Non-adiabatic Arbitrary Geometric Phase Gate in 2-qubit NMR Model

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We study a 2-qubit nuclear spin system for realizing an arbitrary geometric quantum phase gate by means of non-adiabatic operation. A single magnetic pulse with multi harmonic frequencies is applied to manipulate the quantum states of 2-qubit instantly. Using resonant transition approximation, the time dependent Hamiltonian of two nuclear spins can be solved analytically. The time evolution of the wave function is obtained without adiabatic approximation. The parameters of magnetic pulse, such as the frequency, amplitude, phase of each harmonic part as well as the time duration of the pulse, are determined for achieving an arbitrary non-adiabatic geometric phase gate. The derivation of non-adiabatic geometric controlled phase gates and A-A phase are also addressed.

Taking the advantage of quantum superposition and entanglement, a powerful new computational algorithms, such as factoring large numbers and searching an unsorted database, has been created. Further study of quantum information processing and realization of quantum computer has attracted large numbers of theoretical and experimental scientists. For implementation of quantum computing, the ability to perform any single quantum bit (qubit) rotations (SU(2) transformation) and 2-qubit controlled operations, i.e. controlled not (CNOT) or controlled phase gate (CPG), is the key requirement. Moreover, each individual qubit should have a long decoherence time to prevent the deformation of quantum information in qubits for enough long time. In order to implement a controlled quantum gate (CNOT or CPG), the “interaction” between qubits is necessary. In this letter, we are interested in the phase gate of two nuclear spin system. In general, the phase shift of the quantum state stored in qubits after a cyclic time evolution includes both the dynamical and geometrical part. In some condition, the phase can be dependent only on the path of the state evolution, not the dynamics at all. In the case, the relevant transformation of the quantum state is called as a geometric phase gate, which has been discussed and implemented in many schemes including trapped ion, cavity QED and nuclear magnetic resonance. However, the adiabatic implementation of geometric phase gate may create some considerable errors. Non-adiabatic implementation of quantum information procession is required in the practice since any quantum computing is requested as fast as possible. Hence, the theoretical study of non-adiabatic process in quantum information process is important and has attracted many scientists. In this paper, we focus on the study of the implementation of non-adiabatic geometric phase gate.

Since the nuclear spins are well isolated from the environment, their decoherence time are far longer. Meanwhile, nuclei with spin 1/2 are the natural as qubits in quantum information processing. In terms of nuclear magnetic resonance (NMR), the system of nuclear spins has been a good candidate to demonstrate the quantum computational algorithms. Over the recent several years, many kinds of complex quantum information processing have been realized by using NMR, ranging from two to seven qubits in size, in liquid samples and in solid state samples. The physical manipulation of nuclear spin state can be realized by sequences of magnetic pulses with some active resonant frequencies.

In this paper, we study the 2-qubit system that is composed by two weak coupled nuclear spins in an external magnetic field. We present details of the deduction of the time evolution of the quantum state of two nuclear spins manipulated by an external transverse magnetic pulse with some selective resonance frequencies, and show how to achieve an arbitrary non-adiabatic geometric quantum phase gate. Then, as a results, the controlled geometric phase gate as well as A-A phase are easily obtained.

We first recall the definition of the quantum phase gate (QPG). Denote $T$ as an unitary transformation evolving the input quantum state $|\Psi(0)\rangle$ to output one $|\Psi(t)\rangle = T|\Psi(0)\rangle$, where $T$ is a $2^n \times 2^n$ matrix ($n$ the number of qubits). The $T$ defines a quantum gate. The gate is called as a phase gate if $T_{ij} = e^{i\phi_i} \delta_{ij}$, $i,j = 1,2,\cdots,2^n$, where $\{\phi_i : i = 1,2,\cdots,2^n\}$ are the phases that are dependent on the evolution path in parameter space as well as the dynamics. Thereby each phase $\phi_i$ includes both the geometric and dynamical part in general. But, the dynamical part of $\phi_i$ can be vanished in some condition. In the case, the phase becomes pure geometric and the transformation $T$ is called as a geometric phase gate.
(GPG). If the evolution of the state is instantaneous, \( T \) the non-adiabatic GPG. In our present work, we study the implementation of non-adiabatic GPG.

