Noncyclic geometric quantum computation in a nuclear-magnetic-resonance system

Z. S. Wang, G. Q. Liu, and Y. H. Ji

College of Physics and Communication Electronics, Jiangxi Normal University, Nanchang 330022, People's Republic of China and Key Laboratory of Optoelectronic and Telecommunication of Jiangxi, Nanchang, Jiangxi 330022, People's Republic of China

(Received 28 December 2008; published 1 May 2009)

A scheme is proposed to include both cyclic and noncyclic geometric quantum computations in nuclear-magnetic-resonance system by the invariant theory. By controlling magnetic field and arbitrary parameters in the invariant operator, the phases accumulated in the entangling quantum gates for single- and two-qubit systems are pure geometric phases. Thus, fault tolerance may occur in some critical magnetic field parameters for either cyclic or noncyclic evolution by differently choosing for gate time.

DOI: 10.1103/PhysRevA.79.054301 PACS number(s): 03.67.Lx, 03.65.Vf, 03.65.Yz

Geometric quantum computation is built in fault-tolerant quantum gates by using geometric phase shifts. A geometric quantum gate can be achieved by using only adiabatic evolution [1]. However, it is difficult to experimentally realize quantum computation with the adiabatic evolution because a long operation time is required [2–4]. This is especially true given that the evolution has to be repeated several times in order to cancel the dynamical phase. Decoherence is the most important limiting factor for quantum computation because its effect is that quantum superpositions decay into statistical mixtures [5]. It may be better, therefore, to construct geometric quantum gates by using the nonadiabatic geometric phase [6–9] since this allows for shortening gate times.

It is worth noting that the nonadiabatic evolutions result in errors that typically destroy cyclicity so as to cause the evolutions for which the conventional theory of the nonadiabatic geometric phase fails to apply [10,11]. Therefore, it is interesting in extending our studies to the noncyclic geometric computation [12–14]. Such extension may be helpful in the design of geometric quantum gates due to an enhanced flexibility in choice of evolutions. It also avoids the problems about some types of errors that do not preserve cyclicity and therefore may be conceptually useful in that it makes possible to analyze the fault tolerance associated with such errors [15–17].

In the conventional theory for quantum computation, the total phase between the final and initial states is a sum of the geometric and dynamical phases. In some methods of geometric quantum computation, it is necessary to remove or control the dynamical component. In noncyclic case, the phase shifts are usually nonlinear, so that it is difficult to achieve a built-in geometric quantum gate, especially, for the two-qubit entangling quantum gate [16].

In a real quantum system, a useful tool to solve Schrödinger equation is the theory of dynamical invariant to treat time-dependent Hamiltonian [18–20]. Indeed, the dynamically invariant theory was recently used in a proposal of implementation of cyclic geometric quantum gates [21,22]. In the present work, a scheme is proposed to implement quantum gates based on noncyclic geometric phases by the invariant theory, which is a generalization of the results in cyclic Aharanov-Anandan phase. We show that both single- and two-qubit geometric gates may be achieved by a unified scheme which is valid in both cyclic and noncyclic evolutions, and the dynamic phases could be cancelled by appropriately choosing the parameters of the applied magnetic field in nuclear-magnetic-resonance (NMR) system.

Let us start from a dynamically invariant theory. The Hermitian invariant $I(t)$ operator satisfies

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

where $H(t)$ is Hamiltonian of the system. It is known that $I(t)$ is one of the complete set of commuting observables, so that there exists a complete set of eigenstates of $I(t)$ [18–20]. Furthermore, $I(t)$ should not involve in time-derivative operators because $\frac{dI(t)}{dt}=\frac{\partial I(t)}{\partial t}-i[I(t),H(t)]=0$. The nondegenerate eigenvalue equation of the time-dependent invariant operator is given by

$$I(t)|\lambda_n,t\rangle = \lambda_n|\lambda_n,t\rangle, \tag{2}$$

which is used to construct the solution of Schrödinger equation because the eigenstate, $|\lambda_n,t\rangle$, is also the eigenstates of Hamiltonian $H(t)$. Thus,

$$|\psi(t)\rangle = \sum_n c_n \exp\left[i\int_0^t dt\langle\lambda_n,t|i\frac{\partial}{\partial t} - H(t)|\lambda_n,t\rangle\right]|\lambda_n,t\rangle, \tag{3}$$

where c_n do not depend on the involving time. The first term in the phase is a geometric phase and the second term is a dynamical phase.

