Invariant-based inverse engineering for fast nonadiabatic geometric quantum computation

Wei Li

School of Physics and Electronic Information, Yanan University, Yanan 716000, People's Republic of China
* Author to whom any correspondence should be addressed.
E-mail: liweixi@126.com

Keywords: geometric quantum computation, quantum gates, inverse engineering approach, Berry phase

Abstract

In this paper, based on first given Lewis–Riesenfeld invariant depicted by a unit vector in parameter space, we inverse engineering the time-dependent Hamiltonian of a system with su(2) Lie algebraic structure. The introduced method is then applied to investigate nonadiabatic Abelian geometric quantum computation. We demonstrate that, by employing the nonadiabatic Berry phase generated through nonadiabatic periodic evolution, a driven two-level system which undergoes a single cyclic evolution along a loop path in Bloch space can realize a universal set of one-qubit gates. Subsequently, under consideration of the influence of the systematic error and dissipation on nonadiabatic process, the result reveals arbitrary one-qubit gate can be implemented with a high fidelity. Moreover, to complete the universal set, arbitrary controlled-U gate is designed by utilizing a driven system consisted of a pair of coupled spin subsystems.

1. Introduction

Fast and robust control of the dynamics of quantum systems is one of the most fundamental elements to implement universal qubits manipulations for quantum computing [1]. To achieve high-fidelity quantum control, the physical systems driven by special pulse sequences with well-designed strength and time duration should be resistant to certain kinds of noises and errors. Geometric quantum computation (GQC), which utilizes the Abelian or non-Abelian geometric phase [2–4] depending only on the global geometrical feature of a cyclic evolution, is taken as one promising proposal for quantum control for maintaining the robustness against local disturbances during the evolution [5–8].

GQC often involves adiabatic evolution to strongly robust against random noise and systematic error [9–11]. However, the adiabatic process implies low evolution speed, which makes it sensitive to the environment-induced decoherence. To speed up the adiabatic process, shortcuts to adiabaticity [12, 13] in terms of transitionless algorithm [14–17] or counter-diabatic protocol [18, 19] was presented to generate exact dynamical evolution which aims at the adiabatic eigenstates of a given Hamiltonian by introducing auxiliary fields to remove the nonadiabatic effect. In addition, relying on the non-Abelian geometric phase depicted by a matrix [20], various non-Abelian nonadiabatic geometric approaches have been proposed, including nonadiabatic holonomic quantum computation (NHQC) [21, 22], single-loop multiple-pulse NHQC [23] and composite NHQC [24]. These schemes can realize arbitrary holonomic one-qubit gate operation confined to the Hilbert subspace of a three-level system, where two levels encoding a qubit are coupled to an excited state by elaborate pulses. Nevertheless, the disadvantage of these approaches is to impose rigorous conditions on the driving Hamilton of the system, for instance, Hamiltonian matrix in dynamics basis must vanish. Recently, an extensive approach called NHQC+ has been put forward to relax the restriction and still maintain robustness against certain noises, but may need to introduce auxiliary a set of time-dependent basis [25].

The Abelian GQC approaches, which employ only a two-level system, can implement the desired gate operations through either Berry phase [26] in an adiabatic process or Aharonov–Anandan phase [3] in a nonadiabatic process, thus it is simple relative to the above non-Abelian nonadiabatic proposals requiring
systems with three-dimensional Hilbert space. In this paper, based on first given Lewis–Riesenfeld (LR) invariant [27] depicted by a unit vector in parameter space, we inverse designing the suitable Hamiltonian of a system with su(2) Lie algebraic structure and demonstrate that the nonadiabatic periodic evolution can generate the Berry phase in a nonadiabatic manner. What more interesting is that our study also reveals that a driven two-level system undergoing a single cyclic evolution along a loop path in Bloch space can realize a universal set of one-qubit.

The rest of the paper is organized as follows. Section 2 is contributed to a detailed introduction our scheme for fast universal geometric single-qubit gates. We will construct time-dependent Hamiltonian based on invariant (section 2.1). Subsequently, certain constraint on the driven external field is obtained for purely geometric evolution (section 2.2). We further investigate the nonadiabatic geometric phase induced by a cycle evolution and manifest its geometric feature focusing on the two-level system. Based on the nonadiabatic geometric phase, the system can achieve a universal set of non-adiabatic geometric gates (section 2.3). To illustrate the efficiency of the approach, we design special Hamiltonians for a two-level system to implement the appropriate one-qubit gates (section 2.4). The influence of the systematic error and dissipation on nonadiabatic process is then explored in section 2.5. In section 3 we demonstrate that arbitrary controlled-U gate is designed by utilizing a driven system consisted of a pair of coupled spin subsystems. Finally, a summary of the manuscript is presented in section 4.

