ISOHOLONOMIC PROBLEM AND HOLONOMIC QUANTUM COMPUTATION

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Geometric phases accompanying adiabatic processes in quantum systems can be utilized as unitary gates for quantum computation. Optimization of control of the adiabatic process naturally leads to the isoholonomic problem. The isoholonomic problem in a homogeneous fiber bundle is formulated and solved completely. [Proceedings of International Conference on Topology in Ordered Phases organized by Hokkaido University in March 2005.]

1. Introduction

The isoholonomic problem was proposed in 1991 by a mathematician, Montgomery\(^1\). The isoholonomic problem is a generalization of the isoperimetric problem, which requests finding a loop in a plane that surrounds the largest area with a fixed perimeter. On the other hand, the isoholonomic problem requests finding the shortest loop in a manifold that realizes a specified holonomy. This kind of problem naturally arose in studies of the Berry phase\(^2\text{–}^4\) and the Wilczek-Zee holonomy\(^5\), which appear in a state of a controlled quantum system when the control parameter is adiabatically changed and returned to the initial value. Experimenters tried to design efficient experiments for producing these kinds of holonomy. Montgomery formulated the isoholonomic problem in terms of differential geometry and gauge theory. Although he gave partial answers, construction of a concrete solution has remained an open problem.

Recently, in particular after the discovery of factorization algorithm by Shor\(^6\) in 1994, quantum computation grows into an active research area. Many people have proposed various algorithms of quantum computation and various methods for their physical implementation. Zanardi, Rasetti\(^7\) and Pachos\(^8\) proposed utilizing the Wilczek-Zee holonomy for implementing unitary gates and they named the method holonomic quantum computation. Since holonomy has its origin in geometry, it dose not depend on
detail of dynamics and hence it does not require fine temporal tuning of control parameters.

It should be noted, however, that holonomic quantum computation requires two seemingly contradicting conditions. The first one is the adiabaticity condition. To suppress undesirable transition between different energy levels we need to change the control parameter quasi-stationarily. Hence a safer control demands longer execution time to satisfy adiabaticity. The second one is the decoherence problem. When a quantum system is exposed to interaction with environment for a long time, the system loses coherence and a unitary operator fails to describe time-evolution of the system. Hence a safer control demands shorter execution time to avoid decoherence. To satisfy these two contradicting conditions we need to make the loop in the control parameter manifold as short as possible while keeping the specified holonomy. Thus, we are naturally led to the isoholonomic problem.

We would like to emphasize that a quantum computer is actually not a digital computer but an analog computer in its nature. Hence, the geometric and topological approaches are useful for building and optimizing quantum computers.

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2. Wilczek-Zee holonomy

A state vector $\psi(t) \in \mathbb{C}^N$ evolves according to the Schrödinger equation

$$ i\hbar \frac{d}{dt} \psi(t) = H(t)\psi(t). \quad (1) $$

The Hamiltonian admits a spectral decomposition $H(t) = \sum_{l=1}^{L} \varepsilon_l(t)P_l(t)$ 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 $\varepsilon_1$. 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 $t$, we have the eigenvectors such that

$$ H(t)v_\alpha(t) = \varepsilon_1(t)v_\alpha(t), \quad (\alpha = 1, \ldots, k). \quad (2) $$
We assume that they are normalized as $v^\dagger_\alpha(t)v_\beta(t) = \delta_{\alpha\beta}$. Then

$$V(t) = \begin{pmatrix} v_1(t), \ldots, v_k(t) \end{pmatrix}$$

(3)

forms an $N \times k$ matrix satisfying $V^\dagger(t)V(t) = I_k$ and $V(t)V^\dagger(t) = P(t)$. Here $I_k$ is the $k$-dimensional unit matrix. The adiabatic theorem guarantees that the state remains the eigenstate associated with the eigenvalue $\varepsilon_1(t)$ of the instantaneous Hamiltonian $H(t)$ if the initial state was an eigenstate with $\varepsilon_1(0)$. Therefore the state vector is a linear combination

$$\psi(t) = \sum_{\alpha=1}^k \phi_\alpha(t) v_\alpha(t) = V(t)\phi(t).$$

(4)

The vector $\phi = (\phi_1, \ldots, \phi_k) \in \mathbb{C}^k$ is called a reduced state vector. By substituting it into the Schrödinger equation (1) we get

$$\frac{d\phi}{dt} + V^\dagger \frac{dV}{dt} \phi(t) = -\frac{i}{\hbar} \varepsilon_1(t) \phi(t).$$

(5)

Its solution is formally written as

$$\phi(t) = \exp\left(-\frac{i}{\hbar} \int_0^t \varepsilon_1(s) ds\right) T \exp\left(-\int_0^t V^\dagger \frac{dV}{ds} ds\right) \phi(0),$$

(6)

where $T$ stands the time-ordered product. Then $\psi(t) = V(t)\phi(t)$ becomes

$$\psi(t) = e^{-\frac{i}{\hbar} \int_0^t \varepsilon_1(s) ds} V(t) T e^{-\int_0^t V^\dagger \frac{dV}{ds} V^\dagger(0)} \psi(0).$$