Consider the Hamiltonian for a single-qubit system in NMR system; we have

$$H(t) = -\frac{1}{2}\Omega_0(\sigma_x \sin\theta\cos\omega t + \sigma_y \sin\theta\sin\omega t) - \frac{1}{2}\Omega_1\sigma_z\cos\theta, \tag{4}$$

where $\Omega_i = g(\mu)B_i/\hbar$ with $g(\mu)$ are the gyromagnetic, B_i ($i=1,2$) and θ act as the external controllable parameters and can be experimentally changed, and σ_i ($i=x,y,z$) are the Pauli operators.

It is known that any 2×2 matrix may be expanded by a unit $1_{2\times2}$ and three Pauli matrices. Thus, the invariant operator may be constructed by

$$I(t) = b_0(t) + b_x(t)\sigma_x + b_y(t)\sigma_y + b_z(t)\sigma_z, \tag{5}$$

where $b_0(t)$, $b_x(t)$, $b_y(t)$, and $b_z(t)$ are expansion coefficients and will be determined by the invariant equation.

Inserting Eqs. (4) and (5) into Eq. (1), we find that $\dot{b}_0 =0$, $b_x(t)=\omega_0 \cos \omega t$, $b_y(t)=\omega_0 \sin \omega t$, and $b_z(t)=\omega_1$ with $\omega_1=\Omega_1 \cos \theta+\omega$ and $\omega_0=\Omega_0 \sin \theta$. Furthermore, its eigenvalues may be obtained by $\lambda_{\pm}=b_0\pm\sqrt{\omega_0^2+\omega_1^2}$ with corresponding eigenvectors $|\lambda_+,t\rangle=\cos\frac{\chi}{2}|0\rangle+e^{i\omega t}\sin\frac{\chi}{2}|1\rangle$ and $|\lambda_-,t\rangle=-\sin\frac{\chi}{2}|0\rangle+e^{i\omega t}\cos\frac{\chi}{2}|1\rangle$, respectively, where $\chi =2 \arctan \omega_0/(\omega_1+\sqrt{\omega_0^2+\omega_1^2})$. Using these eigenvectors, the corresponding geometric phases in the region of $[0,\tau]$ may be expressed as [20–22]

$$\gamma_{\pm}^{g} = -\frac{\omega\tau}{2}(1 \mp \cos \chi), \tag{6}$$

where τ is gate operation time, for the cyclic geometric phase $\tau=2\pi/\omega$, and the dynamical phases are given by

$$\gamma_{\pm}^{d} = \pm\frac{\tau}{2}\delta, \tag{7}$$

where $\delta=\omega_2 \cos \chi+\omega_0 \sin \chi$ with $\omega_2=\Omega_1 \cos \theta$.

It is noted that χ, ω_0, and ω_2 are functions of Ω_i ($i=1,2$) and θ. In the geometric quantum computation, we may adjust these external controllable parameters to satisfy the following relations:

$$(\omega_2 \cos \chi + \omega_0 \sin \chi) = 2k\omega, \tag{8}$$

where $k=0$ for both the noncyclic and cyclic cases and $k=1,2,\ldots$, only for the cyclic case. When $k=0$, the dynamical phases $\gamma_+^d=\gamma_-^d=0$. This means that the physical system is at dark state. Under the case, it is adapted to implement both the cyclic and noncyclic geometric quantum computations by operating gate timing. Under condition (8), according to Eq. (3), the wave function for single-qubit system may be expressed as

$$\psi(t) = c_+e^{i\gamma_+^g}|\lambda_+,t\rangle + c_-e^{i\gamma_-^g}|\lambda_-,t\rangle, \tag{9}$$