The Hamiltonian of two nuclear spins with a weak Heisenberg type interaction in a constant longitudinal magnetic field along \( z \) direction is

\[
H^{(2)} = H_z^{(2)} + H_{xy}^{(2)},
\]

\[
H_z^{(2)} = -\frac{1}{2}(\omega_1 \sigma_1^z + \omega_2 \sigma_2^z + J \sigma_1^y \sigma_2^y),
\]

\[
H_{xy}^{(2)} = -\frac{1}{2}(J \sigma_1^y \sigma_2^z + J \sigma_1^z \sigma_2^y),
\]

where isotropic coupling is assumed, \( \omega_1 \) and \( \omega_2 \) are the Larmor frequencies of two nuclear spins, \( J \) the coupling constant, \( \{\sigma_i^x, \sigma_i^y, \sigma_i^z : i = 1, 2\} \) the Pauli matrices, and \( \hat{h} = 1 \). In the experiments, two different nuclear spins are selected, \( \omega_1 \neq \omega_2 \), we assume \( \omega_1 > \omega_2 \) and the longitudinal constant magnetic field is in the order of 1 THz, so \( \omega_1, \omega_2 \) are much large than \( J \) and \( \eta = J/(\omega_1 - \omega_2) << 1 \). The experiment numbers of these parameters will be given in late. \( H_2^{(2)} \) is non-diagonal in \( \sigma_i \) representation and gives the quantum fluctuation which yields a correction of order \( \eta^2 \), hence it can be ignored. Thus, the Ising part \( H_z^{(2)} \) of the Hamiltonian is a well precise approximation. \( H^{(2)} (\sim H_z^{(2)}) \) has four eigenstates: \( \{00, 01, 10, 11\} \), where 0 denotes the spin up and 1 the spin down. These states correspond to following \( 4 \) eigenvalues respectively:

\[
\epsilon_1 = - (\omega_1 + \omega_2 + J)/2, \quad \epsilon_2 = - (\omega_1 - \omega_2 - J)/2, \\
\epsilon_3 = (\omega_1 - \omega_2 + J)/2, \quad \epsilon_4 = (\omega_1 + \omega_2 - J)/2.
\]

In this paper, we want to find out an appropriate magnetic pulse to achieve arbitrary non-adiabatic geometric QPG. Therefor a rectangular transversal magnetic pulse with 4-frequency \( \{\Omega_1, \Omega_2, \Omega_3, \Omega_4\} \) is applied to the system. The Hamiltonian becomes

\[
H_{\text{total}} = H_z^{(2)} + H_{\text{pulse}}(t),
\]

where

\[
H_{\text{pulse}}(t) = -\frac{1}{4} \sum_{i=1}^{4} \sum_{k=1}^{4} h_{ik}(t),
\]

\[
h_{ik}(t) = h_{ik} f_k(t) \sigma_i^+ \sigma_k^-.
\]

\( H_{\text{pulse}}(t) \) is the external magnetic pulse where \( f_k(t) = e^{i(\Omega_k t + \Phi_k)} \), \( \sigma_i^\pm = \sigma_i^x \pm i \sigma_i^y \) and \( \sigma_i^y \) are Pauli operators. \( h_{1k} = \gamma_1 \bar{h}_k \) and \( h_{2k} = \gamma_2 \bar{h}_k \) and \( \bar{h}_k \) the amplitudes of magnetic pulse. \( \gamma_1 \) and \( \gamma_2 \) are the gryomagnetic ratio of two different nuclear spins. It is assumed that the magnetic pulse is applied in the duration \( [0, \tau] \):

\[
\bar{h}_k \neq 0, t \in [0, \tau] \\
\bar{h}_k = 0, t \notin [0, \tau], k = 1, 2, 3, 4.
\]

\[
\begin{array}{c}
\Omega_1 \\
\Omega_2 \\
\Omega_3 \\
\Omega_4
\end{array}
\]

\[
\begin{array}{c}
00 \\
01 \\
10 \\
11
\end{array}
\]

**FIG. 1**: The sketch of the energy levels of the Hamiltonian \( H_{\text{total}} \) and two multi-photon transition schemes

The phases \( \{\Phi_k\} \) and duration \( \tau \) of the magnetic pulse will be designed below in detail. Set

\[
\begin{align*}
\Omega_1 &= \epsilon_3 - \epsilon_1 = \omega_1 + J, \quad |00 \rangle \leftrightarrow |10 \rangle \quad (6) \\
\Omega_2 &= \epsilon_4 - \epsilon_3 = \omega_2 - J, \quad |10 \rangle \leftrightarrow |11 \rangle, \quad (7) \\
\Omega_3 &= \epsilon_2 - \epsilon_1 = \omega_1 - J, \quad |00 \rangle \leftrightarrow |01 \rangle, \quad (8) \\
\Omega_4 &= \epsilon_4 - \epsilon_2 = \omega_1 - J, \quad |01 \rangle \leftrightarrow |11 \rangle. \quad (9)
\end{align*}
\]

