Nonadiabatic conditional geometric phase shift with NMR

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Abstract

A conditional geometric phase shift gate, which is fault tolerant to certain types of errors due to its geometric nature, was realized recently via nuclear magnetic resonance (NMR) under adiabatic conditions. By the adiabatic requirement, the result is inexact unless the Hamiltonian changes extremely slowly. However, in quantum computation, everything must be completed within the decoherence time. High running speed of every gate in quantum computation is demanded because the power of a quantum computer can be exponentially proportional to the maximum number of logic gate operations that can be made sequentially within the decoherence time. The adiabatic condition makes any fast conditional Berry phase (cyclic adiabatic geometric phase) shift gate impossible. Here we show that by using a newly designed sequence of simple operations with an additional vertical magnetic field, the conditional geometric phase shift gate can be run nonadiabatically. Therefore geometric quantum computation can be done

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at the same rate as usual quantum computation.

A fault-tolerant quantum logic gate [1] is the central issue in realizing the basic constituents of a quantum information processor. Quantum computation via the controlled geometric phase shift [2] provides a nice scenario to this purpose. Due to its geometric property, a geometric phase [3,4] shift can be robust with respect to certain types of operational errors. In particular, suppose that the spin(qubit) undergoes a random fluctuation about its path in the evolution. Then the final value of the geometric phase shift will not be affected provided that the random fluctuation does not change the total area [2].

Recently, it was reported [2,5–9] that the conditional Berry phase (adiabatic cyclic geometric phase) shift can be used in quantum computation. In particular, in ref [2], an experiment was done with NMR [10–14] under the adiabatic condition.

Demanding on both running speed and precision of every gate in a quantum computer is quite high. It has been reported recently that [2], due to the requirement of adiabatic condition, faster running speed causes severe distortions to the results [2]. The adiabatic condition makes the fast speed and high precision conflict each other in the conditional Berry phase shift gate. Increasing the running speed of the logic gate can exponentially increase the power of a quantum computation such as quantum factorization [15]. It seems that the geometric phase shift gate will only be practical if it can run at a speed comparable to that of the usual quantum gate. Therefore one is tempted to find an easy way to make the conditional geometrical phase shift through nonadiabatic state evolution. In this letter, we present an easy scheme to make the geometric phase shift nonadiabatically with NMR. We start from the exact control of the state evolution on a cone.

**Exact state evolution on the cone.** It is well known that a spin half nucleus can gain a geometric phase shift in the conical evolution. We now assume that the initial spin state is on the cone and we will demonstrate a method to make it evolve nonadiabatically. The
Hamiltonian for a spin in a constantly rotating magnetic field is

$$H(t) = \left[ \omega_0 \sigma_z + \omega_1 \sigma_x(t) \right]/2.$$  \hfill (1)

Here \( \sigma_x(t) = \begin{pmatrix} 0 & e^{-i\gamma t} \\ e^{i\gamma t} & 0 \end{pmatrix} \), \( \omega_0 \) is the amplitude of vertical field and \( \omega_1 \) is the amplitude of the horizontal field, which is rotating around \( z \)-axis in the constant angular speed \( \gamma \). The initial state \( |\psi_0\rangle \) is an eigenstate of \( H_0 = H(0) \). Explicitly, \( |\psi_0\rangle = \cos \frac{\theta}{2} |\uparrow\rangle + \sin \frac{\theta}{2} |\downarrow\rangle \), \( \cos \theta = \omega_0 / \sqrt{\omega_0^2 + \omega_1^2} \). To know the cause of the state distortion, we study the time evolution first.\(^1\) The similar idea has been used for the adiabatic rotational splitting with NQR previously.\(^1\)

The time evolution operator \( U \) generated by the Hamiltonian \( H_0 \) is determined by the time-dependent Schrödinger equation

$$i \frac{\partial}{\partial t} U_0 = H(t) U_0.$$  \hfill (2)

Solving this equation we obtain

$$U_0(t) = e^{i\gamma \sigma_z t} e^{-i(H_0 - \gamma \sigma_z/2)t}.$$  \hfill (3)