which implies that a pair of orthogonal states $|\lambda^{\pm},t\rangle$ can evolve in terms of the relations $u(\tau)|\lambda_{\pm},t=0\rangle =\exp[i\gamma_{\pm}^g(\tau)]|\lambda_{\pm},t=\tau\rangle$, where $u(\tau)$ is a unitary transformation. Thus an arbitrary initial state can be expressed as $|\psi_i\rangle =c_+|\lambda_+,t=0\rangle+c_-|\lambda_-,t=0\rangle$ with $c_{\pm}=\langle\lambda_{\pm},t=0|\psi_i\rangle$. According to Eq. (9), the final state at time τ is calculated as $|\psi_f\rangle =c_+e^{i\gamma_+^g(\tau)}|\lambda_+,t=\tau\rangle+c_-e^{i\gamma_-^g(\tau)}|\lambda_-,t=\tau\rangle$. Under the computational basis $\{|0\rangle,|1\rangle\}$, the unitary matrix $u(\gamma_+^g,\gamma_-^g,\tau)$, between the input and output states, can be written as

$$u(\gamma_+^g,\gamma_-^g,\tau) = \begin{pmatrix} a_1 & b \\ b & a_2 \end{pmatrix}, \tag{10}$$

where $a_1=e^{i\gamma_+^g}\cos^2\frac{\theta}{2}+e^{i\gamma_-^g}\sin^2\frac{\theta}{2}$, $a_2=e^{i\gamma_+^g}\sin^2\frac{\theta}{2}+e^{i\gamma_-^g}\cos^2\frac{\theta}{2}$, and $b=\frac{1}{2}\sin\theta(e^{i\gamma_+^g}-e^{i\gamma_-^g})$. Differently from the cyclic geometric quantum gate for single-qubit system [23], Eq. (10) includes both the cyclic and noncyclic cases for the different gate timing τ. It is noted that there exists the relation $\gamma_+= -\gamma_- -\omega\tau$ between the geometric phases of the eigenstates. Substituting this relation into Eq. (10), one may simplify the quantum gates, so that the result actually recovers Berry's result $\gamma_+=-\gamma_-$ up to 2π under the adiabatic condition.

For two-qubit system in NMR, in order to simplify our computation but without loss of generality, we only consider the spin-spin coupling interaction between the target and control qubits. The total Hamiltonian is

$$H_{12}(t) = -\frac{1}{2}\Omega_0(\sigma_{1x}\sin\theta\cos\omega t+\sigma_{1y}\sin\theta\sin\omega t) -\frac{1}{2}\Omega_1\sigma_{1z}\cos\theta+\lambda\vec{\sigma}_1\cdot\vec{\sigma}_2, \tag{11}$$

where λ is the strength of the interaction between two qubits. According to the closed algebra theory and Eq. (1), the Hermitian invariant operator for the two-qubit system may be constructed as

$$I_{12}(t) = c_0+\Omega_0(\sigma_{1x}\sin\theta\cos\omega t+\sigma_{1y}\sin\theta\sin\omega t) +(\Omega_1\cos\theta+\omega)\sigma_{1z}+c_I\vec{\sigma}_1\cdot\vec{\sigma}_2, \tag{12}$$

where $\dot{c}_0=0$ and $\dot{c}_I=0$ are arbitrary constants and will be determined in the following.

Under the computational basis $\{|00\rangle,|01\rangle,|10\rangle,|11\rangle\}$, the invariant operator $I_{12}(t)$ may be rewritten as

$$I_{12}(t) = \begin{pmatrix} c_0+c_I+\omega_1 & 0 & \omega_0e^{-i\omega t} & 0 \\ 0 & c_0-c_I+\omega_1 & 2c_I & \omega_0e^{-i\omega t} \\ \omega_0e^{i\omega t} & 2c_I & c_0-c_I-\omega_1 & 0 \\ 0 & \omega_0e^{i\omega t} & 0 & c_0+c_I-\omega_1 \end{pmatrix}, \tag{13}$$