2. Invariant-based inverse engineering for universal one-qubit gates

2.1. Explicit construction of Hamiltonian for su(2) Lie algebraic system

We address that a driven quantum system with su(2) Lie algebraic structure takes the following form of time-dependent Hamiltonian

\[ H(t) = \Omega_x(t)J_x + \Omega_y(t)J_y + \Omega_z(t)J_z, \]

in which the generators satisfy the commutation relation \([J_i, J_j] = i\epsilon_{ijk}J_k\). The pulse parameters \(\{\Omega_x(t), \Omega_y(t), \Omega_z(t)\}\) related to driving field assume analytical forms with time dependent. The dynamics of the system is governed by the Schrödinger equation (here we have set \(\hbar = 1\))

\[ i\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle. \]

To implement desired dynamics with respect to exact nonadiabatic passage, we inverse engineer Hamiltonian \(H(t)\) based on L–R dynamical invariant [27] satisfying

\[ \frac{\partial I(t)}{\partial t} - i[I(t), H(t)] = 0. \]

In view of the Lie algebraic structure of the Hamiltonian, L–R invariant can be expressed as a linear combination of generators of su(2) Lie algebraic, here \(I(t)\) may be given by [28]

\[ I(t) = R(t) \cdot J, \]

where the vector \(R(t) = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)\) depicts the evolution trajectory of \(I(t)\) on a surface of unit sphere \(S^2\) with \(\theta(t)\) and \(\varphi(t)\) being the azimuthal and polar angles, respectively. It is mentioned that, consider a space spanned by the generators, \(I(t)\) can be obtained via \(J_z\) rotating around the axis \(J_y\) by \(\theta\) angle and \(J_y\) by \(\varphi\) successively. In this way, by introducing a unitary operator \(G(t) = e^{-i\varphi(t)J_y}e^{-i\theta(t)J_z}\), \(I(t)\) can be recast as

\[ I(t) = G(t)J_zG^\dagger(t), \]

with the instantaneous eigenstate

\[ |\psi_m(t)\rangle = G(t)|m\rangle. \]

Here the state \(|m\rangle\) represents the eigenvector of \(J_z\) with magnetic quantum number \(m\). It is noticed that, the general form of Hamiltonian can be constructed in two parts: one commutes with operator \(I(t)\) in equation (5) and the other satisfies the equation (3). Therefore, one has

\[ H(t) = f(t)I(t) - iG(t)\partial_t G^\dagger(t). \]

with \(f(t)\) being an arbitrary real function with time dependent. The pulse parameters are thus explicitly expressed according to equations (1) and (7),
\[ \Omega_x(t) = \beta(t) \sin \theta(t) \cos \varphi(t) - \dot{\varphi}(t) \sin(\theta(t)), \]
\[ \Omega_y(t) = \beta(t) \sin \theta(t) \sin \varphi(t) + \dot{\varphi}(t) \cos(\theta(t)), \]
\[ \Omega_z(t) = \beta(t) \cos \theta(t) + \dot{\varphi}(t), \]

where \( \beta(t) = f(t) - \dot{\varphi}(t) \).

In general, \( I(t) \) will evolve along a prescribed path characterized by the parameters \( \theta(t) \) and \( \varphi(t) \). For a given invariant, equation (7) indicates that there are many possible Hamiltonians corresponding to different choices of real functions \( f(t) \). Take the proposed reverse engineering protocols \([29–32]\) as an example, the choice of the function \( f(t) \) is constrained by imposing the Hamiltonian and invariant commutating for the initial time and final time, which aims at the adiabatic eigenstates of the given Hamiltonian. In comparison, the function \( f(t) \) should be restricted to the desired nonadiabatic GQC in our scheme. Next, we will obtain the constraint by exploring the dynamical evolution.

### 2.2. Constraint of GQC

Let us investigate the dynamics of the driven system with Hamiltonian presented in equations (1) and (8). The invariant method \([27]\) manifests that the basic solution to the Schrödinger equation differs from the function \( f(t) \) only by a nonadiabatic counterpart to the adiabatic eigenstates of the given Hamiltonian. In contrast, focusing on the two-level system, we demonstrate that a universal set of one-qubit gates can be realized.

To implement the desired nonadiabatic GQC, the kernel of the latter of the L–R phase, accounting for the nonadiabatic energy levels of the system, is expected to vanish:

\[ \langle \phi_m(t)|H(t)|\phi_m(t) \rangle = 0. \]  

Due to not all eigenvalues of Hamiltonian (1) being equal to zero, the dynamical basis \( \{|\psi_m(t)\}\} \) can never recover the adiabatic instantaneous eigenstate \( \{|\psi_m(0)\}\} \) of the Hamiltonian as the parameters \( (\theta, \varphi) \) change slowly with respect to time. We confirm that the dynamics of the system is essentially nonadiabatic. Accordingly, plugging equations (6) and (7) into (10) leads to the explicit expression of constraint

\[ \Omega_x(t)\hat{R}_x(t) + \Omega_y(t)\hat{R}_y(t) + \Omega_z(t)\hat{R}_z(t) = 0. \]  

Employing equation (8), the constraint (11) can also be recast as

\[ f(t) = 2\dot{\varphi}(t)\sin^2 \left( \frac{\theta(t)}{2} \right), \]

which ensures that the evolution is purely geometric. It is mentioned that, different from \([33, 34]\) which cancels the dynamical phase at the final time of the cyclic evolution by designing the special angular parameters in parameter space, there is no restriction on these angles but \( f(t) \) meets the constraint, and thus it is convenience to construct the desired non-adiabatic geometric gates.