Corresponding transitions are shown in figure. The Schrödinger equation is

\[
\hat{H}(t) = \sum_j \epsilon_j(t) |m_j\rangle \langle m_j|
\]

The solution can be expanded as follows

\[
|\Psi(t)\rangle = \sum_j \epsilon_j(t) |m_j\rangle \quad (j = 1, 2, 3, 4)
\]

where \( |m_1\rangle, |m_2\rangle, |m_3\rangle, |m_4\rangle \) respectively corresponds to the state \( |00\rangle, |01\rangle, |10\rangle, |11\rangle \). When the system is initially at the state \( |\Psi(0)\rangle = |00\rangle \), the pulse with 4 frequencies \( \{\Omega_i : i = 1, 2, 3, 4\} \) leads a coherent evolution of four states \( |00\rangle, |01\rangle, |10\rangle, |11\rangle \). Since those transitions satisfying resonant condition are dominating, we can ignore all other minor detuned transitions. This is so-called resonant transition approximation (RTA). In RTA, the states transferred each other by the magnetic pulse are called as the active states, the rest the inactive. When we apply an magnetic pulse with 4 frequencies (see Fig.1), in RTA the Hamiltonian \( H_{\text{total}} \) can be well approximated by following \( \hat{H}(t) \):

\[
\begin{pmatrix}
\epsilon_1 & -\frac{\hbar}{2} f_3(t) & -\frac{\hbar}{2} f_4(t) & 0 \\
-\frac{\hbar}{2} f_3(t) & \epsilon_2 & 0 & -\frac{\hbar}{2} f_1(t) \\
-\frac{\hbar}{2} f_4(t) & 0 & \epsilon_3 & -\frac{\hbar}{2} f_2(t) \\
0 & -\frac{\hbar}{2} f_1(t) & -\frac{\hbar}{2} f_2(t) & \epsilon_4
\end{pmatrix}
\]

where \( \hbar = h_{11}, h_2 = h_{22}, h_3 = h_{13}, h_4 = h_{24} \) and \( f_k(t) \) is the complex conjugate of \( f_k(t) \).

Now we want to find out the exact solution of Hamiltonian without adiabatic approximation. We do an unitary transformation \( U(t) \) as follows

\[
|\Psi(t)\rangle = U(t) |\psi(t)\rangle.
\]
From Schrödinger equation $i\hbar \partial (|\Psi(t)\rangle) / \partial t = \hat{H}(t)|\Psi(t)\rangle$, we obtain an equation of $|\psi(t)\rangle$:

$$i\hbar \partial (|\psi(t)\rangle) / \partial t = H_{rot}(t)|\psi(t)\rangle,$$

(13)

where

$$H_{rot}(t) = U(t)\hat{H}(t)U^+(t) - iU(t)\partial U^+ / \partial t.$$  (14)

It is assumed that the matrix $U(t)$ is diagonal: $U_{ij}(t) = \delta_{ij} e^{i(\varphi_j + \theta_j)}$ where $\{\varphi_i, \theta_i\}$ are some parameters to be determined. When the parameters $\{\varphi_i, \theta_i\}$ satisfy the following relations:

$$\Omega_1 = \varphi_3 - \varphi_1, \Phi_1 = \theta_3 - \theta_1$$
$$\Omega_2 = \varphi_4 - \varphi_3, \Phi_2 = \theta_4 - \theta_3$$
$$\Omega_3 = \varphi_2 - \varphi_1, \Phi_3 = \theta_2 - \theta_1$$
$$\Omega_4 = \varphi_4 - \varphi_2, \Phi_4 = \theta_4 - \theta_2$$

(15), (16), (17), (18)

It can be easily found that

$$H_{rot}(t) = \left( \begin{array}{cccc}
\epsilon_1 - \varphi_1 & -\epsilon_2 & -\epsilon_3 & -\epsilon_4 \\
-\epsilon_2 & \epsilon_1 - \varphi_2 & 0 & 0 \\
-\epsilon_3 & 0 & \epsilon_1 - \varphi_3 & 0 \\
0 & -\epsilon_4 & 0 & \epsilon_1 - \varphi_4
\end{array} \right).$$