which has eigenvalues $\lambda_{1\pm}=c_0+c_I\pm\sqrt{\omega_0^2+\omega_1^2}$ and $\lambda_{2\pm}=c_0-c_I\pm\sqrt{4c_I^2+\omega_0^2+\omega_1^2}$. The corresponding eigenvectors are given by

$$|\lambda_{1+},t\rangle = \cos^2\frac{\chi}{2}|00\rangle+\frac{1}{2}e^{i\omega t}\sin\chi(|01\rangle+|10\rangle) +e^{2i\omega t}\sin^2\frac{\chi}{2}|11\rangle, \tag{14}$$

$$|\lambda_{1-},t\rangle = \sin^2\frac{\chi}{2}|00\rangle-\frac{1}{2}e^{i\omega t}\sin\chi(|01\rangle+|10\rangle) +e^{2i\omega t}\cos^2\frac{\chi}{2}|11\rangle, \tag{15}$$

$$|\lambda_{2\pm},t\rangle = \frac{1}{\sqrt{2}}\cos\alpha_{\pm}(|00\rangle -e^{2i\omega t}|11\rangle)\mp e^{i\omega t}\sin\alpha_{\pm}(\cos\beta_{\pm}|01\rangle-\sin\beta_{\pm}|10\rangle), \tag{16}$$

where $\alpha_{\pm}=\arccos\omega_0/\sqrt{2[(\sqrt{4c_I^2+\omega_0^2+\omega_1^2}\mp c_I)^2-c_I^2]}$ and $\beta_{\pm}=\arctan(\mp 2c_I\mp\omega_1+\sqrt{4c_I^2+\omega_0^2+\omega_1^2})/(\mp 2c_I\pm\omega_1 +\sqrt{4c_I^2+\omega_0^2+\omega_1^2})$.

Using these eigenvectors, the corresponding geometric phases may be expressed as

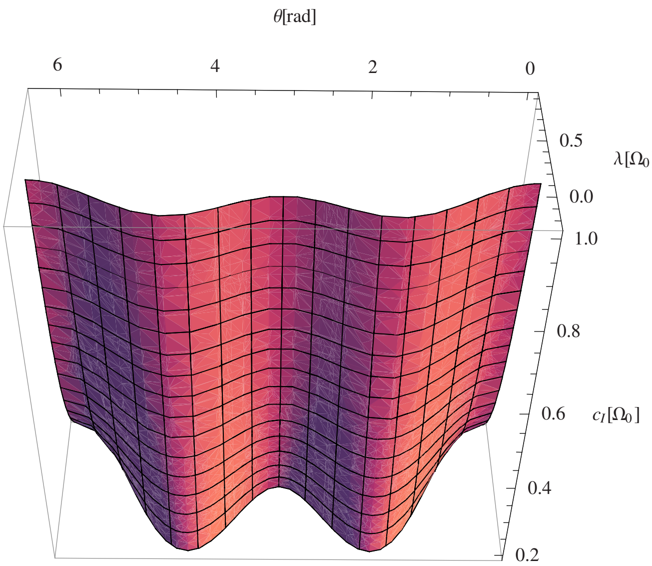

FIG. 1. (Color online) Invariant coupling constant c_I (for only $c_I \geq 0$) is shown as a function of θ and λ, where $\omega=\frac{1}{2}\Omega_0=\frac{1}{2}\Omega_1$ are taken and c_I and λ are in units of Ω_0. A similar situation is for $c_I < 0$.

$$\gamma^g_{1+}=2\gamma^g_+, \quad \gamma^g_{1-}=2\gamma^g_-, \quad \gamma^g_{2+}=\gamma^g_{2-}=-\omega\tau. \tag{17}$$

It is noted that the geometric phases for the two-qubit system are two times of the ones for the single-qubit system. In the cyclic evolution with $\tau=2\pi/\omega$, it is obvious that γ^g_{1+} and γ^g_{1-} are proportional to the area of Bloch sphere with the azimuthal angles $\theta=\chi$ and $\theta=\pi+\chi$, respectively, while $\gamma^g_{2+}=-2\pi$ and $\gamma^g_{2-}=-2\pi$ are -2 times of the area in the parameter space with the azimuthal angles $\theta=\pi/2$ and $\theta=3\pi/2$, respectively.