To proceed, the first term of the integration of the L–R phase, which denotes a nonadiabatic counterpart of the geometric phase of the adiabatic evolution, can be worked out from equations (6) and (9). In the following section, we will calculate the nonadiabatic geometric phase and manifest its geometric feature focusing on the two-level system. Furthermore, we demonstrate that a universal set of one-qubit gates can be realized.

### 2.3. Implementation of arbitrary one-qubit gate

Let us first explore the geometric phase induced by the dynamical evolution. To be specific, we focus on the case of a two-level system with \( j = \frac{1}{2} \). The corresponding instantaneous eigenstates of \( I(t) \) are shown to be

\[ |\phi_{\pm}(t)\rangle = \cos \left( \frac{\theta(t)}{2} \right) |\pm\rangle \pm e^{\pm i\varphi(t)} \sin \left( \frac{\theta(t)}{2} \right) |\mp\rangle, \]

where the notation \(|+\rangle\) and \(|-\rangle\) denote the spin up \((1, 0)^T\) for \( m = \frac{1}{2} \) and spin down state \((0, 1)^T\) for \( m = -\frac{1}{2} \), respectively. Considering a cyclic evolution of states \(|\phi_{\pm}(t)\rangle\) from the initial time \( t_0 \) to the final time \( t_f \), that is, \(|\phi_{\pm}(t_0)\rangle = |\phi_{\pm}(t_f)\rangle\), for the overall evolution the nonadiabatic geometric phase can be worked out to be
\[
\Phi_{\pm}(t_f, t_0) = \int_{t_0}^{t_f} \langle \phi_{\pm}(t') | i \partial_t | \phi_{\pm}(t') \rangle \, dt'
\]
\[
= \pm \frac{1}{2} \int_{t_0}^{t_f} f(t') \, dt'.
\] (14)

To reveal the geometric feature of the phase factor, we will concentrate to the evolution along an arbitrary smooth and continuous closed curve \(L\) depicted by the unit vector \(R(\theta, \varphi)\) in parameter space. The integral in the first line of equation (14) can be recast as the line integral along the curve \([26]\),

\[
\Phi_{\pm}(t_f, t_0) = i \int_{R(t_0)}^{R(t_f)} \langle \phi_{\pm}(R) | \frac{\partial}{\partial R} | \phi_{\pm}(R) \rangle \, dR
\]
\[
= \oint_{L} A_{\pm}(R) \cdot dR
\] (15)

in which \(A_{\pm}(R) = i \langle \phi_{\pm}(R) | \frac{\partial}{\partial R} | \phi_{\pm}(R) \rangle\) can be regarded as the ‘vector potential’ in the parameter space. It is noted that we have assumed the path \(L\) is counterclockwise, otherwise add a minus sign before the integral. According to equation (13), it is straightforward to obtain \(A_{\pm}(R) = \mp \frac{1}{\sin \frac{\varphi}{2}} e_{\varphi}\) with the unit vector \(e_{\varphi}\) pointing in the direction of increase of azimuthal angle \(\varphi\). To apply the Stokes theorem, the geometric phase can be then calculated by surface integral over the enclosed surface \( \Sigma \) bounded by \(L\),

\[
\Phi_{\pm}(t_f, t_0) = i \int_{\Sigma(L)} \frac{\partial}{\partial R} \times A_{\pm}(R) \cdot dS.
\] (16)

It is readily to obtain \(\Phi_{\pm}(t_f, t_0) = \mp \Omega(L)/2\) with the solid angle \(\Omega(L)\) swept by the loop evolution. The geometric phase is just Berry phase in a nonadiabatic manner.

Next, we will show that a universal set of one-qubit gates can be realized in the above two-level system. To this goal, we consider that the system evolves along a loop path \(L\), the evolution operator is given by

\[
U(t, t_0) = \sum_{\pm} e^{i \Phi_{\pm}(t, t_0)} | \phi_{\pm}(t) \rangle \langle \phi_{\pm}(t_0) |.
\] (17)

Due to the Lie algebraic structure of the Hamiltonian, the operator at the final time \(t = t_f\) takes the form

\[
U(L) = n_0 I - n_1 \cdot \sigma,
\] (18)

in which \(I\) and \(\sigma = (\sigma_x, \sigma_y, \sigma_z)\) are the identity and Pauli matrices, respectively. According to the states (13), the coefficients of these matrices are then worked out to be \(n_0 = \cos \Phi\) and \(n_1 = i n \sin \Phi\) with \(\Phi = \Omega(L)/2, \bar{\theta} = \theta(t_0), \bar{\varphi} = \varphi(t_0),\) and the unit vector \(\mathbf{n} = (\sin \bar{\theta} \cos \bar{\varphi}, \sin \bar{\theta} \sin \bar{\varphi}, \cos \bar{\theta})\). The time evolution operator is finally recast as

\[
U(L) = e^{-in \cdot \sigma \omega t/2}.
\] (19)

