pmatrix}
\]

(4.12)

and the projected curve in \(S^2\) becomes

\[
P(t) = V(t) V^\dagger(t)
\]

\[
= \frac{1}{2} I + \frac{1}{2} \mathbf{\sigma} \cdot [\mathbf{n}(\mathbf{n} \cdot \mathbf{e}_3) + (\mathbf{e}_3 - \mathbf{n}(\mathbf{n} \cdot \mathbf{e}_3)) \cos 2 \rho t - (\mathbf{n} \times \mathbf{e}_3) \sin 2 \rho t],
\]

(4.13)

where \(\mathbf{e}_3 = (0, 0, 1)\). We see from (4.13) that the point \(P(t)\) in \(S^2\) starts at the north pole \(\mathbf{e}_3\) of the sphere and moves along a small circle with the axis \(\mathbf{n}\) in the clockwise sense by the angle \(2 \rho t\). The point \(P(t)\) comes back to the north pole when \(t\) satisfies \(2 \rho t = 2 \pi n\) with an integer \(n\). To make a closed loop, namely, to satisfy the loop condition (4.1) at \(t = T = 1\), the control parameters must satisfy

\[
\rho = \|\mathbf{w}\| = n\pi \quad (n = \pm 1, \pm 2, \ldots).
\]

(4.14)

Then, the point \(P(t)\) travels the same small circle \(n\) times during \(0 \leq t \leq 1\). Therefore, the integer \(n\) counts the winding number of the loop. At \(t = 1\), \(\cos \rho = (-1)^n\) and the holonomy (4.2) is evaluated as

\[
V_0^\dagger e^{X} V_0 e^{-\Omega} = e^{itw_3}(-1)^n e^{-2itw_3} = e^{-i(w_3 - n\pi)} = U_{\text{gate}} = e^{i\gamma}.
\]

(4.15)

Thus, to generate the holonomy \(U_{\text{gate}} = e^{i\gamma}\), the controller parameters are fixed as

\[
w_3 = n\pi - \gamma, \quad w_1 + iw_2 = e^{-i\phi} \sqrt{(n\pi)^2 - (n\pi - \gamma)^2}.
\]

(4.16)
This is the solution to the inverse problem defined by (4.1) and (4.2). Here the nonvanishing integer $n$ must satisfy $(n\pi)^2 - (n\pi - \gamma)^2 > 0$. The real parameter $\phi$ is not fixed by the loop condition and the holonomy condition. The phase $h_2 = e^{i\phi}$ parametrizes solutions in an equivalence class as observed in (4.8). The integer $n$ classifies inequivalent classes.

The length of the loop, (3.39), is now evaluated as

$$S = \text{tr} \left(W^\dagger W \right) T = (n\pi)^2 - (n\pi - \gamma)^2. \quad (4.17)$$

For a fixed $\gamma$ in the range $0 \leq \gamma < 2\pi$, the simple loop with $n = 1$ is the shortest one among the extremal loops. Thus, we conclude that the controller of $U_{\text{gate}} = e^{i\gamma}$ is

$$X = \begin{pmatrix}
2i(\pi - \gamma) & ie^{i\phi}\sqrt{\pi^2 - (\pi - \gamma)^2} \\
-ie^{-i\phi}\sqrt{\pi^2 - (\pi - \gamma)^2} & 0
\end{pmatrix}. \quad (4.18)$$

We call this solution a small circle solution because of its geometric picture mentioned above.

### 4.3 $U(k)$ holonomy

Here we give a prescription to construct a controller matrix $X$ that generates a specific unitary gate $U_{\text{gate}}$. In other words, we give a systematic method to solve the inverse problem (4.2). It turns out that the working space should have a dimension $N \geq 2k$ to apply our method. In the following we assume that $N = 2k$. The time interval is normalized as $T = 1$ as before.

Our method consists of three steps: first, diagonalize the unitary matrix $U_{\text{gate}}$ to be implemented, second, construct a diagonal controller matrix by combining small circle solutions, third, undo diagonalization of the controller.