The dynamical phases may be obtained by

$$\gamma^d_{1\pm}=\tau\left(\lambda \pm \frac{1}{2}\delta\right), \tag{18}$$

$$\gamma^d_{2\pm}=\tau\Bigg[\lambda\cos 2\alpha_\pm - \frac{1}{2}\omega_2\sin^2\alpha_\pm\cos 2\beta_\pm \mp \frac{1}{2\sqrt{2}}\omega_0\sin 2\alpha_\pm(\cos\beta_\pm+\sin\beta_\pm) - 2\lambda\sin^2\alpha_\pm\sin 2\beta_\pm\Bigg]. \tag{19}$$

After choosing the external controllable parameters according to Eq. (8), we further set the arbitrary constant c_I to satisfy

$$8\lambda c_I - \omega_2\omega_1 + \frac{2\omega_0^2 c_I}{\sqrt{4c_I^2+\omega_0^2+\omega_1^2}}=0, \tag{20}$$

which leads to $\gamma^d_{2+}=\gamma^d_{2-}=\gamma^d_2$. From Fig. 1, we see that there exist, indeed, some physically meaningful solutions to Eq. (20).

It is noted that the eigenvectors $|\lambda_{1+},t\rangle$ and $|\lambda_{1-},t\rangle$ depend only on the magnetic field parameters while $|\lambda_{2+},t\rangle$ and $|\lambda_{2-},t\rangle$ are determined by both the magnetic field parameters and the constant c_I in invariant operator. Therefore, we may separate the system into two subspaces. Under conditions (8) and (20), thus, the wave functions may be expressed by

$$|\Psi_1(t)\rangle = c_{1+}e^{i\gamma^g_{1+}}|\lambda_{1+},t\rangle + c_{1-}e^{i\gamma^g_{1-}}|\lambda_{1-},t\rangle, \tag{21}$$

$$|\Psi_2(t)\rangle = e^{i(\gamma^g_2-\gamma^d_2)}(c_{2+}|\lambda_{2+},t\rangle + c_{2-}|\lambda_{2-},t\rangle), \tag{22}$$

where $e^{i(\gamma^g_2-\gamma^d_2)}$ may be regarded as an overall phase and dropped out in quantum computation. It is noted that $\langle\Psi_1(t)|\Psi_2(t)\rangle=0$. Therefore, the two subspaces are orthogonal. Thus, under the basis $\{|\lambda_{1+},t\rangle,|\lambda_{1-},t\rangle,|\lambda_{2+},t\rangle,|\lambda_{2-},t\rangle\}$, a geometric controlled-u gate may be expressed as

$$U(\tau)=\begin{pmatrix} u(\tau) & O \\ O & E \end{pmatrix}, \quad u(\tau)=\begin{pmatrix} e^{i\gamma^g_{1+}(\tau)} & 0 \\ 0 & e^{i\gamma^g_{1-}(\tau)} \end{pmatrix}, \tag{23}$$

where E and O represent the 2×2 unit and zero matrices, respectively. The controlled-u gate is either the cyclic geometric gate or the noncyclic one for the different gate time τ.

In terms of the computational basis $\{|00\rangle,|01\rangle,|10\rangle,|11\rangle\}$, where the first (second) bit represents the state of the target (control) qubit, the two initial states are $|\Psi_{1i}(0)\rangle=c_{1+}|\lambda_{1+},0\rangle+c_{1-}|\lambda_{1-},0\rangle$ and $|\Psi_{2i}(0)\rangle=c_{2+}|\lambda_{2+},0\rangle+c_{2-}|\lambda_{2-},0\rangle$ and the corresponding final states are $|\Psi_{1f}(\tau)\rangle=c_{1+}e^{i\gamma^g_{1+}(\tau)}|\lambda_{1+},\tau\rangle+c_{1-}e^{i\gamma^g_{1-}(\tau)}|\lambda_{1-},\tau\rangle$ and $|\Psi_{2f}(\tau)\rangle=c_{2+}|\lambda_{2+},\tau\rangle+c_{2-}|\lambda_{2-},\tau\rangle$, respectively. Inserting Eqs. (14)–(17) into $|\Psi_{1f}(\tau)\rangle$ and $|\Psi_{2f}(\tau)\rangle$, we find that the final states may be completely expressed by the geometric phases. Thus, the geometric unitary transformation $U(\gamma^g_{1\pm},\gamma^g_2,\tau)$ up to a relative phase factor, between the input and output states, can be written as