It is seen that, as both \(\alpha\) and \(\mathbf{n}\) can take any value, \(U(L)\) denotes an arbitrary single-qubit gate in the qubit space. For instance, up to an unimportant overall phase factor, the choice of \(\mathbf{n} = (0, 0, 1)\) leads to the phase shift gate \(|l\rangle \rightarrow e^{i\alpha} |l\rangle\) with \(l = 0\) or \(l = 1\). By selecting \(\alpha = \pi\) and \(\mathbf{n} = (1, 0, 0)\), the NOT gate \(|l\rangle \rightarrow |l \oplus 1\rangle\), \(l = 0, 1\), can be implemented. The Hadamard gate \(|l\rangle \rightarrow \frac{1}{\sqrt{2}} (|0\rangle + |l \oplus 1\rangle)\), \(l = 0, 1\), can be realized by setting \(\alpha = -\pi/2\) and \(\mathbf{n} = (0, 1, 0)\).

In the following section, we will compute the nonadiabatic geometric phase and further implement appropriate one-qubit gates for specific examples.

### 2.4. Examples

Let us first consider that a spin \(\frac{1}{2}\) system driven by a rotating magnetic field is described by the Hamiltonian (here we have set Bohr magneton \(\mu_B = \frac{1}{2}\) in the system of units)

\[
H(t) = B(t) \cdot \mathbf{S},
\] (20)

where \(B(t) = B_0 (\sin \alpha \cos \omega t, \sin \alpha \sin \omega t, \cos \alpha)\) with \(B_0 = \omega \cos \alpha\) and \(\alpha\) an arbitrarily real constant limited within the interval \([0, \frac{\pi}{2}]\). The explicit expression of magnetic field is obtained by choosing \(\theta = \frac{\pi}{2} + \alpha\) and \(\varphi(t) = \omega t\). Considering the overall evolution from \(t_0 = 0\) to \(t_f = \frac{\pi}{\omega}\), the integration presented in equation (14) gives rise to the nonadiabatic Berry phase \(\Phi_{\pm}(t_f, t_0) = \mp \pi (1 + \sin \alpha)\). It is seen that there are many possible one-qubit gates corresponding to different choices of real constant \(\alpha\). For instance, by setting \(\alpha = \frac{\pi}{2}\), the gate \(U = \frac{i}{\sqrt{2}} \sigma_z\) can be implemented.
For the second example, we consider the system is driven by a classical external field with

\[
\Omega_x(t) = \frac{\omega \sin^2 \omega t}{2\sqrt{1 - \sin^4 \frac{\omega t}{2}}} \left(1 - \frac{1}{2} \cos \omega t \left(1 + \sin^2 \frac{\omega t}{2}\right)\right),
\]

\[
\Omega_y(t) = -\frac{\omega \sin \omega t}{2\sqrt{1 - \sin^4 \frac{\omega t}{2}}} \left(1 - 2\sin^2 \frac{\omega t}{2}\right),
\]

\[
\Omega_z(t) = \omega \left(1 + \sin^2 \frac{\omega t}{2}\right) \cos^2 \frac{\omega t}{2}.
\]

The above expression is obtained by setting \( \theta(t) = \arccos(\sin^2 \frac{\omega t}{2}) \) and \( \varphi(t) = \omega t \) in equation (8). The orientation of \( I(t) \) goes from \( (\theta, \varphi) = (\frac{\pi}{2}, 0) \) at \( t_0 = 0 \) to \( (\theta, \varphi) = (0, \pi) \) at \( t = \frac{\pi}{2} \), and then returns to the initial orientation \( (\theta, \varphi) = (\frac{\pi}{2}, 2\pi) \) at \( t = \frac{\pi}{2} \). To the process, the geometric phase can be worked out to be \( \Phi^d_{\theta}(t_0, t_0) = \pm \frac{\pi}{2} \). Up to an overall phase factor \( e^{-i\pi} \), the NOT gate \( |\rangle \rightarrow |\bar{\rangle} \), \( l = 0, 1 \), can be implemented. It is mentioned that, the Z gate is also realized by setting \( \theta(t) = \arccos(\sin^2 \frac{\omega t}{2}) \) and \( \varphi(t) = \pi - \omega t \) with \( \omega t \in [-\pi, \pi] \). Correspondingly, the pulse parameters should be modulated as \( \Omega(t) = (\Omega_x(t), -\Omega_y(t), -\Omega_z(t)) \).

### 2.5. The effects in the presence of the systematic error and dissipation

Consider that a two-level system with energy gap \( \omega_0 \) is driven by a classical external field \( E(t) = E_0(t) \cos \left[ \int_0^t \omega(t') dt' + \phi(t) \right] \) with time-dependent amplitude \( E_0(t) \), frequency \( \omega(t) \) and phase \( \phi(t) \).

