Nonadiabatic Conditional Geometric Phase Shift with NMR

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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. However, in quantum computation, everything must be completed 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 at the same rate as usual quantum computation.

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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. Because of 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.

Demand on both the running speed and the precision of every gate in a quantum computer is quite high. It has been reported recently that [2], due to the requirement of the adiabatic condition, faster running speed causes severe distortions to the results [2]. The adiabatic condition makes the fast speed and high precision conflict with 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 be practical only 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

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

(We shall extend it to the case of arbitrary time-dependent rotating speed in the end of this section.) Here $\sigma_x(t) = \left(\begin{smallmatrix} 0 & e^{-i\gamma t} \\ e^{i\gamma t} & 0 \end{smallmatrix}\right)$, ω_0 is the amplitude of the vertical field, and ω_1 is the amplitude of the horizontal field, which is rotating around the z axis in the constant angular speed γ. 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. (A similar idea has been used for the adiabatic rotational splitting with nuclear quadrupole resonance previously [16].) At time $\tau = 2\pi/\gamma$, when the external field completes a 2π rotation, the state is evolved to

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

The adiabatic approximation assumes that at time τ, the state completes a cyclic evolution provided that γ is small. However, due to the decoherence time limitation, γ cannot be too small. The nonzero γ distorts the state in the evolution and makes it *noncyclic* at time τ. This nonzero γ in the adiabatic approximation causes two types of errors. One is that the noncyclic completion of the evolution at time τ will cause further errors in the succeeding operations in the sequence. (We have to make a sequence of operations to remove the dynamic phase in realizing the geometric quantum gate [2].) The other is that the geometric phase acquired over period τ 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 the 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 the 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

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$$i\frac{\partial}{\partial t}U_W(t) = H_W(t)U_W(t) \tag{3}$$

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:

$$i\partial(RU_W)/\partial t = H_0(RU_W). \tag{4}$$

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

$$U_W(t) = e^{-i\gamma t\sigma_z/2}e^{-iH_0t}. \tag{5}$$

Consequently, at any time t, state $|\psi(t)\rangle = e^{-i\lambda t} \times e^{-i\gamma t\sigma_z/2}|\psi_0\rangle$ is exactly the instantaneous eigenstate of Hamiltonian $H(t)$, where λ is the eigenvalue of H_0 for eigenstate $|\psi_0\rangle$. In particular, at time τ, $|\psi(\tau)\rangle = e^{-i\pi-i\lambda\tau}|\psi_0\rangle$. It differs only 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 γ plays an important role. Without this field, the time evolution operator generated by $H(t)$ is

$$U(t) = e^{-i\gamma t\sigma_z/2}e^{-iH_1t} \tag{6}$$

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 γ. So, we have two ways to control the spin evolution exactly. We can use the additional field γ, 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 $|\psi_0\rangle$. (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 ω_1. For this purpose, only the method using an additional vertical field will work.)

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 $\gamma_a(t)$, $\int_0^\tau \gamma_a(t)\,dt = 2\pi$. In this case, we need only change the term γt in $H_W(t)$, $U_W(t)$, R, and $\psi(t)$ into $\int_0^t \gamma_a(t')\,dt'$ accordingly. Consequently, 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 [5]) in a constant angular speed. Punctual results can be obtained here through the exact feedback system where the value of an 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, an additional vertical field should be in the inverse direction $(-z)$ accordingly.

NMR system and the rotational framework.—Consider the interacting nucleus spin 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., ω_a can be 500 MHz [2]), J is the interacting constant between nuclei and $\sigma_{za} = \sigma_{zb} = \sigma_z = \left(\begin{smallmatrix}1 & 0\\ 0 & -1\end{smallmatrix}\right)$. After adding a circularly polarized rf field in the horizontal plane, the Hamiltonian for spin a in static framework is

$$H' = \frac{1}{2}\omega_0\sigma_z + \frac{1}{2}\omega_a'\sigma_z + \frac{1}{2}\omega_1\begin{pmatrix}0 & e^{-i\omega_a't}\\ e^{i\omega_a't} & 0\end{pmatrix}. \tag{7}$$