(19)

which is time independent. We simply denote $H_{rot}(t)$ as $H_{rot}$. Due to $\Omega_1 = \epsilon_3 - \epsilon_1$, $\Omega_2 = \epsilon_4 - \epsilon_3$, $\Omega_3 = \epsilon_2 - \epsilon_1$, $\Omega_4 = \epsilon_4 - \epsilon_2$, then considering the relations of (15)-(18), we get

$$\epsilon_2 - \varphi_2 = \Omega_3 + \epsilon_1 - \varphi_1 = \epsilon_1 - \varphi_1,$$
$$\epsilon_3 - \varphi_3 = \Omega_1 + \epsilon_1 - \varphi_3 = \epsilon_1 - \varphi_1,$$
$$\epsilon_4 - \varphi_4 = \Omega_3 + \Omega_4 + \epsilon_1 - \varphi_4 = \epsilon_1 - \varphi_1.$$

Setting $\varphi_1 = \epsilon_1$, equation (19) becomes

$$H_{rot}(t) = H_{rot} = \left( \begin{array}{cccc}
-\frac{\hbar^2}{2} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{array} \right).$$

(20)

From equations (15)-(18), we have

$$\varphi_2 = \Omega_3 + \varphi_1, \varphi_3 = \Omega_1 + \varphi_1,$$
$$\varphi_4 = \Omega_3 + \varphi_1, \varphi_1 = \Omega_1 + \varphi_1,$$
$$\theta_2 = \Phi_1 + \Phi_2, \theta_3 = \Phi_1 + \theta_1,$$
$$\theta_4 = \Phi_1 + \Phi_2 - \theta_1.$$

Four eigenvalues of $H_{rot}$ can be found as follows

$$E_1 = -\frac{\sqrt{2}}{4} \sqrt{A + \sqrt{B + C}},$$
$$E_2 = \frac{\sqrt{2}}{4} \sqrt{A - \sqrt{B + C}},$$
$$E_3 = -\frac{\sqrt{2}}{4} \sqrt{A - \sqrt{B + C}},$$
$$E_4 = \frac{\sqrt{2}}{4} \sqrt{A + \sqrt{B + C}},$$

where

$$A = \sum_{i=1}^{4} h_i^2, B = \sum_{i=1}^{4} h_i^4,$$
$$C = 8h_1 h_2 h_3 h_4 + 2h_1 h_2^2 + 2h_1^2 h_3^2 - 2h_1 h_3 h_4 + 2h_1 h_2 + 2h_3 h_4 + 2h_2 h_3^2$$

we further set $h_1 = h_4$ and $h_2 = h_3$. It results

$$E_1 = -\frac{1}{2}(h_1 + h_2), E_2 = \frac{1}{2}(h_1 + h_2),$$
$$E_3 = -\frac{1}{2}(h_1 - h_2), E_4 = \frac{1}{2}(h_1 - h_2).$$

(21), (22)

Four corresponding eigenfunctions are $|\psi_i\rangle = \sum_{j=1}^{4} C_{ij}|m_j\rangle, i = 1, 2, 3, 4$. The coefficients matrix $C$ and its inverse $C^{-1}$ are

$$C = C^{-1} = \frac{1}{2} \left( \begin{array}{cccc}
1 & 1 & 1 & 1 \\
1 & -1 & -1 & -1 \\
1 & -1 & -1 & -1 \\
1 & 1 & 1 & 1
\end{array} \right).$$

(23)

$$|m_i\rangle = \sum_{j=1}^{4} C_{ij}^{-1}|\psi_j\rangle, i = 1, 2, 3, 4. \text{ If the system is initially at one of the eigenstates: } |\Psi^{(i)}(0)\rangle = |m_i\rangle, (i = 1, 2, 3, 4), \text{ the state of system at time } t \text{ will be }$$

$$|\Psi^{(i)}(t)\rangle = U(t) \exp[-iH_{rot} t]|m_i\rangle = \sum_{j=1}^{4} C_{ij}^{-1} U(t) \exp[-iH_{rot} t]|\psi_j\rangle = \sum_{j=1}^{4} C_{ij}^{-1} |m_j\rangle U(t)|\psi_j\rangle \exp(-iE_j t) = \sum_{j=1}^{4} C_{ij}^{-1} e^{-i(\varphi_j t + \theta_j)} \exp(-iE_j t) C_{jk}|m_k\rangle = \sum_{j=1}^{4} C_{ij}^{-1} e^{-i(\varphi_j t + \theta_j)} \exp(-iE_j t) C_{jk}|m_k\rangle$$