In particular, at time \( t = \tau = 2\pi/\gamma \), when the external field completes a \( 2\pi \) rotation, the state is evolved to

$$\psi(\tau) = e^{-i\pi - i(H_0 - \gamma \sigma_z/2)\tau} |\psi_0\rangle.$$  \hfill (4)

The adiabatic approximation assumes that at time \( \tau \), the state completes a cyclic evolution provided that \( \gamma \) is small. However, due to the decoherence time limitation, \( \gamma \) cannot be too small. The non-zero \( \gamma \) distorts the state in the evolution and makes it noncyclic at time \( \tau \). This non-zero \( \gamma \) in the adiabatic approximation causes two types of errors. One is that the noncyclic

\(^1\)We shall extend it to the case of arbitrary time-dependent rotating speed in the end of this section.
completion of the evolution at time $\tau$ will cause further errors in the succeeding operations in the sequence. (A sequence of operations is used to remove the dynamic phase in realizing the geometric quantum gate [2].) The other is that the geometric phase acquired over period $\tau$ is not $-\pi(1 - \cos \theta)$, as for the ideal adiabatic cyclic evolution.

Now we give an easy way to exactly control the state evolution on the cone. Here the external field can be rotated around $z$–axis arbitrarily fast. We use $|\psi_0\rangle$, the eigenstate of $H_0$ for the initial state. We switch on a static vertical magnetic field $\omega_z = \gamma$ while the external field is rotated around $z$–axis. In this way, the new time-dependent Hamiltonian is $H_W(t) = \frac{1}{2}[(\omega_0 + \gamma)\sigma_z + \omega_1\sigma_x(t)]$. The time evolution operator $U_W(t)$ generated by this Hamiltonian satisfies the Schrödinger equation

$$i\frac{\partial}{\partial t}U_W(t) = H_W(t)U_W(t)$$

with the boundary condition $U_W(0) = 1$. The state at time $t$ is related to the state at time 0 by $|\psi(t)\rangle = U_W(t)|\psi_0\rangle$, $\psi_0 = \psi(0)$. Denoting $R = e^{i\gamma t\sigma_z/2}$ we obtain the following equivalent equation

$$i\partial(RU_W)/\partial t = H_0(RU_W).$$

Noting that $H_0$ is time-independent therefore we have $RU_W(t) = e^{-iH_0t}$. This is equivalent to

$$U_W(t) = e^{-i\gamma t\sigma_z/2}e^{-iH_0t}.$$  

Consequently, at any time $t$, state $|\psi(t)\rangle = e^{-i\lambda t}e^{-i\gamma t\sigma_z/2}|\psi_0\rangle$ is exactly the instantaneous eigenstate of Hamiltonian $H(t)$, where $\lambda$ is the eigenvalue of $H_0$ for eigenstate $|\psi_0\rangle$. In particular, at time $\tau$, $|\psi(\tau)\rangle = e^{-i\pi-i\lambda \tau}|\psi_0\rangle$. It only differs to $|\psi_0\rangle$ by a phase factor. Note that the time evolution operator $U_W(t)$ here is generated by the Hamiltonian $H_W(t)$ instead of $H(t)$.

Here the additional vertical field $\gamma$ plays an important role. Without this field, the time evolution operator generated by $H(t)$ is
\[ U(t) = e^{-i\gamma \sigma_z / 2} e^{-iH_1 t} \]  

and \( H_1 = H_0 - \gamma \sigma_z / 2 \). Obviously, this time evolution operator \( U(t) \) will distort a qubit with the initial state \( |\psi_0\rangle \) in the evolution. But this \( U(t) \) can exactly control the qubit with the initial state \( |\psi_1\rangle \), the eigenstate of \( H_1 \). If initially we set the spin state to \( |\psi_1\rangle \), then the spin will evolve exactly on its cone without the additional field \( \gamma \). So, we have two ways to control the spin evolution exactly. We can use the additional field \( \gamma \), if the initial state is set to be \( |\psi_0\rangle \). Alternatively, we can also set the initial state to be \( |\psi_1\rangle \) and then we need not add any additional field when the external field is rotated. In this letter, we adopt the former one, i.e. we set the initial spin state to \( |\psi_0\rangle \).