In the first step, we diagonalize a given unitary matrix $U_{\text{gate}} \in U(k)$ as

$$R^\dagger U_{\text{gate}} R = U_{\text{diag}} = \text{diag}(e^{i\gamma_1}, \ldots, e^{i\gamma_k}) \quad (4.19)$$

with $R \in U(k)$. Each eigenvalue $\gamma_j$ is taken in the range $0 \leq \gamma_j < 2\pi$. In the second step, we combine single loop solutions associated with the Berry phase to construct two $k \times k$ matrices

$$\Omega_{\text{diag}} = \text{diag}(i\omega_1, \ldots, i\omega_k), \quad \omega_j = 2(\pi - \gamma_j), \quad (4.20)$$

$$W_{\text{diag}} = \text{diag}(i\tau_1, \ldots, i\tau_k), \quad \tau_j = e^{i\phi_j}\sqrt{\pi^2 - (\pi - \gamma_j)^2}. \quad (4.21)$$

Then we obtain a diagonal controller

$$X_{\text{diag}} = \begin{pmatrix}
\Omega_{\text{diag}} & W_{\text{diag}} \\
-W_{\text{diag}}^\dagger & 0
\end{pmatrix}. $$
In the third step, we construct the controller $X$ as

$$X = \begin{pmatrix} R & 0 \\ 0 & I_k \end{pmatrix} \begin{pmatrix} \Omega_{\text{diag}} & W_{\text{diag}} \\ -W_{\text{diag}}^\dagger & 0 \end{pmatrix} \begin{pmatrix} R^\dagger & 0 \\ 0 & I_k \end{pmatrix} = \begin{pmatrix} R \Omega_{\text{diag}} R^\dagger & R W_{\text{diag}} \\ -W_{\text{diag}}^\dagger R^\dagger & 0 \end{pmatrix}, \quad (4.22)$$

which is a $2k \times 2k$ matrix. We call the set of equations, (4.19), (4.20), (4.21) and (4.22), constructing equations of the controller. This is the main result of this paper.

It is easily verified that the controller $X$ constructed above satisfies the holonomy condition (4.2). The diagonal controller $X_{\text{diag}}$ is actually a direct sum of controllers (4.18), which generate Berry phases $\{e^{i\gamma_j}\}$. Hence, its holonomy is also a direct sum of the Berry phases (4.15) as

$$V_0^\dagger e^{X_{\text{diag}}} V_0 e^{-\Omega_{\text{diag}}} = U_{\text{diag}},$$

and hence we have

$$V_0^\dagger e^{X} V_0 e^{-\Omega} = R V_0^\dagger e^{X_{\text{diag}}} V_0 R^\dagger R e^{-\Omega_{\text{diag}}} R^\dagger = R U_{\text{diag}} R^\dagger = U_{\text{gate}}.$$

## 5 Optimizing holonomic quantum computation

Now we apply the prescription developed so far to construct controllers of several specific unitary gates, which are fundamental ingredients of quantum computation. Our examples are the Hadamard gate, the CNOT gate, and the two-qubit discrete Fourier transformation (DFT) gate. For each unitary gate $U_{\text{gate}}$, we need to calculate the diagonalizing matrix $R$. Then the constructing equations of the controller, (4.19)-(4.22), provide the desired optimal controller matrices.

### 5.1 Hadamard gate

The Hadamard gate is a one-qubit gate defined as

$$U_{\text{Had}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (5.1)$$

It is diagonalized by

$$R = \begin{pmatrix} \cos \frac{\pi}{8} & -\sin \frac{\pi}{8} \\ \sin \frac{\pi}{8} & \cos \frac{\pi}{8} \end{pmatrix}, \quad (5.2)$$

as

$$R^\dagger U_{\text{Had}} R = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (5.3)$$

Needless to say,

$$\cos \frac{\pi}{8} = \frac{\sqrt{2} + \sqrt{2}}{2}, \quad \sin \frac{\pi}{8} = \frac{\sqrt{2} - \sqrt{2}}{2}. \quad (5.4)$$

Therefore, we have $\gamma_1 = 0$ and $\gamma_2 = \pi$. We may put $\phi_1 = \phi_2 = 0$. The ingredients of the constructing equations of the controller, (4.19)-(4.22), are calculated as

$$\Omega_{\text{diag}} = \text{diag}(2i\pi, 0), \quad W_{\text{diag}} = \text{diag}(0, i\pi), \quad (5.5)$$
Substituting these into (4.22), we obtain the optimal controller of the Hadamard gate.