(24)

where

$$\epsilon_k^{(i)}(t) = \frac{1}{4} \left( \begin{array}{cccc}
C_{ij}^{-1} & -C_{ij}^{-1} & -C_{ij}^{-1} & -C_{ij}^{-1} \\
-C_{ij}^{-1} & C_{ij}^{-1} & C_{ij}^{-1} & C_{ij}^{-1} \\
-C_{ij}^{-1} & C_{ij}^{-1} & C_{ij}^{-1} & C_{ij}^{-1} \\
-C_{ij}^{-1} & C_{ij}^{-1} & C_{ij}^{-1} & C_{ij}^{-1}
\end{array} \right) e^{-i(\varphi_j t + \theta_j)}$$

(25)

$$\tilde{\epsilon}_k^{(i)}(t) = \frac{1}{4} \sum_{j=1}^{4} C_{ij}^{-1} e^{-iE_j t} C_{jk}.$$  

(26)

The initial condition is $|\epsilon_k^{(i)}(0)|^2 = 1$ and $|\tilde{\epsilon}_k^{(i)}(0)|^2 = 0 (k \neq i)$. For a cyclic evolution after time $\tau$,

$$|\Psi^{(i)}(\tau)\rangle = e^{i\beta(\tau)}|\Psi^{(i)}(0)\rangle = \epsilon_k^{(i)}(\tau)|\psi_k\rangle,$$

(27)

where the total phase is $\beta(\tau) = \arg \langle \Psi^{(i)}(0) | \Psi^{(i)}(\tau) \rangle = \delta_D^{(i)}(\tau) + \delta_G^{(i)}(\tau)$. $\delta_D^{(i)}(\tau)$ is the geometric phase. The
geometric phase gate is achieved.

\[ \delta_D^{(i)}(\tau) = - \int_0^\tau dt \langle \Psi^{(i)}(t) | \tilde{H}(t) | \Psi^{(i)}(t) \rangle \]
\[ = - \int_0^\tau dt \sum_{k,k'} c_k^{(i)}(t) c_{k'}^{(i)}(t) (m_k | \tilde{H}(t) | m_{k'}) \]  

In appendix A, we obtain

\[ \begin{align*}
\tilde{c}_1^{(1)}(t) &= \tilde{c}_2^{(2)}(t) = \tilde{c}_3^{(3)}(t) = \tilde{c}_4^{(4)}(t) \\
&= \cos \left( \frac{h_1 t}{2} \right) \cos \left( \frac{h_2 t}{2} \right) \\
\tilde{c}_2^{(1)}(t) &= \tilde{c}_1^{(2)}(t) = \tilde{c}_4^{(3)}(t) = \tilde{c}_3^{(4)}(t) \\
&= i \cos \left( \frac{h_1 t}{2} \right) \sin \left( \frac{h_2 t}{2} \right) \\
\tilde{c}_3^{(1)}(t) &= \tilde{c}_4^{(2)}(t) = \tilde{c}_3^{(3)}(t) = \tilde{c}_2^{(4)}(t) \\
&= i \sin \left( \frac{h_1 t}{2} \right) \cos \left( \frac{h_2 t}{2} \right) \\
\tilde{c}_4^{(1)}(t) &= \tilde{c}_3^{(2)}(t) = \tilde{c}_2^{(3)}(t) = \tilde{c}_1^{(4)}(t) \\
&= \sin \left( \frac{h_1 t}{2} \right) \sin \left( \frac{h_2 t}{2} \right)
\end{align*} \]

When \( t = \tau \) and satisfies \( h_1 \tau = 2m\pi, h_2 \tau = 2n\pi \), namely

\[ \tau = \frac{2m\pi}{h_1}, \frac{n\pi}{h_2}, m, n = 1, 2, 3, \ldots \]  

we have

\[ |\tilde{c}_i^{(i)}(\tau)| = 1 : i = 1, 2, 3, 4, \]
\[ |\tilde{c}_i^{(j)}(\tau)| = 0 : i \neq j. \]

It directly yields

\[ |\Psi^{(i)}(\tau)\rangle = \sum_k e^{-i(\varphi_i t + \theta_k)} \tilde{c}_k^{(i)}(t) |m_k\rangle \]
\[ = e^{-i(\varphi_i + \theta_i)} |m_1\rangle, i = 1, 2, 3, 4. \]