Here ω_a' and ω_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 the z axis in speed ω_a'. We assume ω_a' close to ω_a but obviously different from ω_b. The Hamiltonian for spin a in the rotational framework is

$$H_a = R'H'R'^{-1} + i(\partial R'/\partial t)R'^{-1} = H_0 \tag{8}$$

and $R' = e^{i\omega_a'\sigma_z t/2}$. Note here H_0 is dependent on the state of spin b through ω_0. In the rotational framework, if the horizontal field is rotated in the angular speed γ, the Hamiltonian for spin a is just $H(t)$, as defined in Eq. (1). In the NMR system, we require $|\psi_0\rangle$ to be the eigenstate of H_0 in the rotational framework. Previously [2], 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 the 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 θ. (For simplicity we will call the following sequence S operation later on.) We have $S =$

$$\left[\frac{\pi}{2}\right]^y \to J'[\varphi_\pm(t_c)] \to [-\delta\cdot t_c]^z \to \left[\frac{\pi}{2}\right]^x \to [-\varphi']^y. \tag{9}$$

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 the z axis for an angle $\varphi_\pm = (\delta \pm J)t_c$. (Or $\varphi_\pm +$

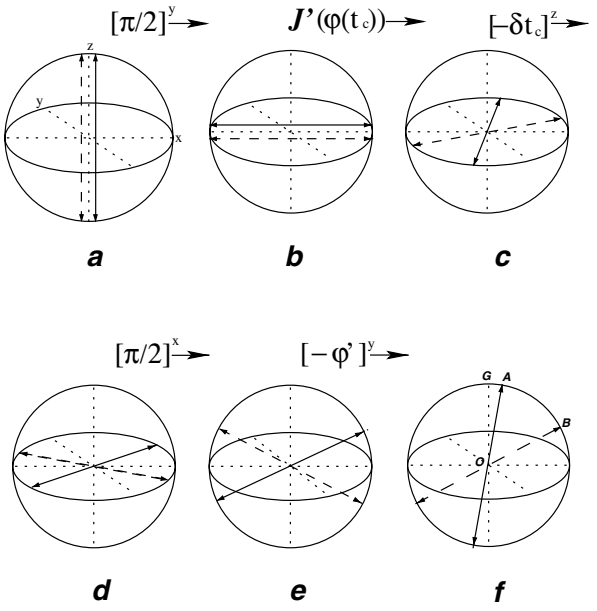

FIG. 1. Using the S operation to produce the eigenstate of H_0 nonadiabatically: (a) shows the possible initial state for spin a. The up (down) arrow on the solid line represents the up (down) state for spin a while spin b is up. The up (down) arrow on the dashed line represents the up (down) state for spin a while spin b is down. In (f), angle GOA is $\theta_+ = \arctan\frac{\omega_1}{\delta+J}$ and angle GOB is $\theta_- = \arctan\frac{\omega_1}{\delta-J}$.

π, 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 the eigenstate of Hamiltonian H_0 after the 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

$$\begin{cases} Jt_c = \left(\arctan\frac{\delta+J}{\omega_1} - \arctan\frac{\delta-J}{\omega_1}\right) \Big/ 2, \\ \varphi' = \left(\arctan\frac{\delta+J}{\omega_1} + \arctan\frac{\delta-J}{\omega_1}\right) \Big/ 2. \end{cases} \tag{10}$$

From this constraint, given specific values of δ, J, and ω_1, we can easily obtain the scaled time $J \cdot t_c$ (Fig. 2) and the angle φ' (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 ω_1 and φ' vs ω_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. With this S operation and the way to nonadiabatically control the state evolution on the cone, we propose the following scheme to make the nonadiabatic conditional geometric phase shift:

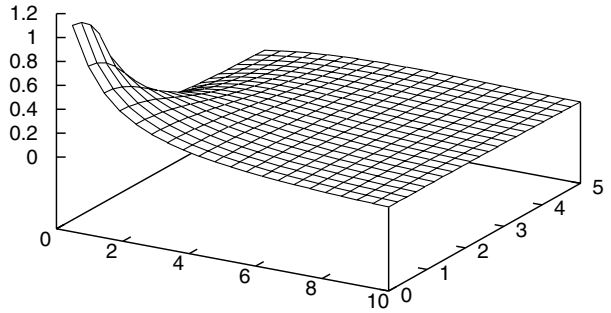

FIG. 2. The time control in the S operation: Parameter ω_1/J varies from 0 to 10; δ/J varies from 0 to 5. The vertical axis is for the scaled time Jt_c.

$$S \to \begin{pmatrix} \omega_z \\ C \end{pmatrix} \to \pi_a \to \begin{pmatrix} \bar{\omega}_z \\ \bar{C} \end{pmatrix} \to S^{-1} \to$$
$$\pi_b \to S \to \begin{pmatrix} \omega_z \\ C \end{pmatrix} \to \pi_a \to \begin{pmatrix} \bar{\omega}_z \\ \bar{C} \end{pmatrix} \to S^{-1} \to \pi_b \,. \tag{11}$$