We have assumed above that the field rotates at a constant speed. Actually, we can easily modify the above scheme for arbitrary time-dependent rotating speed \( \gamma_a(t) \), \( \int_0^T \gamma_a(t) dt = 2\pi \). In this case, we need only change the term \( \gamma t \) in \( H_W(t) \), \( U_W(t) \), \( R \) and \( \psi(t) \) into \( \int_0^t \gamma_a(t') dt' \) accordingly. Consequently, the the additional vertical field is now a time-dependent field \( \omega_z(t) = \gamma_a(t) \) instead of a static field. This extension is important in case it is difficult to rotate the field (or the fictitious field \( \omega \)) in a constant angular speed. Punctual results can be obtained here through the exact feedback system where the value of additional vertical field is always instantaneously equal to the angular velocity of the rotating field.

Thus we see, by adding an additional magnetic field that is equal to the rotating frequency of the external field, we do get the exact result. Obviously if we rotate the field inversely, additional vertical field should be in the inverse direction\((-z)\) accordingly.

**NMR system and the rotational framework.** Consider the interacting nucleus spin

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\(^2\)Our main motivation is to give the nonadiabatic quantum gate in the most general case, i.e., we shall allow the time-dependent rotation of horizontal field \( \omega_1 \). For this purpose, only the method using additional vertical field will work.
pair (spin \(a\) and spin \(b\)) in the NMR quantum computation \([10,13]\). If there is no horizontal field the Hamiltonian for the two qubit system is

\[
H_i = \frac{1}{2}(\omega_a \sigma_{za} + \omega_b \sigma_{zb} + J \sigma_{za} \cdot \sigma_{zb}),
\]

where \(\omega_a (\omega_b)\) is the resonance frequency for spin \(a (b)\) in a very strong static magnetic field (e.g. \(\omega_a\) can be 500MHz \([2]\) ), \(J\) is the interacting constant between nuclei and \(\sigma_{za} = \sigma_{zb} = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\).

After adding a circularly polarized RF field in horizontal plane, the Hamiltonian for spin \(a\) in static framework is

\[
H' = \frac{1}{2} \omega_0 \sigma_z + \frac{1}{2} \omega'_a \sigma_z + \frac{1}{2} \omega_1 \begin{pmatrix} 0 & e^{-i\omega'_a t} \\ e^{i\omega'_a t} & 0 \end{pmatrix}.
\]

(9)

Here \(\omega'_a\) and \(\omega_1\) are the angular frequency and amplitude of the RF field respectively, \(\omega_0 = \omega_a - \omega'_a \pm J\) and the ” \(\pm\”\) sign in front of \(J\) is dependent on the specific state of spin \(b\), up or down respectively. To selectively manipulate spin \(a\), we shall use the rotational framework that is rotating around \(z-\)axis in speed \(\omega'_a\). We assume \(\omega'_a\) close to \(\omega_a\) but obviously different from \(\omega_b\). The Hamiltonian for spin \(a\) in the rotational framework is

\[
H_a = R' H' R'^{-1} + i(\partial R'/\partial t) R'^{-1} = H_0
\]

(10)

and \(R' = e^{i\omega'_a \sigma_z t/2}\). Note here \(H_0\) is dependent on state of spin \(b\) through \(\omega_0\). In the rotational framework, if the horizontal field is rotated in the angular speed \(\gamma\), the Hamiltonian for spin \(a\) is just \(H(t)\), as defined in eq(11). In the NMR system, we require \(|\psi_0\rangle\) to be the eigenstate of \(H_0\) in rotational the framework. Previously \([3]\), state \(|\psi_0\rangle\) for spin \(a\) was produced adiabatically.

In the following we demonstrate how to nonadiabatically produce the state \(|\psi_0\rangle\).