5.2 CNOT gate

One of the most important 2-qubit gates is the CNOT gate defined as

\[ U_{\text{CNOT}} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \] (5.7)

It is diagonalized by

\[ R = \frac{1}{\sqrt{2}} \begin{pmatrix} \sqrt{2} & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 1 \end{pmatrix} \] (5.8)

as

\[ R^\dagger U_{\text{CNOT}} R = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}. \] (5.9)

Therefore, we have \( \gamma_1 = \gamma_2 = \gamma_3 = 0 \) and \( \gamma_4 = \pi \). The ingredients of the controller are

\[ \Omega_{\text{diag}} = \text{diag}(2i\pi, 2i\pi, 2i\pi, 0), \quad W_{\text{diag}} = \text{diag}(0, 0, 0, i\pi), \] (5.10)

and hence

\[ R\Omega_{\text{diag}} R^\dagger = i\pi \begin{pmatrix} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \quad RW_{\text{diag}} = \frac{i\pi}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \] (5.11)

Substituting these into (4.22), we obtain the optimal controller of the CNOT gate.

5.3 DFT2 gate

Discrete Fourier transformation (DFT) gates are important in many quantum algorithms including Shor’s algorithm for integer factorization. The two-qubit DFT (DFT2) is a unitary transformation

\[ U_{\text{DFT2}} = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix}. \] (5.12)
It is diagonalized by
\[
R = \frac{1}{2} \begin{pmatrix}
1 & \sqrt{2} & -1 & 0 \\
1 & 0 & 1 & -\sqrt{2} \\
-1 & \sqrt{2} & 1 & 0 \\
1 & 0 & 1 & \sqrt{2}
\end{pmatrix}
\] (5.13)
as
\[
R^\dagger U_{\text{DFT2}} R = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & -1 & 0 \\
0 & 0 & 0 & i
\end{pmatrix}.
\] (5.14)

Therefore, we have \(\gamma_1 = \gamma_2 = 0, \gamma_3 = \pi\) and \(\gamma_4 = \pi/2\). Thus the ingredients of the controller are
\[
\Omega_{\text{diag}} = \text{diag}(2i\pi, 2i\pi, 0, i\pi), \quad W_{\text{diag}} = \text{diag}(0, 0, i\pi, i\pi \sqrt{3}/2),
\] (5.15)
and hence
\[
R\Omega_{\text{diag}} R^\dagger = \frac{i\pi}{2} \begin{pmatrix}
3 & 1 & 1 & 1 \\
1 & 2 & -1 & 0 \\
1 & -1 & 3 & -1 \\
1 & 0 & -1 & 2
\end{pmatrix}, \quad RW_{\text{diag}} = \frac{i\pi}{2} \begin{pmatrix}
0 & 0 & -1 & 0 \\
0 & 0 & 1 & -\sqrt{3}/2 \\
0 & 0 & 1 & 0 \\
0 & 0 & 1 & \sqrt{3}/2
\end{pmatrix}.
\] (5.16)

Substituting these into (4.22), we finally obtain the optimal controller of the DFT2 gate.

### 6 Summary and discussions

Let us summarize our argument. We briefly reviewed the WZ holonomy and discussed that it may be utilizable for implementation of quantum computation. The WZ holonomy is neatly described in terms of differential geometry of a homogeneous bundle, which consists of Stiefel and Grassmann manifolds and is equipped with the canonical connection. We formulated the optimization problem of control in holonomic quantum computation in a form of the isoholonomic problem in the homogenous bundle. We would like to emphasize that it had been left unsolved for more than a decade after the first proposal. We derived a set of equations, (3.21) and (3.27), that characterizes the optimal control and solved it to obtain the horizontal extremal curve (3.37). The curve must satisfy two boundary conditions, (4.1) and (4.2), to be a closed loop in the control manifold and to produce a specified unitary gate as a holonomy. We solved this inverse problem by combining small circle solutions (4.18) to \(U(1)\) holonomy into a direct sum. We provided a prescription (4.19)-(4.22) to construct exactly an optimal controller for any unitary gate. Finally we applied our prescription to several important quantum gates. transform gate.

We would like to discuss prospective development of the results presented above. Although our prescription is applicable to arbitrarily large qubit gates, the homogeneous
bundle seems rather over-idealized for practical applications. A realistic quantum system may have smaller control manifold $M$ than the Grassmann manifold. The restricted control manifold $M$ is embedded in the Grassmann manifold by an embedding map $f : M \to G_{N,k}(\mathbb{C})$ and we need to study the isoholonomic problem in the pullbacked bundle $f^*S_{N,k}(\mathbb{C})$. Furthermore, the available working Hilbert space in a realistic system may not have dimensions as large as $N \geq 2k$. Actually, even when $N < 2k$, sequential operations of single loop solutions can generate any unitary gate. However, such a patched solution could not be optimal. These problems will be treated separately in our future publications.

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