Equation (33) is the condition to achieve a phase gate. In appendix B, we give the proof of that the dynamical phases also vanish at same condition (33):

\[ \delta_D^{(i)}(\tau) = 0, i = 1, 2, 3, 4. \]  

Hence, for any initial state \( |\Psi(0)\rangle = \sum_i c_i(0) |m_i\rangle \) the wave function \( |\Psi(\tau)\rangle \) is

\[ |\Psi(\tau)\rangle = A \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & e^{-i\Theta_2} & 0 \\
0 & e^{-i\Theta_3} & 0 & 0 \\
0 & 0 & 0 & e^{-i\Theta_4}
\end{pmatrix} |\Psi(0)\rangle. \]  

Where \( A = \cos(m\pi/2) \cos(n\pi/2), A = \pm 1 \) only contributes a global phase. The phases \( \{\Theta_i = \varphi_i + \theta_i : i = 1, 2, 3, 4\} \) are all geometric. Hence a non-adiabatic geometric phase gate is achieved.

From equations (15) to (18), there are relations \( \varphi_2 = \Omega_2 + \varphi_1, \varphi_3 = \Omega_1 + \varphi_1, \varphi_4 = \Omega_1 + \Omega_2 - \varphi_1, \varphi_1 = \epsilon_1. \) It is similar to have \( \theta_2 = \Phi_2 - \theta_1, \theta_3 = \Phi_3 + \Phi_1, \theta_4 = \Phi_4 + \theta_1. \) Since all \( \{\Omega_i\} \) and \( \epsilon_1 \) are fixed, all \( \{\varphi_i\} \) are changeless. \( \{\Phi_i\} \) are the phases of four harmonic waves of the external magnetic pulse and can be freely adjusted. Hence we can use four free parameters \( \{\Phi_i\} \) to change the values of \( \theta_i : i = 1, 2, 3, 4 \), then to alter four phases \( \Theta_i(= \varphi_i + \theta_i) \) in gate individually. As a result the arbitrary non-adiabatic geometric phase gate of two qubits is implemented by means of NMR. The duration time \( \tau \) of magnetic pulse is determined by equations (33):

\[ \tau = 2m\pi/h_1, h_2 = \frac{n\pi}{m} h_1 \text{ where } h_1 \text{ and } h_2 \text{ are related to the amplitude of magnetic pulse and are adjustable. Taking } m = n = 1, \text{ it gives } h_1 = h_2 \text{ and } \tau = 2\pi/h_1. \]

Set \( \theta_1 = -\varphi_1 \tau \text{ and } \theta_2 = -\varphi_2 \tau \) in equation (35), we obtain an arbitrary geometric controlled phase gate (CPG) by changing the parameters \( \{\theta_3, \theta_4\} \):

\[ T_{CPG} = A \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & e^{-i(\varphi_3 \tau + \theta_3)} & 0 \\
0 & 0 & 0 & e^{-i(\varphi_4 \tau + \theta_4)}
\end{pmatrix}, A = \pm 1. \]

Further, if we adjust the parameters \( \{\theta_i\} \) to satisfy following conditions

\[ \varphi_i \tau + \theta_i = \varphi_1 \tau + \theta_1 : i = 2, 3, 4. \]

The wave function at time \( \tau \) is recovered to initial state with a phase difference only.

\[ |\Psi(\tau)\rangle = \pm e^{-i(\varphi_1 \tau + \theta_1)} |\Psi(0)\rangle. \]

Where \( \varphi_1 \tau + \theta_1 \) is just the A-A phase.

Finally, we give brief discussion on the validity of Ising model and our RTA and some estimation of the time \( \tau \) to achieve the geometric arbitrary phase gate. It is known that the nuclei \( ^1\text{H}, ^1\text{H}, ^1\text{C}, ^1\text{C}, ^1\text{N}, ^1\text{N}, ^1\text{F}, ^3\text{F}, ^3\text{F}, ^1\text{P}, \text{ etc.} \) have spin \( S = 1/2 \). Taking the \( ^1\text{H} \) and \( ^1\text{C} \) as an example, the Larmor precession frequency of nucleus \( ^1\text{H} : \omega_2 \sim 500\text{MHz} \) at field \( B_0 = 1.87T \). The gyromagnetic ratio of \( ^1\text{C} \) has only 25% of \( ^1\text{H} \), so \( \omega_2 \sim 125\text{MHz} \), \( \omega_1 - \omega_2 \sim 375\text{MHz} \). Assume the coupling \( J \sim 200\text{Hz} \) (in the references \( J \sim 200\text{Hz} \), we have \( J/(\omega_2 - \omega_2) \sim 0.54 \times 10^{-6} (<< 1) \)). Hence the quantum fluctuation from \( H_{xy} \) can be ignored. It shows that our Ising model Hamiltonian can well describe the physics.