The term $\binom{\omega_z}{C}$ or $\binom{\bar{\omega}_z}{\bar{C}}$ represents doing operation C or $\bar{C}$ with an additional vertical field ω_z parallel or antiparallel to the $+z$ direction. C represents rotating the external field around the z axis for 2π; $\bar{C}$ is the inverse rotation of C. $\pi_{a,b}$ is to flip the spin a, b, respectively. The instantaneous value of the vertical field ω_z is equal to the value of the instantaneous rotating speed in loop C or $\bar{C}$. If loop C is traveled in a uniform angular velocity, the value of ω_z is a constant. The net dynamic phase shift after the whole sequence of operations is 0. Similar to that in [2,9], the sequence of operations 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 Γ, $-\Gamma$, $-\Gamma$, and Γ, respectively, for the four different initial states $(|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle)$, $\Gamma = 2\pi(\cos\theta_+ - \cos\theta_-)$,

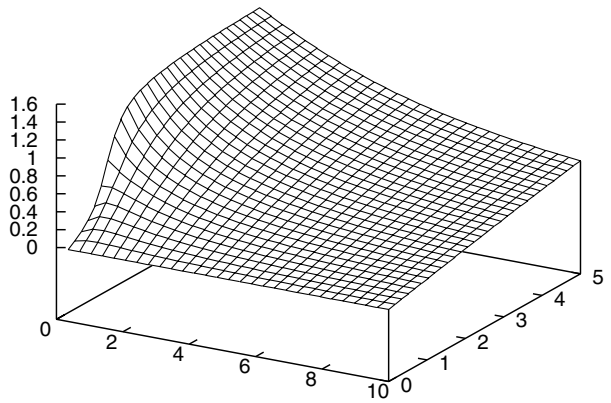

FIG. 3. The rotating angle control in the S operation: Parameter ω_1/J varies from 0 to 10; δ/J varies from 0 to 5. The vertical axis is for the angle φ'.

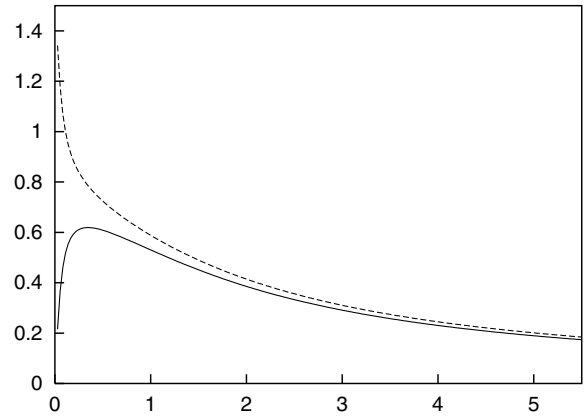

FIG. 4. The time and rotating angle control in the S operation for a specific δ/J value: The horizontal axis represents ω_1/J. The vertical axis is for the scaled control Jt_c (solid line) or the angle φ' (dashed line). Here $\delta/J = 1.058$, as for the experimental condition [2]. By this figure, given the specific values of ω_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 φ') in the S operation.

$\cos\theta_{\pm} = \{(\delta \pm J)/[\sqrt{(\delta \pm J)^2 + \omega_1^2}]\}$. This is just the result in Refs. [2,9].

As was pointed out earlier [2,9], for a given value of δ/J, the controlled phase shift Γ will first rise and then fall while ω_1 is increased. The value of ω_1 at the optimized point had been used in the laboratory for an adiabatic case [2], because operational error of the first order is zero there. If we do not care about the optimization point, we can set $\omega_a' = \omega_a$ and the S operation can be simplified to $S_0 = [\frac{\pi}{2}]^y \rightarrow J[\pm\varphi(t_c)] \rightarrow [\frac{\pi}{2}]^x$. Term $J[\pm\varphi(t_c)]$ represents the time evolution over period t_c under the interaction between spin a and b, i.e., under Hamiltonian $\pm\frac{1}{2}J\sigma_z$.

Conclusion.—To make the conditional geometric phase shift gate we need to 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 quantum gate in a speed comparable to that of the normal quantum gate. The idea on the nonadiabatic geometric phase shift gate demonstrated by the NMR system here should in principle also work for the other two level systems, such as the Josephson junction system [5] and the harmonic oscillator system [6,17], where the decoherence time can be much shorter.

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