The Hamiltonian of the system in interaction picture reads

\[
H(t) = \frac{1}{2} \{-\Omega(t) \cos \phi(t) \sigma_x + \Omega(t) \sin \phi(t) \sigma_y + \Delta(t) \sigma_z\},
\]

with the Rabi frequency \( \Omega(t) = \langle 0 | -d \cdot E(t) |1 \rangle \) (\( d \) is the atomic transition dipole moment) and the detuning \( \Delta(t) = \omega - \omega_0 \). Compared the above expression of Hamiltonian with equation (8), one can see that the Rabi frequency and the detuning are also corresponding to \( \Omega(t) = \sqrt{\Omega_x(t)^2 + \Omega_y(t)^2} \) and \( \Delta(t) = \Omega_z(t) \), and thus the exact driven external field \( E(t) \) can be subtly designed according to the prescribed \( \Omega_{x,y,z} \). An ideal cyclic evolution of a two-level system can implement arbitrary one-qubit gate with 100% fidelity if does not exist two qualitatively different sources of errors. One is systematic error which stems from the imperfect control quantities such as the Rabi frequency \( \Omega(t) \), the detuning \( \Delta(t) \) and the phase characterized as \( \phi(t) = \arccos \left( \frac{\Omega_z(t)}{\Omega_{x,y,z}} \right) \) \( (i = x, y, z) \). The other is dissipation of open system due to the interaction with surrounding environment. In this section, we will explore the impact on the system in the presence of the systematic error and dissipation.

The system with the Hamiltonian represented as equation (22) will evolve along a prescribed path characterized by the parameters \( \{\Omega(t), \Delta(t), \phi(t)\} \) or \( \{\theta(t), \varphi(t)\} \). We first consider the effects the polar angle deviation \( \delta\varphi = \varphi'(t) - \varphi(t) \) on the Rabi frequency, detuning and phase of the driven two-level system. Here the small quantity \( \delta\varphi \) is assumed as constant during the overall evolution due to the parameter fluctuating slowly as compared to the gate operation. Applying \( \varphi'(t) \) into equation (8), the pulse parameters become

\[
\Omega_x'(t) = \Omega_x(t) \cos \delta\varphi - \Omega_y(t) \sin \delta\varphi,
\]

\[
\Omega_y'(t) = \Omega_x(t) \sin \delta\varphi + \Omega_y(t) \cos \delta\varphi,
\]

\[
\Omega_z'(t) = \Omega_z(t).
\]

This result shows that the Rabi frequency and the detuning are robust against the deviation of the parameter \( \varphi(t) \) due to \( \Omega'(t) = \Omega(t) \) and \( \Delta'(t) = \Delta(t) \). The geometric phase in equation (14) is also immune to this deviation for \( \phi'(t) = \varphi(t) \). Nevertheless, it leads to the imperfect control the phase \( \phi(t) \) of the driven field owing to

\[
\cos \varphi'(t) = \cos \phi(t) \cos \delta\varphi - \sin \phi(t) \sin \delta\varphi,
\]

where \( \varphi'(t) = \phi(t) + \delta\phi \) leads to the relation \( \delta\phi = \delta\varphi \). It reveals that the systematic error of the phase can be completely reflected by the deviation of control parameter \( \varphi(t) \).

To proceed, only with the system error \( \delta\phi \) being included, the real evolution is then depicted by an imperfect operator \( V = e^{-i\varphi'(t)/2} \) with erroneous rotation axis \( \mathbf{n}' = n'(\theta, \varphi', \delta\phi) \), which yields the imperfect effect on the desired geometric quantum control. To characterize the influence of the systematic error \( \delta\phi \) on gate operations, one defines the fidelity [35, 36]

\[
F_s = \frac{1}{2} \text{Tr}(VU^\dagger),
\]

where \( U = e^{i\pi \varphi(t)/2} \dagger \).
to evaluate the overlap of the operator $V$ and an ideal operator $U$ in equation (19). The gate fidelity is then calculated to be

$$F_s = 1 - \frac{1}{2} \sin^2 \delta \phi \sin^2(\delta \phi)^2.$$  \hfill (26)

Here we have used the approximations $\sin x \approx x$, $\cos x \approx 1 - \frac{1}{2}x^2$ as $x \ll 1$ and neglected no less than third order small quantities. It is seen that the fidelity takes the maximum as $F_s = 1$ at $\delta = 0$, and a minimum fidelity $F_s = 1 - \frac{1}{2}(\delta \phi)^2$ at $\Phi = \theta = \frac{\pi}{2}$. Thus, the one-qubit gate is robust to first order in error in phase $\delta \phi(t)$ or parameter $\varphi(t)$.

To reveal the sensitivity to the systematic error of the phase, we compare our scheme with nonadiabatic non-Abelian geometric gates $U_B = -\sin \theta \cos \varphi \sigma_x - \sin \theta \sin \varphi \sigma_y + \cos \theta \sigma_z$ [21] and the dynamical gates $U_\Gamma = -i\sin \Phi \cos \varphi \sigma_x - i\sin \Phi \sin \varphi \sigma_y + \cos \Phi \sigma_z$ [39]. By employing $\varphi' = \varphi + \delta \varphi$ and the equation (25), the corresponding fidelities are calculated to be $F_B = 1 - \frac{1}{2} \sin^2 \Phi(\delta \phi)^2$ and $F_\Gamma = 1 - \frac{1}{2} \sin^2 \theta(\delta \phi)^2$. It indicates that, with the same value $\theta = \bar{\theta}$ and $\Phi = \bar{\Phi}$, the geometric gates we constructed are more robust against the systematic error of the phase than the above gate implementations.