**Creating the conditional initial state with NMR.** In rotating the state around \(z-\)axis, we have started from state \(|\psi_0\rangle\), which is the eigenstate of \(H_0\). State \(|\psi_0\rangle\) must be created from the spin state \(|\uparrow\rangle\) or \(|\downarrow\rangle\). We need a nonadiabatic way to create state \(|\psi_0\rangle\) for spin \(a\). Note that we are working in the rotational framework. We denote \(\delta = \omega_a - \omega'_a\). We can use the
following sequence of operations to create the conditional angle $\theta$. (For simplicity we will call the following sequence as $S$ operation later on.) We have $S = \begin{align*} \left[ \frac{\pi}{2} \right]^y & \rightarrow J'(\varphi_\pm(t_c)) \rightarrow [-\delta \cdot t_c]^z \rightarrow \left[ \frac{\pi}{2} \right]^x \rightarrow [-\varphi']^y \end{align*} \tag{11} \]

Here all terms inside the $\cdots$ represent the Bloch sphere rotation angles caused by RF pulses. The superscripts indicate the axis the Bloch sphere is rotated around. $J'(\varphi_\pm(t_c))$ is the time evolution over period $t_c$ by the Hamiltonian $\frac{1}{2}(\delta \pm J)\sigma_z$. This evolution rotates spin $a$ around $z-$axis for an angle $\varphi_\pm = (\delta \pm J)t_c$. (Or $\varphi_\pm + \pi$, if spin $a$ is down initially. For clarity we omit this case and always assume spin $a$ is initially up.) After this $S$ operation, the angle between spin $a$ and the $z$-axis is $\theta_\pm = \frac{\pi}{2} - (\varphi' + \varphi_\pm)$ (see Fig. 1). To ensure the state to be eigenstate of Hamiltonian $H_0$ after $S$ operation we require $\tan(\varphi' + Jt_c) = \frac{\delta + J}{\omega_1}$ and $\tan(\varphi' - Jt_c/2) = \frac{\delta - J}{\omega_1}$ simultaneously. This is equivalent to

\[
\begin{cases} 
Jt_c = \frac{(\arctan \frac{\delta + J}{\omega_1} - \arctan \frac{\delta - J}{\omega_1})}{2} \\
\varphi' = \frac{(\arctan \frac{\delta + J}{\omega_1} + \arctan \frac{\delta - J}{\omega_1})}{2}.
\end{cases} \tag{12}
\]

From this constraint, given specific values of $\delta$, $J$ and $\omega_1$, we can easily obtain the scaled time $J \cdot t_c$ (Fig. 2) and the angle $\varphi'$ (Fig. 3) in controlling the $S$ operation. In particular, for $\delta/J = 1.058$, the value adopted in the recent NMR experiment, the relation curves for $Jt_c$ vs $\omega_1$ and $\varphi'$ vs $\omega_1$ are shown in Fig. 4.

**The nonadiabatic conditional geometric phase shift.** After the $S$ operation, the state of spin $a$ is an eigenstate of Hamiltonian $H_0$ no matter whether spin $b$ is up or down. After this $S$ operation we can use the additional magnetic field to nonadiabatically control the state evolution on the cone. However, after the state completes a loop, the total phase shift includes both dynamic and geometric contribution \[\text{[17]}\]. It is possible for the state to evolve on the dynamic phase path if we choose certain specific value of the rotating speed $\gamma$ (and also the additional field $\gamma$). For this task, we require
\[ \gamma = -\frac{\omega_1^2 + \omega_0^2}{\omega_0}. \] (13)

The negative sign in the right hand side indicates that the additional field \( \gamma \) is anti-parallel with the field \( \omega_0 \). By this setting, the total magnetic field in \( H_1 \) is always "perpendicular" to the state vector expressed in the Bloch ball. One can easily show that the instantaneous dynamical phase

\[ \langle \psi_0 | U_W(t)^\dagger H(t) U_W(t) | \psi_0 \rangle = 0. \] (14)

In case that \( \gamma \) is time dependent, to remove the dynamical phase, we can use the time-dependent magnetic field \( \omega_1(t) \) and \( \omega_0(t) \). We require

\[ \gamma(t) = \frac{\omega_1^2(t) + \omega_0^2(t)}{\omega_1(t)} \] (15)

and

\[ \omega_0(t)/\omega_1(t) = \omega_0(0)/\omega_1(0) = \tan \theta \] (16)

The two qubit case is a bit different from the single qubit case. Qubit \( b \) could be either up or down. We need choose the appropriate \( \gamma \) value so that the instantaneous dynamic phase for qubit \( a \) is always zero no matter qubit \( b \) is up or down. For this purpose, besides equation(13), we require

\[ \omega_1 = \sqrt{\delta^2 - J^2}. \] (17)