(7)

In particular, when the control parameter comes back to the initial point as $P(T) = P(0)$, the state vector $\psi(T)$ also comes back in the same eigenspace as $\psi(0) = V(0)\phi(0)$. The Wilczek-Zee holonomy $\Gamma \in U(k)$ is defined via

$$\psi(T) = e^{-\frac{i}{\hbar} \int_0^T \varepsilon_1(s) ds} V(0) \Gamma \phi(0)$$

(8)

and is given explicitly as

$$\Gamma = V(0)^\dagger V(T) T e^{-\int V^\dagger \frac{dV}{ds}}.$$  

(9)

If the condition $V^\dagger \frac{dV}{dt} = 0$ is satisfied, the curve $V(t)$ is called a horizontal lift of the curve $P(t)$. Then the holonomy (9) is reduced to $\Gamma = V^\dagger(0)V(T)$.

3. Formulation of the problem

The isoholonomic problem is formulated in terms of the homogeneous fiber bundle $(S_{N,k}(\mathbb{C}), G_{N,k}(\mathbb{C}), \pi, U(k))$. The Stiefel manifold $S_{N,k}(\mathbb{C})$ is the
set of orthonormal \( k \)-frames; a \( k \)-frame \( V \) spans the degenerate energy eigenspace in \( \mathbb{C}^N \):

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

where \( M(N,k;\mathbb{C}) \) is the set of \( N \times k \) complex matrices. An element of the unitary group \( h \in U(k) \) acts on \( V \in S_{N,k}(\mathbb{C}) \) from the right as \( (V,h) \mapsto VH \) by means of a matrix product. The Grassmann manifold \( G_{N,k}(\mathbb{C}) \) is defined as the set of projection matrices to \( k \)-dimensional subspaces in \( \mathbb{C}^N \),

\[
G_{N,k}(\mathbb{C}) = \{ P \in M(N,N;\mathbb{C}) \mid P^2 = P, \ P^\dagger = P, \ \text{tr}P = k \}.
\]

The projection map \( \pi : S_{N,k}(\mathbb{C}) \to G_{N,k}(\mathbb{C}) \) is defined as \( \pi : V \mapsto PV \). Then it can be proved that the Stiefel manifold \( S_{N,k}(\mathbb{C}) \) becomes a principal bundle over \( G_{N,k}(\mathbb{C}) \) with the structure group \( U(k) \). The canonical connection form on \( S_{N,k}(\mathbb{C}) \) is defined as a one-form

\[
A = V^\dagger dV,
\]

which takes its value in the Lie algebra \( u(k) \). The holonomy associated with this connection is called the Berry phase in case of \( k = 1 \) and the Wilczek-Zee holonomy in general. We define Riemannian metrics, \( \|dV\|^2 = \text{tr}(dV^\dagger dV) \) for the Stiefel manifold and \( \|dP\|^2 = \text{tr}(dPdP) \) for the Grassmann manifold. For any curve \( P(t) \) in \( G_{N,k}(\mathbb{C}) \), there is a curve \( V(t) \) in \( S_{N,k}(\mathbb{C}) \) such that \( \pi(V(t)) = P(t) \). If the curve \( V(t) \) satisfies

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

it is called a horizontal lift of the curve \( P(t) \). When the curve \( P(t) \) is a closed loop, such that

\[
V(T)V^\dagger(T) = V(0)V^\dagger(0),
\]

the holonomy associated with the loop is defined as \( V(T) = V(0)\Gamma \) and is given as

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

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

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

where \( \Omega(t) \in u(k) \) is a Lagrange multiplier to impose the horizontal condition (13) on the curve \( V(t) \). Thus the isoholonomic problem is stated as follows; find a horizontal curve \( V(t) \) that attains an extremal value of the functional (16) and satisfies the boundary conditions (14) and (15).
4. Derivation and solution of the Euler-Lagrange equation

We derive the Euler-Lagrange equation associated with the functional $S$ 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

$$V_\epsilon(t) = (1 + \epsilon \eta(t))V(t).$$  \hfill (17)

By substituting $V_\epsilon(t)$ into (16) and differentiating with respect to $\epsilon$, the extremal condition yields

$$0 = \left. \frac{dS}{d\epsilon} \right|_{\epsilon=0} = \int_0^T \text{tr} \left\{ \dot{\eta}(VV^\dagger - \dot{V}V^\dagger - \dot{V}\Omega V^\dagger) \right\} dt.$$  \hfill (18)

Thus we obtain the Euler-Lagrange equation

$$\frac{d}{dt}(VV^\dagger - \dot{V}V^\dagger + \dot{V}\Omega V^\dagger) = 0.$$  \hfill (19)

The extremal condition with respect to $\Omega(t)$ reproduces the horizontal equation $V^\dagger \dot{V} = 0$.