$$U(\gamma^g_{1\pm},\gamma^g_2,\tau)=\begin{pmatrix} u_{1+} & u'_{1+} & u'_{1-} & u_{1-} \\ u_{2+} & u'_{2+} & u'_{2-} & u_{2-} \\ u_{3+} & u'_{3+} & u'_{3+} & u_{3-} \\ u_{4+} & u'_{4+} & u'_{4-} & u_{4-} \end{pmatrix}, \tag{24}$$

where $u_{3k-2\pm}=\{\eta_{k+}\pm[\eta_{k-}-(u'_{3k-2+}+u'_{3k-2-})\sin\chi]/\cos\chi\}/2$ $(k=1,2)$, $u_{k+1\pm}=\{\eta_{0-}\pm[\eta_{0+}-(u'_{k+1+}+u'_{k+1-})\sin\chi]/\cos\chi\}/2$ $(k=1,2)$, $u'_{1\pm}=(b_\mp d_\pm+b_\pm a_\mp)/u$, $u'_{2\pm}=(\pm f_\mp d_\pm+f_\pm a_\mp)/u$, $u'_{3\pm}=(\mp h_\mp d_\pm\pm h_\pm a_\mp)/u$, and $u'_{4\pm}=(-p_\mp d_\pm-p_\pm a_\mp)/u$ with $\eta_{0\pm}=\sin\chi(e^{i(\gamma^g_{1+}-\gamma^g_2)}\pm e^{i(\gamma^g_{1-}-\gamma^g_2)})/2$, $\eta_{1\pm}=e^{i\gamma^g_{1+}}\cos^2\frac{\chi}{2}\pm e^{i\gamma^g_{1-}}\times\sin^2\frac{\chi}{2}$, $\eta_{2\pm}=e^{i(\gamma^g_{1+}-2\gamma^g_2)}\sin^2\frac{\chi}{2}\pm e^{i(\gamma^g_{1-}-2\gamma^g_2)}\cos^2\frac{\chi}{2}$, $a_\pm=\sin\alpha_\pm\cos\beta_\pm+\tan\chi/\sqrt{2}$, $d_\pm=\sin\alpha_\pm\sin\beta_\pm-\tan\chi/\sqrt{2}$, $b_\pm=(\cos\alpha_\pm-\eta_{1-}\cos\alpha_\pm/\cos\chi)/\sqrt{2}$, $f_\pm=e^{-i\gamma^g_2}\sin\alpha_\pm\times\cos\beta_\pm\pm\eta_{0+}\cos\alpha_\pm/(\sqrt{2}\cos\chi)$, $h_\pm=e^{-i\gamma^g_2}\sin\alpha_\pm\times\sin\beta_\pm\mp\eta_{0+}\cos\alpha_\pm/(\sqrt{2}\cos\chi)$, $p_\pm=(e^{-2i\gamma^g_2}\cos\alpha_\pm+\eta_{2-}\times\cos\alpha_\pm/\cos\chi)/\sqrt{2}$, and $u=d_+d_--a_+a_-$.

