Nonadiabatic holonomic one-qubit gates

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April 10, 2014

Abstract

Adiabatic quantum gate implementation generally takes longer time, which is disadvantageous in view of decoherence. In this report we implement several essential one-qubit quantum gates nonadiabatically by making use of a dynamical invariant associated with a Hamiltonian. Moreover we require that these gates be holonomic, that is, the dynamical phases associated with the gates vanish. Our implementation is based on our recent work [J. Phys. Soc. Jpn. 83, 034001 (2014)] and the gate parameters required for the implementations are found by numerical optimization.

Keywords: nonadiabatic control, Aharonov-Anandan phase, holonomic quantum gate.

1 Introduction

1.1 Dynamical Invariants

Let $H = H(t) \in M_n(\mathbb{C})$ be a time-dependent Hamiltonian. A time-dependent Hermitian operator $I = I(t) \in M_n(\mathbb{C})$ is called a dynamical invariant (also known as the Lewis-Riesenfeld invariant [11]) if it satisfies

$$i \frac{\partial I}{\partial t} = [H, I]. \quad (1)$$

Let $|\psi(t)\rangle$ be a solution of the time-dependent Schrödinger equation

$$i \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle. \quad (2)$$

Then $\langle \psi(t)|I|\psi(t)\rangle$ is independent of time. In fact,

$$\frac{d}{dt} \langle \psi(t)|I|\psi(t)\rangle \quad = \quad \left( \frac{d}{dt} \langle \psi(t)| \right) I |\psi(t)\rangle + \langle \psi(t)| \frac{d}{dt} |\psi(t)\rangle \quad + \quad \langle \psi(t)|I \left( \frac{d}{dt} |\psi(t)\rangle \right) \quad = \quad \langle \psi(t)| [iHI - i[HI - IH] - iIH] |\psi(t)\rangle \quad = \quad 0.$$

Let $\{\lambda_k\}$ be the set of eigenvalues of $I$ and $\{|\phi_k(t)\rangle\}$ be the corresponding set of normalized eigenvectors; $I |\phi_k(t)\rangle = \lambda_k |\phi_k(t)\rangle$. It might seem
that \( \lambda_k \) depends on time since \( I \) does. Observe, however, that

\[
\dot{\lambda}_k = \frac{d}{dt} \langle \phi_k(t) | I | \phi_k(t) \rangle = \left( \frac{d}{dt} \langle \phi_k(t) | \right) I | \phi_k(t) \rangle + \langle \phi_k(t) | \dot{I}(t) | \phi_k(t) \rangle + \langle \phi_k(t) | I \left( \frac{d}{dt} | \phi_k(t) \rangle \right)
\]

\[
= \lambda_k \left( \frac{d}{dt} \langle \phi_k(t) | \right) | \phi_k(t) \rangle - i \lambda_k \langle \phi_k(t) | (H - H) | \phi_k(t) \rangle + \lambda_k \langle \phi_k(t) | \left( \frac{d}{dt} | \phi_k(t) \rangle \right)
\]

\[
= \lambda_k \frac{d}{dt} \langle \phi_k(t) | \phi_k(t) \rangle = 0,
\]

where use has been made of the normalization condition \( \langle \phi_k(t) | \phi_k(t) \rangle = 1 \).

The dynamical invariant has the following spectral decomposition

\[
I = \sum_k \lambda_k | \phi_k(t) \rangle \langle \phi_k(t) |, \quad \lambda_k \in \mathbb{R}. \tag{3}
\]

### 1.2 Solutions of the Schrödinger Equation

Take \( | \phi_k(0) \rangle \) and consider a solution \( | \psi_k(t) \rangle \) of the Schrödinger equation \( i \partial_t | \psi_k(t) \rangle = H | \psi_k(t) \rangle \) such that \( | \psi_k(0) \rangle = | \phi_k(0) \rangle \). The solution \( | \psi_k(t) \rangle \) should not be confused with the \( k \)-th eigenvector of \( H \). The index \( k \) simply states that the vector was initially the eigenvector \( | \phi_k(0) \rangle \) of \( I(0) \).