Next, we solve the equations (13) and (19). The equation (19) is integrated to yield

$$\dot{V}V^\dagger - \dot{V}V^\dagger + \dot{V}\Omega V^\dagger = \text{const} = X \in u(N).$$  \hfill (20)

Conjugation of the horizontal condition (13) yields $\dot{V}^\dagger V = 0$. Then, by multiplying $V$ on (20) from the right we obtain

$$\dot{V} + \dot{V}\Omega = XV.$$  \hfill (21)

By multiplying $V^\dagger$ on (21) from the left we obtain

$$\Omega = V^\dagger XV.$$  \hfill (22)

We can show $\dot{\Omega} = 0$ by a straightforward calculation. Hence, $\Omega(t)$ is actually a constant matrix. The solution of (21) and (22) is

$$V(t) = e^{tX} V_0 e^{-t\Omega}, \quad \Omega = V_0^\dagger XV_0.$$  \hfill (23)

We call this solution the horizontal extremal curve. Then (20) becomes

$$(XV - \dot{V}\Omega)V^\dagger - V(-V^\dagger X + \Omega V^\dagger) + \dot{V}\Omega V^\dagger = X,$$

which is arranged as

$$X - (VV^\dagger X + XVV^\dagger - VV^\dagger XVV^\dagger) = 0.$$  \hfill (24)
Here we used (22). We may take, without loss of generality,
\[ V_0 = \begin{pmatrix} I_k \\ 0 \end{pmatrix} \in S_{N,k}(\mathbb{C}) \]  
(25)
as the initial point. We can parametrize \( X \in u(N) \), which satisfies (22), as
\[ X = \begin{pmatrix} \Omega & W \\ -W^\dagger & Z \end{pmatrix} \]  
(26)with \( W \in M(k, N-k; \mathbb{C}) \) and \( Z \in u(N-k) \). Then the constraint equation (24) implies that \( Z = 0 \). Finally, we obtained a complete set of solution (23) of the horizontal extremal equation (13) and (19).

5. Solution to the boundary value problem
The remaining problem is to find the controller matrices \( \Omega \) and \( W \) that satisfy the closed loop condition
\[ V(T)V^\dagger(T) = e^{TX}V_0V^\dagger_0 e^{-TX} = V_0V^\dagger_0 \]  
(27)and the holonomy condition
\[ V_0^\dagger V(T) = V_0^\dagger e^{TX}V_0 e^{-T\Omega} = U_{\text{gate}} \]  
(28)for a requested unitary gate \( U_{\text{gate}} \in U(k) \). Montgomery\(^1\) presented this boundary value problem as an open problem. Here we give a prescription to construct a controller matrix \( X \) that produces the specified unitary gate \( U_{\text{gate}} \). 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 \( T = 1 \).

Our method consists of three steps. In the first step, we diagonalize a given unitary matrix \( U_{\text{gate}} \in U(k) \) as
\[ R^\dagger U_{\text{gate}} R = U_{\text{diag}} = \text{diag}(e^{i\gamma_1}, \ldots, e^{i\gamma_k}) \]  
(0 \leq \gamma_j < 2\pi) \]  
(29)with \( R \in U(k) \). The small circle is a circle in a two-sphere \( \mathbb{C}P^1 \subset G_{N,k}(\mathbb{C}) \) that surrounds a solid angle which is equal to twice of the Berry phase. In the second step, combining \( k \) small circles we construct \( k \times k \) matrices
\[ \Omega_{\text{diag}} = \text{diag}(i\omega_1, \ldots, i\omega_k), \quad W_{\text{diag}} = \text{diag}(i\tau_1, \ldots, i\tau_k), \]  
(30)with \( \omega_j = 2(\pi - \gamma_j) \) and \( \tau_j = e^{i\phi_j} \sqrt{\pi^2 - (\pi - \gamma_j)^2} \). We combine them into a \( 2k \times 2k \) matrix
\[ X_{\text{diag}} = \begin{pmatrix} \Omega_{\text{diag}} & W_{\text{diag}} \\ -W_{\text{diag}}^\dagger & 0 \end{pmatrix}. \]
In the third step, we construct the controller \( X \) as
\[
X = \begin{pmatrix} R & 0 \\ 0 & I_k \end{pmatrix} \begin{pmatrix} \Omega_{\text{diag}} & W_{\text{diag}} \\ -W_{\text{diag}}^\dagger & 0 \end{pmatrix} \begin{pmatrix} R^\dagger & 0 \\ 0 & I_k \end{pmatrix} = \begin{pmatrix} R\Omega_{\text{diag}}R^\dagger & RW_{\text{diag}} \\ -W_{\text{diag}}^\dagger & R^\dagger \end{pmatrix}.
\]

\[ \text{(31)} \]

In the paper\(^9\) we calculated explicitly controllers of various unitary gates; the controlled NOT gate, the discrete Fourier transformation gate and so on.

6. Conclusion

We formulated and solved the isoholonomic problem in the homogeneous fiber bundle. The problem was reduced to a boundary value problem of the horizontal extremal equation. We determined the control parameters that satisfy the boundary conditions. This result is applicable for producing arbitrary unitary gates.

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