Furthermore, we show that the evolution is still purely geometric although the system does not completely achieve the target state. In the presence of the systematic error of the phase, the invariant can be written as

$$I'(t) = \frac{1}{2} R'(t) \cdot \sigma,$$  \hfill (27)

with $R'(t) = (\sin \theta(t) \cos \varphi'(t), \sin \theta(t) \sin \varphi'(t), \cos \theta(t))$ and $\varphi'(t) = \varphi(t) + \delta \varphi$. With $\Omega'(t) = (\Omega'_x(t), \Omega'_y(t), \Omega'_z(t))$ represent in equation (23) being considered, it is easily verified that the constraint condition of GQC $R'(t) \cdot \Omega'(t) = 0$ is still guaranteed during the implementation of the gate. Meanwhile, it is remarkable that the error is independent of the angular speed of the evolving state vector or operation time of the gate.

In realistic systems the noise due to the surrounding environment can also affect the fidelity. To investigate the noise effect on the non-adiabatic geometric quantum gate represented in equation (19), we focus on a spin system interaction with its fermionic reservoir [37] in the presence of phase damping noise within the Markovian regime. The evolution of the system is modeled by the Lindblad master equation [38]

$$\frac{\partial \rho(t)}{\partial t} = -i[H(t), \rho(t)] + \sum_i (\Gamma_i \rho(t) \Gamma_i^\dagger - \frac{1}{2} \Gamma_i^\dagger \Gamma_i \rho(t) - \frac{1}{2} \rho(t) \Gamma_i^\dagger \Gamma_i)$$  \hfill (28)

in which $\rho(t)$ is the density operator of the spin system and $\Gamma_i = \sqrt{\gamma_i} \sigma_i$ is the Lindblad operator with $\gamma_i(i = x, y, z)$ accounting for the damping rate of the corresponding phase flip process. The pulse parameters $\Omega_{x,y,z}(t)$ is specified by equation (21) to implement non-adiabatic NOT gate.

To characterize the influence of the noise on the dynamical evolution, one introduce the fidelity

$$F(t) = \{|\psi(t)\rangle |U(t)\rho(t)U^\dagger(t)|\psi(t)\rangle\},$$

where $U(t)$ is given explicitly in equation (17) and the input state takes the form $|\psi\rangle = \cos \mu |0\rangle + \sin \mu |1\rangle$ with $\mu$ uniformly distributed over the range of $[0, \frac{\pi}{2}]$. We compute numerically the fidelity for both the random spin flip process with $\gamma_x = \gamma_y = \gamma_z = \gamma$ and the pure dephasing process with $\gamma_x = \gamma_y = 0, \gamma_z = \gamma$, as illustrated in figure 1(a).
Here we have employed the following experimental parameters: the time duration of the gate is set as \( \tau_c = 40 \pi \) ns, the sweep frequency is taken as \( \omega = 5 \times 10^7 \) Hz and the dephasing rate is chosen as \( \gamma = 5 \) kHz for the electron spin in nitrogen-vacancy color centers in diamond [40]. The fidelities of NOT gate can reach about \( F(\tau_c) = 99.99\% \) for the pure dephasing process and \( F(\tau_c) = 99.97\% \) for the random spin flip process, respectively.

3. Realization of two-qubit gate along nonadiabatic passage

To implement an arbitrary unitary operation on the state space of \( n \) qubits, a two-qubit entangling gate together with arbitrary one-qubit gates should be constructed to complete the universal set. We now design nonadiabatic geometric controlled-U gate by utilizing a system consisted of a pair of coupled spin subsystems. To this goal, we assume that the system undergoes dynamical evolution with the following time evolution operator

\[
\tilde{U}(t, t_0) = \frac{1}{2}(I^i + \sigma^i_z) \otimes I^j + \frac{1}{2}(I^i - \sigma^i_z) \otimes U(t, t_0),
\]

where the identity operator \( I \) and unitary operator \( U(t, t_0) \) represented as equation (17) acting on the vectors in two-dimensional Hilbert subspace spanned by the basis \( \{ |0\rangle, |1\rangle \} \) of the second spin correspond to the states of first spin being set \( |0\rangle \) and \( |1\rangle \), respectively. The condition \( U(t_f, t_0) = U \) is met for the overall evolution over one period \( t \in [t_0, t_f] \). Due to the time evolution operator \( \tilde{U}(t, t_0) \) and corresponding Hamiltonian \( H(t) \) satisfying \( \tilde{H}(t) = i[\tilde{U}(t, t_0)\tilde{U}^\dagger(t, t_0), \) one has

\[
\tilde{H}(t) = \frac{1}{2}(I^i - \sigma^i_z) \otimes H(t).
\]

As we have discussed in section 2, a two-level system with Hamiltonian \( H(t) = \frac{1}{2}\Omega(t) \cdot \sigma^{(2)} \) and \( \Omega(t) \) satisfying equations (8) and (11), which undergoes exact cyclic evolution along pre-described closed curve \( L \) depicted by \( \{ \theta(t), \varphi(t) \} \) in the parameter space, can implement arbitrary qubit operation. For example, setting \( \theta(t) = \arccos(\sin^2 \frac{t}{\Omega}) \) and \( \varphi(t) = \omega t \) with \( \omega t \in [0, 2\pi] \) in equation (18) leads to \( U(2\pi/\omega, 0) = \sigma_x \), and thus the CNOT gate can be implemented. The corresponding pulse parameters are shown in equation (21).