\[| \psi_k(t) \rangle = e^{i \alpha_k(t)} | \phi_k(t) \rangle \quad \text{for} \quad \alpha_k(t) = \int_0^t \langle \dot{\phi}_k(s) | [i \partial_s - H(s)] | \phi_k(s) \rangle ds. \tag{5}\]

**Theorem 1.** The solution \( | \psi_k(t) \rangle \) of the Schrödinger equation (2) is given by

\[| \psi_k(t) \rangle = e^{i \alpha_k(t)} | \phi_k(t) \rangle \quad \text{for} \quad \alpha_k(t) = \int_0^t \langle \dot{\phi}_k(s) | [i \partial_s - H(s)] | \phi_k(s) \rangle ds. \tag{5}\]
Let $|\psi(t)\rangle$ be an arbitrary solution of the Schrödinger equation. Since $\{|\phi_n(0)\rangle\}$ is a complete set, $|\psi(0)\rangle$ can be expanded as

$$|\psi(0)\rangle = \sum_k c_k |\phi_k(0)\rangle.$$  

From linearity, the solution at arbitrary $t > 0$ is

$$|\psi(t)\rangle = \sum_k c_k e^{i\alpha_k(t)} |\phi_k(t)\rangle,$$  

where $c_k$ is independent of time.

A few remarks are in order. It is a common practice to write $|\psi(t)\rangle$ as

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle, \quad U(t) = T e^{-i \int_0^t H(s) ds},$$

where $U(t)$ is the time-evolution operator. However, analytic evaluation of $U(t)$ is impossible, except for a few simple cases, due to the time-ordering operation $T$. In the above formalism, everything is found by solving the eigenvalue problem $I|\phi_k(t)\rangle = \lambda_k |\phi_k(t)\rangle$ at a given instant of time $t$, however, the difficulty lies in finding $I$.

Since $|\psi_k(0)\rangle$ develops to $|\psi_k(t)\rangle$ at time $t > 0$, the time-evolution operator $U(t)$ can be expressed as

$$\sum_k |\psi_k(t)\rangle\langle\psi_k(0)| = \sum_k e^{i\alpha_k(t)} |\phi_k(t)\rangle\langle\phi_k(0)|.$$  

The evolution of $|\phi_k(t)\rangle$ is transitionless since $U(t)|\phi_k(0)\rangle = e^{i\alpha_k(t)} |\phi_k(0)\rangle$ for any $t > 0$. The solution of the Schrödinger equation always remains in the $k$-th eigenstate of $I$ if $|\psi(0)\rangle = |\phi_k(0)\rangle$. On the other hand, $|\psi(t)\rangle$ is not an eigenvector of $H$ and the time-evolution is nonadiabatic.

1.3 **Aharonov-Anandan Phase and Dynamical Invariants**

Let $U(T)$ be the time-evolution operator at a fixed time $T$ for a given Hamiltonian. $U(T)$ has the spectral decomposition

$$U(t) = \sum_k e^{i\chi_k} |\chi_k\rangle\langle\chi_k|,$$  

where $U(T)|\chi_k\rangle = e^{i\chi_k} |\chi_k\rangle$ and $\langle\chi_k|\chi_{k'}\rangle = \delta_{kk'}$. Since a unitary matrix is normal, the set of normalized eigenvectors $\{|\chi_k\rangle\}$ forms a complete set.

Suppose the initial state of the wave function $|\psi(0)\rangle$ is $|\chi_k\rangle$. Then we find

$$|\psi(T)\rangle = U(T)|\psi(0)\rangle = U(T)|\chi_k\rangle = e^{i\chi_k} |\psi(0)\rangle.$$  

By noting that $|\psi(T)\rangle$ and $|\psi(0)\rangle$ represent the same vector in the projected Hilbert space $\mathbb{C}P^n = \mathbb{C}^n/U(1)$, we find an eigenvector of $U(T)$ executes a cyclic evolution in the projective Hilbert space. Such a vector is called cyclic. In the $U(1)$ fiber over $\{|\psi(0)\rangle, |\psi(0)\rangle\}$ and $|\psi(T)\rangle$ differ by a phase $e^{i\chi_k}$, which is called the Aharonov-Anandan phase [2].