We set the intensity of the external transverse magnetic pulse \( h_1 \sim 10^{-2}T \), it yields \( h_1 \sim 2.8\text{MHz} \). From the equation (33), we have

\[ \tau = 2m\pi/h_1 \sim 2.2 \times m \times 10^{-6} \text{ sec}. \]

Meanwhile, \( h_2 \) should be adjusted to meet the condition \( h_2 = \frac{m}{n} h_1 \). Since gyromagnetic ratio of \( ^1\text{C} \) is 0.25 of the one of \( ^1\text{H} \), the amplitude \( h_2 \) must be four times of \( h_1 \) (\( h_2 \geq 4h_1 \)), then the condition \( h_2 = \frac{m}{n} h_1 \) can be satisfied. We choose the one of solutions, \( n = 1, m = 1 \), that yields
Due to \( \Omega \sim 10^2 \), order of 10\(^2\), but the operating time \( \tau \) of such non-adiabatic geometric phase gate is only the order of 10\(^{-6}\) sec. The ratio \( \tau / \tau_c \sim 10^{10} - 10^{9} \) in NMR is high.

To summarize, We have studied Ising model of two nuclear spins. A single transverse rf magnetic pulse with multi-frequency is applied to manipulate quantum state simultaneously. By means of RTA, an arbitrary non-adiabatic geometric phase gate as a result, the controlled phase gate as well as A-A phase are also addressed. From estimation of parameters, we believe that our RTA is good approximation and the operation time of GPG \( \tau \) is order of 10\(^{-6}\) - 10\(^{-5}\) sec. The absence of dynamical contributions to the phase gate can decrease the error of dynamical fluctuation in quantum information process. Meanwhile, the non-adiabatic manipulation of quantum state in practice quantum computing is required that leads the study of non-adiabatic manipulation to implement the geometric phase gate.

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Appendix A

In this appendix, we would prove \( |c_k(t)| = \delta_k^i \) when \( h_1 \tau = 2m\pi \) and \( h_2 \tau = 2n\pi \) where \( m \) and \( n \) are integer numbers. According to eq.(26), \( c_{k}^{(i)}(t) = \frac{1}{4} \sum_{j=1}^{4} C_{i,j}^{(1)} e^{-iE_j t} C_{j,k} \), and eq.(23) of matrix \( C \), we get

\[
\begin{align*}
|c_{1}(t)| & = |c_{2}(t)| = |c_{3}(t)| = |c_{4}(t)| \\
\delta_1^i & = \delta_2^i = \delta_3^i = \delta_4^i = \frac{1}{2} \left( \cos \left( \frac{h_1 t + h_2}{2} \right) + \cos \left( \frac{h_1 t - h_2}{2} \right) \right) \\
& = \cos \left( \frac{h_1 t}{2} \right) \cos \left( \frac{h_2 t}{2} \right)
\end{align*}
\]

It is similar to obtain following results:

\[
\begin{align*}
|c_{1}(t)| & = |c_{2}(t)| = |c_{3}(t)| = |c_{4}(t)| \\
\delta_1^i & = \delta_2^i = \delta_3^i = \delta_4^i = \frac{1}{2} \left( \cos \left( \frac{h_1 t + h_2}{2} \right) + \cos \left( \frac{h_1 t - h_2}{2} \right) \right) \\
& = \cos \left( \frac{h_1 t}{2} \right) \cos \left( \frac{h_2 t}{2} \right)
\end{align*}
\]

When \( t = \tau, h_1 \tau = 2m\pi \) and \( h_2 \tau = 2n\pi \) (\( m, n \) : integer numbers), following results are obtained:

\[
|c_{1}(t)| = 1, \quad |c_{j}(t)| = 0, \quad i \neq j.
\]

Appendix B

In this appendix, we want to prove the equation (28):

\[
\delta_D^{(i)} = 0 : i = 1, 2, 3, 4.
\]