With this setting we propose the following scheme to make the nonadiabatic conditional geometric phase shift.

\[ S \rightarrow \begin{pmatrix} \omega_z \\ C \end{pmatrix} \rightarrow S^{-1}. \] (18)
The term \[ \left( \begin{array}{c} \omega_z \\ C \end{array} \right) \] represents doing operation \( C \) with an additional vertical field \( \gamma \). \( C \) represents rotating the external field around \( z \)-axis for \( 2\pi \) in a uniform speed \( \gamma \). We should choose the rotating direction so that additional field \( \gamma \) is anti-parallel the field \( \delta \pm J \), \((\delta > J)\). The dynamical phase shift after the operations is 0. So the scheme raised here can remove the dynamic phase and retain only the geometric phase. It can be shown that the geometric phase acquired after the total sequence of operations is \( \Gamma_{\pm}, \Gamma_{-} \) and \( -\Gamma_{+} \) respectively for the four different initial state \((|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle)\), \( \Gamma_{\pm} = -\pi \mp 2\pi \cos \theta_{\pm}, \cos \theta_{\pm} = \frac{\delta \pm J}{\sqrt{(\delta \pm J)^2 + \omega_z^2}} = \sqrt{\frac{\delta \pm J}{2\omega_z}} \).

**Concluding remark.** To make the conditional geometric phase shift gate we need be able to control two elementary operations. One is to exactly control the cyclic state evolution on a cone; the other is to produce the initial state on the cone with an angle \( \theta_{\pm} \) conditional on the other bit. Previously \([2]\), these two elementary operations were done adiabatically. We have shown that both of these two tasks can be done nonadiabatically. We have designed a new scheme for the nonadiabatic conditional geometric phase shift gate. This makes it possible to run the geometric quattum gate in a speed comparable to that of the normal quantum gate. The idea on nonadiabatic geometric phase shift gate demonstrated by the NMR system here should in principle also work for the other two level systems, such as Josephson Junction system \([5]\) and the harmonic oscillator system \([3,18]\), where the decoherence time can be much shorter.

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*Note added:* This manuscript is a revised version of Ref. \([19]\) with corrections made according to Ref. \([20]\). In this version, we removed all unpublished contents in the old versions therefore
the new version includes only the contents published in [19,20]. For an extended version with all details, one may refer to quant-ph/0108111 [21], which was posted to the arXiv one year ago. The original scheme appeared in Ref. [19] does not filter the dynamical phase. This was first pointed out by Tim Piller et al in August 2001. We then replaced the old multiloop scheme by a new single loop scheme with dynamical phase free path. This correction was first presented as the version 4 of this manuscript and also as quant-ph/0108111 in August 2001, and finalized in 2002 [20].
FIG. 1. Using $S$ operation to produce the eigenstate of $H_0$ nonadiabatically. Picture $a$ shows the possible initial state for spin $a$. The up(down) arrow on the solid line represents the up(down) state for spin $a$ while spin $b$ is up. The up(down) arrow on the dashed line represents the up(down) state for spin $a$ while spin $b$ is down. In picture $f$, angle $GOA$ is $\theta_+ = \arctan \frac{\omega_1}{\delta + J}$ and angle $GOB$ is $\theta_- = \arctan \frac{\omega_1}{\delta - J}$. 
FIG. 2. The time control in $S$ operation. Parameter $\omega_1/J$ varies from 0 to 10, $\delta/J$ varies from 0 to 5. Vertical axis is for the scaled time $Jt_c$.

FIG. 3. The rotating angle control in $S$ operation. Parameter $\omega_1/J$ varies from 0 to 10, $\delta/J$ varies from 0 to 5. Vertical axis is for the angle $\varphi'$.
FIG. 4. The time and rotating angle control in $S$ operation for specific $\delta/J$ value. Horizontal axis represents $\omega_1/J$. Vertical axis is for the scaled control $Jt_c$(the solid line) or the angle $\varphi'$(dashed line). Here $\delta/J = 1.058$, as for the experimental condition[2]. By this figure, given the specific values of $\omega_1/J$, we can always find the corresponding point in the two curves thus we can take the suitable time control(for $t_c$) and rotation control(for $\varphi'$) in the $S$ operation.
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