Let $|\phi(t)\rangle$ be a closed curve in the projective Hilbert space ($|\phi(T)\rangle = |\phi(0)\rangle$) such that $|\psi(t)\rangle = e^{i\alpha(t)} |\phi(t)\rangle$, where $|\psi(t)\rangle$ is a solution of the Schrödinger equation. This $\alpha(t)$ is identified with the Lewis-Riesenfeld phase, meaning there is a dynamical invariant $I$ whose eigenvector is $|\phi(t)\rangle$. In fact $U(T)$ can be written as

$$U(T) = \sum_k |\psi_k(T)\rangle\langle\psi_k(0)|$$

$$= \sum_k e^{i\alpha(T)} |\phi_k(T)\rangle\langle\phi_k(0)|$$

$$= \sum_k e^{i\chi_k} |\phi_k(0)\rangle\langle\phi_k(0)|.$$  


Thus we have the following correspondences
\[ |\phi_k(0)\rangle \leftrightarrow |\chi_k\rangle, \]
\[ e^{i\alpha_k(T)} \leftrightarrow e^{i\chi_k}. \]

Let
\[ \alpha_k(T) = \int_0^T \langle \phi_k(t)|(i\partial_t - H)|\phi_k(t)\rangle dt \] (11)
be the Lewis-Riesenfeld phase associated with the eigenvector \(|\phi_k(t)\rangle\) of \(I\). The first term
\[ \gamma^g_k = i \int \langle \phi_k(t)|d|\phi_k(t)\rangle \] (12)
is reparameterization \((t \rightarrow \tau(t))\) invariant and geometric in nature (geometric phase), while
\[ \gamma^d_k = -\int_0^T \langle \phi_k(t)|H|\phi_k(t)\rangle dt \] (13)
is the dynamical phase.

When \(\gamma^d_k = 0\) for all \(k\), the time-evolution is called holonomic or geometric [3]. A quantum gate satisfying this condition is called a holonomic (geometric) gate.

2 Nonadiabatic Holonomic One-Qubit Gates

For definiteness, let us consider [4]
\[ H = \frac{1}{2}(\Omega \cos \omega t \sigma_x + \Omega \sin \omega t \sigma_y + \Delta \sigma_z). \] (14)

It is easy to verify that
\[ I = \Omega \cos \omega t \sigma_x + \Omega \sin \omega t \sigma_y + (\Delta - \omega) \sigma_z \] (15)
is a dynamical invariant of \(H\). The eigenvalues and eigenvectors of \(I\) are
\[ \pm \lambda, \quad |\phi_\pm(t)\rangle = \left( \frac{e^{-i\omega t \cos \theta_\pm}}{\sin \theta_\pm} \right), \] (16)
where \(\lambda = \sqrt{\Omega^2 + (\Delta - \omega)^2}\), \(\cos \theta_\pm = \xi_\pm/\sqrt{1 + \xi_\pm^2}\), \(\sin \theta_\pm = 1/\sqrt{1 + \xi_\pm^2}\) with \(\xi_\pm = [(\Delta - \omega) \pm \lambda]/\Omega\). The Lewis-Riesenfeld phases are readily evaluated as
\[ \alpha_\pm(t) = (\omega \mp \lambda)t/2. \] (17)

Note that \(H, I\) and \(|\phi_\pm(t)\rangle\) are cyclic with a period \(T = 2\pi/\omega\).