Thus, we achieve the entangling universal quantum gates based entirely on purely geometric operations. Geometric quantum computation demands that logical gates in computing are realized by using geometric phase shifts, so that it may have the built-in fault-tolerant advantage due to the fact that the geometric phases depend only on some global geometric features. As an example, we choose the parameters in terms of Eqs. (8) and (20) as $\Omega_0=\Omega_1$, $\omega=\Omega_0\sin\theta$

$-\Omega_1\cos\theta$, $c_I=-\Omega_0/2$, and $\lambda=0.034\Omega_0$, so that $\theta=3\pi/4$, $\chi=\pi/4$, $\alpha_+=81.58°$, $\beta_+=28.68°$, $\alpha_-=31.4°$, and $\beta_-=-75.36°$. Thus the elements of unitary transformation matrix (24) may be written as

$$u_{1+}=2.07-1.47e^{i\gamma_{1+}^g}+0.40e^{i\gamma_{1-}^g},$$

$$u'_{1+}=0.64-0.77e^{i\gamma_{1+}^g}+0.13e^{i\gamma_{1-}^g},$$

$$u'_{1-}=-4.79+5.78e^{i\gamma_{1+}^g}-0.99e^{i\gamma_{1-}^g},$$

$$u_{1-}=-2.07+2.33e^{i\gamma_{1+}^g}-0.25e^{i\gamma_{1-}^g},$$

$$u_{2+}=2.29e^{-i\gamma_2^g}-0.55e^{i(\gamma_{1+}^g-\gamma_2^g)}-0.91e^{i(\gamma_{1-}^g-\gamma_2^g)},$$

$$u'_{2+}=-0.78e^{-i\gamma_2^g}-0.43e^{i(\gamma_{1+}^g-\gamma_2^g)}-0.43e^{i(\gamma_{1-}^g-\gamma_2^g)},$$

$$u'_{2-}=-3.80e^{-i\gamma_2^g}+2.39e^{i(\gamma_{1+}^g-\gamma_2^g)}+2.39e^{i(\gamma_{1-}^g-\gamma_2^g)},$$

$$u_{2-}=2.29e^{-i\gamma_2^g}+0.91e^{i(\gamma_{1+}^g-\gamma_2^g)}+0.55e^{i(\gamma_{1-}^g-\gamma_2^g)},$$

$$u_{3+}=1.34e^{-i\gamma_2^g}-0.61e^{i(\gamma_{1+}^g-\gamma_2^g)}-0.96e^{i(\gamma_{1-}^g-\gamma_2^g)},$$

$$u'_{3+}=0.11e^{-i\gamma_2^g}-0.32e^{i(\gamma_{1+}^g-\gamma_2^g)}-0.32e^{i(\gamma_{1-}^g-\gamma_2^g)},$$

$$u'_{3-}=-2.80e^{-i\gamma_2^g}+2.39e^{i(\gamma_{1+}^g-\gamma_2^g)}+2.39e^{i(\gamma_{1-}^g-\gamma_2^g)},$$

$$u_{3-}=-1.34e^{-i\gamma_2^g}+0.96e^{i(\gamma_{1+}^g-\gamma_2^g)}+0.61e^{i(\gamma_{1-}^g-\gamma_2^g)},$$

$$u_{4+}=-2.07e^{-2i\gamma_2^g}-0.25e^{i(\gamma_{1+}^g-2\gamma_2^g)}+2.33e^{i(\gamma_{1-}^g-2\gamma_2^g)},$$

$$u'_{4+}=-0.64e^{-2i\gamma_2^g}-0.13e^{i(\gamma_{1+}^g-2\gamma_2^g)}+0.77e^{i(\gamma_{1-}^g-2\gamma_2^g)},$$

$$u'_{4-}=4.79e^{-2i\gamma_2^g}+0.99e^{i(\gamma_{1+}^g-2\gamma_2^g)}-5.78e^{i(\gamma_{1-}^g-2\gamma_2^g)},$$

$$u_{4-}=2.07e^{-2i\gamma_2^g}+2.04e^{i(\gamma_{1+}^g-2\gamma_2^g)}-1.47e^{i(\gamma_{1-}^g-2\gamma_2^g)},$$

We see that $U(\gamma_{1\pm}^g,\gamma_2^g,\tau)$ is a nontrivial geometric phase gate.