We further test the performance of CNOT gate, consider the decoherence effect on two coupled spin systems by applying the master equation

\[
\frac{\partial \rho(t)}{\partial t} = -i[H(t), \rho(t)] + \sum_{ij} (\Gamma^i_0 \rho(t) \Gamma^j_0) - \frac{1}{2} \Gamma^i_0 \Gamma^j_0 \rho(t) - \frac{1}{2} \rho(t) \Gamma^j_0 \Gamma^i_0,
\]

where \( \Gamma^i_0 = \sqrt{\gamma_i} \sigma^i_z \otimes I^j \) and \( \Gamma^j_0 = \sqrt{\gamma_j} I^i \otimes \sigma^j_z \) are Lindblad operators with \( \gamma_i(i = x, y, z; j = 1, 2) \) accounting for the damping rate of the corresponding phase flip process of the \( j \)th spin system. Similar to the single-qubit case, we introduce two-qubit gate fidelity \( F_2(t) = |\langle \psi_2 | \tilde{U}^\dagger(t) \rho(t) \tilde{U}(t) | \psi_2 \rangle| \), where the initial state is characterized as \( |\psi_2 \rangle = \cos \alpha_1 |00\rangle + \sin \alpha_1 \sin \alpha_2 \cos \alpha_3 |01\rangle + \sin \alpha_1 \sin \alpha_2 \sin \alpha_3 |10\rangle + \sin \alpha_1 \cos \alpha_2 |11\rangle \) with parameters \( \alpha_1, \alpha_2 \in [0, 2\pi] \) and \( \alpha_3 \in [0, \pi] \) evenly distributed over the corresponding interval. Realistically, we still set the sweep frequency as \( \omega = 5 \times 10^7 \) Hz, the time duration of the gate as \( \tau_c = 40\pi \) and the dephasing rate as \( \gamma = 5 \) kHz. After numerical calculation, the fidelities of CNOT gate can reach about 99.92\% for the pure dephasing process with \( \gamma^c_4 = \gamma^c_5 = \gamma^c_7 = \gamma \) and 99.71\% for the random spin flip process with \( \gamma^c_4 = \gamma^c_5 = 0, \gamma^c_7 = \gamma \), respectively. The dynamics of gate fidelity is shown in figure 1(b).

4. Conclusion

In summary, we have inverse designed the general form of time-dependent Hamiltonian of one-qubit and two-qubit systems. The Schrödinger equation of the systems can be solved exactly by virtue of presupposition owning of L–R dynamical invariant. While serving as a protocol for nonadiabatic GQC, our scheme is shown to implement an arbitrary unitary operation on the state space of \( n \) qubits and possess the following distinct advantages: (1) no auxiliary time-dependent basis or state is involved; (2) only the diagonal elements of the Hamiltonian in the instantaneous eigenstate of \( H(t) \) are required to vanish, which relaxes the constraint on the driving Hamiltonian; (3) a driven two-level system which undergoes only single loop evolution in Bloch space can realize a universal set of one-qubit gates, hence it is readily achievable for experimental implementation; and (4) arbitrary one-qubit gate can be realized with high fidelity against systematic error and dephasing.
ORCID iDs