Let us require that \(U(T)\) is a holonomic gate, that is
\[ \gamma^d_\pm = -\int_0^T \langle \phi_\pm(t)|H|\phi_\pm(t)\rangle dt = 0. \] (18)

This is satisfied if and only if
\[ \Omega^2 + \Delta(\Delta - \omega) = 0. \] (19)
In fact, this condition not only satisfies \(\gamma^d_\pm = 0\) but also a stronger condition that the integrand \(\langle \phi_\pm(t)|H|\phi_\pm(t)\rangle\) vanishes for \(\forall t \in [0, T]\). We find from this condition that \(\Delta \in [0, \omega]\), from which we also find \(\Omega^2 \sim \Delta\omega\). Adiabaticity cannot be attained under this condition and hence such a gate cannot be realized within the adiabatic regime.

When the above conditions are met, the resulting gate is [4]
\[ U_\beta(T) = \sum_{\pm} e^{i\alpha_{\pm}(T)}|\phi_{\pm}(0)\rangle\langle \phi_{\pm}(0)| \]
\[ = -e^{i\pi \sin \beta[\cos \beta \sigma_x + \sin \beta \sigma_z]}, \] (20)
where \(\cos^2 \beta = \Delta/\omega, \beta \in [0, \pi/2]\).

\(U_\beta(T)\) generates a 1-dimensional trajectory in SU(2) manifold as shown in Fig. 1.
By noting that \([U_{\beta_1}(T), U_{\beta_2}(T)] \neq 0\) in general, the set \(\{U_{\beta}(T)\}\) generates all SU(2) group elements and hence forms a universal set of one-qubit gates.

3 Examples

In this section, we consider several important one-qubit gates. Since \(U_\beta\) given in Eq. (20) implements a one-dimensional subset of SU(2), we need to employ several \(U_\beta\) to implement arbitrary one-qubit gates.

In what follows, we list \(\{\beta_i\} = \{\beta_1, \ldots, \beta_N\}\) with the convention that \(\beta_1\) acts first and \(\beta_N\) acts last, and we give the gate fidelity \(F = \text{tr}(U^\dagger U_{\text{ideal}})/\text{tr}(U_{\text{ideal}}^\dagger U_{\text{ideal}})\). The numerical results below are high-fidelity implementations of the desired gates.

3.1 NOT gate

The NOT gate

\[
e^{i\pi/2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\] (21)

can be realized by using 4 gates with \(\{\beta_i\} = \{0.423, 0.680, 0.236, 0.222\}\). The fidelity is 0.99999999990.

3.2 Hadamard gate

A Hadamard gate

\[
e^{i\pi/2} \sqrt{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}
\] (22)

with good fidelity 0.999999999791 requires 7 gates, with \(\{\beta_i\}\) given as \(\{0.331, 0.783, 0.300, 0.926, 0.174, 0.851, 0.347\}\).

3.3 Phase gate

The phase gate

\[
e^{-i\pi/4} \begin{pmatrix} 1 & 0 \\ 0 & i \end{pmatrix}
\] (23)

implemented using 4 gates \(\{\beta_i\} = \{0.827, 0.102, 0.287, 0.777\}\) has the fidelity 0.99999999993.

3.4 \(\pi/8\)-gate

Similar to the NOT gate, \(\pi/8\)-gate

\[
e^{-i\pi/8} \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{pmatrix}
\] (24)

can be implemented using 3 elementary gates with \(\{\beta_i\} = \{0.788, 0.514, 0.788\}\) and fidelity 0.99999999996.
4 Summary

A review of holonomic gates implemented by using the dynamical invariants is given. An interesting relation between the dynamical phase and the Aharonov-Anandan phase is clarified. We have explicitly shown that important one-qubit gates can be implemented by combining holonomic quantum gates.

Analysis of the robustness of our one-qubit gates under noise is an important issue and will be published elsewhere.

Acknowledgement

We are grateful to Yasushi Kondo for careful reading of the manuscript. UG and MN are grateful to the Japan Society for the Promotion of Science (JSPS) for partial support from a Grant-in-Aid for Scientific Research (Grant No. 24320008). MN also thanks JSPS for a Grant-in-Aid for Scientific Research (Grant No. 23540470). UG acknowledges the financial support of the Ministry of Education, Culture, Sports, Science and Technology (MEXT) Scholarship for foreign students.

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