In conclusion, we have proposed a way to realize both the cyclic and noncyclic geometric computations based on the dynamical invariant theory, where the invariant operators are constructed by the closed algebra. For the cyclic geometric gate, the gate time is $\tau=2\pi/\omega$. For the noncyclic gate, the gate time is arbitrary. The idea of the noncyclic geometric gate may be helpful to reduce some errors from the gate timing operation. By controlling magnetic field and arbitrary parameters in the invariant operator, the phase accumulated in the entangling quantum gate is a pure geometric phase. Thus, the fault tolerance may occur in some critical magnetic field parameters for the NMR implementations of either noncyclic or cyclic geometric phase-shift gate in the single- and two-qubit systems.

In the conventional geometric gate, it is a big question how to remove the dynamical component by using some operations or dark states. The experimental errors are, obviously, increased because of the operational process. More worryingly, the dynamical phase accumulated in the gate operation for the entangled two-qubit system under the noncyclic evolution is possibly nonzero and cannot be eliminated. Our approach does not need any such process, which leads to a possible reduction in experimental errors as well as gate timing.

This work was supported by the National Natural Science Foundation of China under Grant No. 10864002.

[1] P. Zanardi and M. Rasetti, Phys. Lett. A **264**, 94 (1999).
[2] L. M. Duan, J. I. Cirac, and P. Zoller, Science **292**, 1695 (2001).
[3] G. Falci, R. Fazio, G. M. Palma, J. Siewert, and V. Vedral, Nature (London) **407**, 355 (2000).
[4] D. Leibfried *et al.*, Nature (London) **422**, 412 (2003).
[5] Z. S. Wang, L. C. Kwek, C. H. Lai, and C. H. Oh, Eur. Phys. J. D **33**, 285 (2005); Europhys. Lett. **74**, 958 (2006); Z. S. Wang, C. Wu, X. L. Feng, L. C. Kwek, C. H. Lai, and C. H. Oh, Phys. Rev. A **75**, 024102 (2007).
[6] Wang Xiang-Bin and M. Keiji, Phys. Rev. Lett. **87**, 097901 (2001).
[7] S. L. Zhu and Z. D. Wang, Phys. Rev. A **66**, 042322 (2002).
[8] Z. S. Wang, Chunfeng Wu, Xun-Li Feng, L. C. Kwek, C. H. Lai, C. H. Oh, and V. Vedral, Phys. Rev. A **76**, 044303 (2007).
[9] Xun-Li Feng, Z. S. Wang, Chunfeng Wu, L. C. Kwek, C. H. Lai, and C. H. Oh, Phys. Rev. A **75**, 052312 (2007).
[10] Y. Aharonov and J. Anandan, Phys. Rev. Lett. **58**, 1593 (1987).
[11] A. Blais and A.-M. S. Tremblay, Phys. Rev. A **67**, 012308 (2003).
[12] J. Samuel and R. Bhandari, Phys. Rev. Lett. **60**, 2339 (1988).
[13] N. Mukunda and R. Simon, Ann. Phys. (N.Y.) **228**, 205 (1993).
[14] A. Mostafazadeh, J. Phys. A **32**, 8157 (1999).
[15] E. Sjöqvist, Phys. Lett. A **286**, 4 (2001).
[16] A. Friedenauer and E. Sjöqvist, Phys. Rev. A **67**, 024303 (2003).
[17] S. L. Zhu and Z. D. Wang, Phys. Rev. Lett. **91**, 187902 (2003).
[18] H. R. Lewis and W. B. Riesenfeld, J. Math. Phys. **10**, 1458 (1969).
[19] H. R. Lewis, Jr., J. Math. Phys. **9**, 1976 (1968).
[20] Z. S. Wang, L. C. Kwek, C. H. Lai, and C. H. Oh, Phys. Scr. **75**, 494 (2007).
[21] L. B. Shao, Z. D. Wang, and D. Y. Xing, Phys. Rev. A **75**, 014301 (2007).
[22] Z. S. Wang, Phys. Rev. A **79**, 024304 (2009).
[23] S. L. Zhu and Z. D. Wang, Phys. Rev. Lett. **89**, 097902 (2002).