When \( h_1 = h_4, h_2 = h_3 \), the definition of \( \bar{H}(t) \) becomes (see eq.(11))

\[
\bar{H}(t) = \begin{pmatrix}
\epsilon_1 & -\frac{h_1}{2} f_3(t) & -\frac{h_2}{2} f_3(t) & 0 \\
-\frac{h_1}{2} f_3(t) & \epsilon_2 & 0 & -\frac{h_2}{2} f_1(t) \\
-\frac{h_2}{2} f_1(t) & 0 & \epsilon_3 & -\frac{h_2}{2} f_2(t) \\
0 & -\frac{h_2}{2} f_2(t) & -\frac{h_2}{2} f_2(t) & \epsilon_4
\end{pmatrix}
\]

where \( f_k(t) = e^{i(\Omega_k t + \phi_k)} \). According to the definition of dynamic phase, eq.(28), we have

\[
-\delta_D^{(i)} = \int_{0}^{\tau} dt \sum_{k,k'} c_{k}^{(i)}(t) c_{k'}^{(i)}(t) \langle m_k | \bar{H}(t) | m_{k'} \rangle
\]

\[
= \int_{0}^{\tau} dt \sum_{k=1}^{4} c_{k}^{(i)}(t) c_{k}^{(i)}(t) \epsilon_k
\]

\[
- \frac{h_2}{2} c_{2}^{(i)*}(t) c_{1}^{(i)}(t) e^{-i(\Omega_1 t + \phi_2)} e^{-i(\phi_1 t + \theta_1)} e^{-i(\phi_2 t + \theta_2)}
\]

\[
+ \frac{h_1}{2} c_{1}^{(i)*}(t) c_{2}^{(i)}(t) e^{-i(\Omega_2 t + \phi_1)} e^{-i(\phi_1 t + \theta_1)} e^{-i(\phi_2 t + \theta_2)}
\]

\[
+ \frac{h_1}{2} c_{2}^{(i)*}(t) c_{3}^{(i)}(t) e^{-i(\Omega_3 t + \phi_2)} e^{-i(\phi_2 t + \theta_2)} e^{-i(\phi_3 t + \theta_3)}
\]

\[
+ \frac{h_2}{2} c_{3}^{(i)*}(t) c_{4}^{(i)}(t) e^{-i(\Omega_4 t + \phi_3)} e^{-i(\phi_3 t + \theta_3)} e^{-i(\phi_4 t + \theta_4)}
\]

\[
+ h.c.
\]
We do the following calculations:

\[ \int_0^\tau dt c_1^{(1)*}(t)c_1^{(1)}(t) = \epsilon_1 \int_0^\tau dt \cos^2 \left( \frac{h_3}{2} t \right) \cos^2 \left( \frac{h_4}{2} t \right) = \frac{\epsilon_1}{4} \int_0^\tau dt [1 + \cos(h_3 t)][1 + \cos(h_4 t)] = \frac{\epsilon_1}{4} \left( \tau + \int_0^\tau dt \cos(h_3 t) \cos(h_4 t) \right) = \frac{\epsilon_1}{4} \tau. \]

\[ \int_0^\tau dt c_2^{(1)*}(t)c_2^{(1)}(t) = \epsilon_2 \int_0^\tau dt \cos^2 \left( \frac{h_1}{2} t \right) \sin^2 \left( \frac{h_2}{2} t \right) = \frac{\epsilon_2}{4} \int_0^\tau dt [1 + \cos(h_1 t)][1 - \cos(h_2 t)] = \frac{\epsilon_2}{4} \left( \tau - \int_0^\tau dt \cos(h_1 t) \cos(h_2 t) \right) = \frac{\epsilon_2}{4} \tau. \]

It is similar to have

\[ \int_0^\tau dt c_3^{(1)*}(t)c_3^{(1)}(t) = \epsilon_3 \int_0^\tau dt \sin^2 \left( \frac{h_1}{2} t \right) \cos^2 \left( \frac{h_2}{2} t \right) = \frac{\epsilon_3}{4} \tau, \]

\[ \int_0^\tau dt c_4^{(1)*}(t)c_4^{(1)}(t) = \epsilon_4 \int_0^\tau dt \sin \left( \frac{h_1}{2} t \right) \sin \left( \frac{h_2}{2} t \right) = \frac{\epsilon_4}{4} \tau. \]

Inserting results of (B2-B4) to (B1), we obtain \( \delta_D^{(1)}(\tau) = 0 \). Similar calculations also can show \( \delta_D^{(2,3,4)}(\tau) = 0 \). The conclusion of \( \delta_D^{(i)}(\tau) = 0 \) is proved for all \( i \).

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