Wei Li  https://orcid.org/0000-0001-8342-1000

References

[1] Neilsen M A and Chuang I L 2000 Quantum Computation and Quantum Information (Cambridge: Cambridge University Press) p 279
[2] Zanardi P and Rasetti M 1999 Holonomic quantum computation Phys. Lett. A 264 94
[3] Aharonov Y and Anandan J 1987 Phase change during a cyclic quantum evolution Phys. Rev. Lett. 58 1593
[4] Sjöqvist E 2008 A new phase in quantum computation Physics 135
[5] Chiara G D and Palma G M 2003 Berry phase for a spin 1/2 particle in a classical fluctuating field Phys. Rev. Lett. 91 090404
[6] Zhu S L and Zanardi P 2005 Geometric quantum gates that are robust against stochastic control errors Phys. Rev. A 72 020301(R)
[7] Filipp S, Klepp J, Hasegawa Y, Plonka-Spehr C, Schmidt U, Gelenterp B and Rauch H 2009 Experimental demonstration of the stability of Berry’s phase for a spin-1/2 particle Phys. Rev. Lett. 102 030404
[8] Berger S, Pechal M, Abudumalikov A A, Eichler C, Steffen L, Fedorov A, Wallraff A and Filipp S 2013 Exploring the effect of noise on the Berry phase Phys. Rev. A 87 060303(R)
[9] Jones J A, Vedral V, Ekert A and Castagnoli G 2000 Geometric quantum computation using nuclear magnetic resonance Nature 403 869
[10] Duan L-M, Cirac J I and Zoller P 2001 Geometric manipulation of trapped ions for quantum computation Science 292 1695
[11] Wu L-A, Zanardi P and Lidar D A 2005 Holonomic quantum computation in decoherence-free subspaces Phys. Rev. Lett. 95 130501
[12] Chen X, Lizuain I, Ruschhaupt A, Guéry-Odelin D and Muga J G 2010 Shortcut to adiabatic passage in two- and three-level atoms Phys. Rev. Lett. 105 123003
[13] del Campo A 2013 Shortcuts to adiabaticity by counterdiabatic driving Phys. Rev. Lett. 111 100502
[14] Demirplak M and Rice S A 2003 Adiabatic population transfer with control fields J. Phys. Chem A 107 9937
[15] Berry M V 2009 Transitionless quantum driving J. Phys. A: Math. Theor. 42 365303
[16] Schaff F, Song X L, Vignolo P and Labevec G 2010 Fast optimal transition between two equilibrium states Phys. Rev. A 82 033430
[17] del Campo A and Sen Gupta K 2015 Controlling quantum critical dynamics of isolated systems Eur. Phys. J. Spec. Top. 224 189
[18] Zhang J et al 2013 Experimental implementation of assisted quantum adiabatic passage in a single spin Phys. Rev. Lett. 110 240501
[19] Sun Z, Zhou L, Xiao G, Poletti D and Gong J 2016 Finite-time Landau–Zener processes and counterdiabatic driving in open systems: beyond Born, Markov, and rotating-wave approximations Phys. Rev. A 93 012121
[20] Wólczek F and Zee A 1984 Appearance of Gauge structure in simple dynamical systems Phys. Rev. Lett. 52 2111
[21] Sjöqvist E, Tong D M, Mauritz Andersson L, Hessmo B, Johansson M and Singh K 2012 Non-adiabatic holonomic quantum computation New J. Phys. 14 103035
[22] Xu G F, Zhang J, Tong D M, Sjöqvist E and Kwek L C 2012 Nonadiabatic holonomic quantum computation in decoherence-free subspaces Phys. Rev. Lett. 109 170501
[23] Herterich E and Sjöqvist E 2016 Single-loop multiple-pulse nonadiabatic holonomic quantum gates Phys. Rev. A 94 052310
[24] Xu G F, Zhao P Z, Xing T H, Sjöqvist E and Tong D M 2017 Composite nonadiabatic holonomic quantum computation Phys. Rev. A 95 032311
[25] Liu B-J, Song X-K, Xue Z-Y, Wang X and Yang-M-H 2019 Plug-and-Play approach to nonadiabatic geometric quantum gates Phys. Rev. Lett. 123 100503
[26] Berry M V 1984 Quantal phase factors accompanying adiabatic changes Proc. R. Soc. A 392 45
[27] Lewis H R and Riesenfeld W B 1969 An exact quantum theory of the time-dependent harmonic oscillator and of a charged particle in a time-dependent electromagnetic field J. Math. Phys. 10 1458
[28] Zhao P J, Li W, Cao H, Yao S W and Cen L X 2018 Exotic dynamical evolution in a secant-pulse-driven quantum system Phys. Rev. A 98 022136
[29] Chen X, Ruschhaupt A, Schmidt S, del Campo A, Guéry-Odelin D and Muga J G 2010 Fast optimal frictionless atom cooling in harmonic traps: shortcut to adiabaticity Phys. Rev. Lett. 104 063602
[30] Chen X and Muga J G 2012 Engineering of fast population transfer in three-level systems Phys. Rev. A 86 033405
[31] Martinez-Garaot S, Torrontegui E, Chen X and Muga J G 2014 Shortcuts to adiabaticity in three-level systems using Lie transforms Phys. Rev. A 89 035408
[32] Torrontegui E, Martinez-Garaot S and Muga J G 2014 Hamiltonian engineering via invariants and dynamical algebra Phys. Rev. A 89 043408
[33] Wang Y, Ding Y, Wang J and Chen X 2020 Digital quantum simulation of nonadiabatic geometric gates via shortcuts to adiabaticity Entropy 22 1175
[34] Li S, Chen T and Xue Z Y 2020 Fast holonomic quantum computation on superconducting circuits with optimal control Adv. Quantum Technol. 3 20200001
[35] Dawson C M, Haselgrove H L and Nielsen M A 2006 Noise thresholds for optical cluster-state quantum computation Phys. Rev. A 75 052306
[36] Wang X, Yu C-S and Yi X X 2008 An alternative quantum fidelity for mixed states of qubits Phys. Lett. A 373 58
[37] Yamada N, Sakuma A and Tsujiura H 2007 Decoherence processes of a quantum two-level system coupled to a fermionic environment J. Appl. Phys. 101 09C110
[38] Lindblad G 1976 On the generators of quantum dynamical semigroups Commun. Math. Phys. 48 119
[39] Zheng S B, Yang C P and Nori F 2016 Comparison of the sensitivity to systematic errors between nonadiabatic non-Abelian geometric gates and their dynamical counterparts Phys. Rev. A 93 032313
[40] Buluta I, Ashhab S and Nori F 2011 Natural and artificial atoms for quantum computation Rep. Prog. Phys. 74 104401