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Entanglement and Geometric Phase for Two-Particle System in Nuclear Magnetic Resonance

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Abstract Evolution of entangled degree with geometric phases and initial conditions are investigated for two-particle system in nuclear magnetic resonance under cyclic evolution. We find that a perfect entanglement may be obtained by controlling the geometric phases and initial conditions, which is helpful to implement a universal entangling geometric quantum gate in nuclear magnetic resonance.

Keywords Entangled degree · Geometric phase · Entangling geometric quantum gate

1 Introduction

Entanglement is a quintessential property of quantum mechanics that sets it apart from any classical physical theory. A physical feature of entanglement is that it gives rise to correlations between two physical subsystems, which cannot be explained by any local realistic description in classical mechanics. The idea of non-local correlation among remote particles was originally exploited in a classic paper on the incompleteness of quantum mechanics by Einstein, Podolsky and Rosen (EPR)[1], further conceptualized in a seminal paper by Schrödinger [2, 3], and a subsequent work by Bell [4–6]. For two entangled particles, Einstein and his co-workers [1] would like to show that quantum mechanics cannot in all situations be a complete description of physical reality. Incidentally, these particles (EPR pairs) have now found wide applications in the area of quantum information theory.

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An entangled state is a state of a composite system that cannot be separated into product states in terms of the subsystems. For a bipartite pure state, the degree of entanglement can be found from the Schmidt numbers [4–6]. For a mixed state, there is the Peres-Horodecki theorem [7, 8] concerning partial transposition, which can be used to determine if a state is entangled or separable for the dimension being low, especially 2×2 or 2×3 systems. Indeed, in recent years, quantum entanglement has become an important physical resource for quantum communication and information processing like quantum teleportation [9, 10], superdense coding [11], quantum key distribution [12] and telecoloning [13].

Besides quantum entanglement, quantum mechanics harbors another surprising elegant idea from the acquisition of a purely geometric phase when a state undergoes a closed evolution in parameter space [14]. Recently, the geometric phase has been attracting increasing interest because of its importance for understanding and implementing quantum computation in real physical systems [15–17]. Geometric (Holonomic) quantum computation is a scheme intrinsically fault-tolerant and therefore resilient to certain types of computational errors [18–20]. Once more the holonimies are built up when a quantum system is driven to a cyclic or noncyclic evolution through adiabatic or nonadiabatic change in the controllable parameters in the Hamiltonian. Such holonomies can be either Abelian phase factors or non-Abelian unitary operations if the spectrum of the Hamiltonian is degenerate.

It is known that geometric quantum gate of two-particle system may be constructed based on the geometric quantum gate of single-particle system [21]. However, non-local correlation between the two-qubit system may be lost. Therefore, it is important to construct a universal entangled geometric quantum gate [18–20], where the quantum characters with both entanglement and geometry are fully applied, and it is interesting to study the relation between the entangled degree and the geometric phase.

2 Two-Qubit System in Nuclear Magnetic Resonance System

For two-qubit system in nuclear magnetic resonance system (NMR), the most natural two-qubit gate is directly generated by the spin-spin coupling Hamiltonian [18]. Thus the Hamiltonian is written as

$$\begin{aligned} H(t) = &-\frac{1}{2}\Omega_0((\sigma_{1x}+\sigma_{2x})\sin\theta\cos\omega t + (\sigma_{1y}+\sigma_{2y})\sin\theta\sin\omega t) \\ &- \frac{1}{2}\Omega_1(\sigma_{1z}+\sigma_{2z})\cos\theta + \frac{1}{4}\lambda\vec{\sigma}_1\cdot\vec{\sigma}_2, \end{aligned} \tag{1}$$

where λ is the strength of the interaction between two qubits. While $\Omega_i = g\mu B_i/\hbar$ with $g(\mu)$ are the gyromagnetic, B_i $(i=0,1)$ and θ act as an external controllable parameters and can be experimentally changed, and σ_i $(i=x,y,z)$ are Pauli operators.

By redefining $\vec{J} = \vec{\sigma_1} + \vec{\sigma_2}$, where $[J_m, J_n] = 2i\epsilon_{mnl}J_l (m,n,l = x,y,z)$ are satisfied, we rewrite the Hamiltonian (1) according to J_x, J_y, J_z and $\vec{J}^2$, i.e.,

$$\begin{aligned} H(t) = &-\frac{1}{2}\Omega_0(J_x\sin\theta\cos\omega t + J_y\sin\theta\sin\omega t) \\ &- \frac{1}{2}\Omega_1 J_z\cos\theta + \frac{1}{8}\lambda(\vec{J}^2 - 6). \end{aligned} \tag{2}$$

For the initial time $t=0$ the magnetic field lies in the x–z plane with the Hamiltonian $H(0) = -\frac{1}{2}\Omega_0 J_x\sin\theta - \frac{1}{2}\Omega_1 J_z\cos\theta + \frac{1}{8}\lambda(\vec{J}^2 - 6)$.

As the evolving time t increases the magnetic field rotates in the x–y plane. In order to describe the process, we use the Baker-Campbell-Hausdorff formula to rewrite the Hamiltonian as

$$H(t) = e^{-\frac{i}{2}\omega t J_z} H(0) e^{\frac{i}{2}\omega t J_z}. \tag{3}$$

It is known that the geometric gates based on the nonadiabatic cyclic evolution depend only on some global features, which makes them robust to certain computational errors. Therefore, we are interested in an exact solution of the Schrödinger equation for the wave function $|\psi(t)\rangle$ with a cyclic evolution of NMR system. According to (3), a unitary transformation is given by

$$|\psi'(t)\rangle = e^{\frac{i}{2}\omega t J_z}|\psi(t)\rangle, \tag{4}$$

which corresponds to rotate the state vector $|\psi(t)\rangle$ clockwise by an angle $(-\omega t)$ and keep the observables the same. Thus, $\psi'(t)$ satisfies the following equation,

$$i\frac{\partial|\psi'(t)\rangle}{\partial t} = H_{eff}|\psi'(t)\rangle, \tag{5}$$

where the effective Hamiltonian can be obtained by using (4) and (5). We find

$$H_{eff} = -\frac{1}{2}\Omega e^{-\frac{i}{2}\chi J_y}\left(J_z + \frac{1}{8}\lambda(\vec{J}^2 - 6)\right)e^{\frac{i}{2}\chi J_y}, \tag{6}$$

where $\Omega = (\Omega_0^2 \sin^2\theta + (\Omega_1 \cos\theta + \omega)^2)^{1/2}$ and $\chi = \tan^{-1}\{\Omega_0 \sin\theta / \Omega_1 \cos\theta + \omega)$.

Because the effective Hamiltonian H_{eff} is independent of the evolving time, the wave function can be expressed as

$$|\psi(t)\rangle = e^{-\frac{i}{2}\omega t J_z} e^{-itH_{eff}}|\psi(0)\rangle, \tag{7}$$

where $|\psi(0)\rangle$ is consist of eigenstates of the effective Hamiltonian. The eigenequation can be written as

$$H_{eff}\Phi_{Jk} = \left(-\frac{1}{2}\Omega k + \frac{1}{2}\left(J(J+1) - \frac{3}{2}\right)\right)\Phi_{Jk}, \tag{8}$$

where $J = 1$ with $k = 1, 0, -1$ or $J = 0$ with $k = 0$. The corresponding eigenfunctions for $J = 1$ are expressed respectively by $\Phi_{1+1} = \exp\{-\frac{i}{2}\chi J_y\}|00\rangle = \cos^2\frac{\chi}{2}|00\rangle + \sin\frac{\chi}{2}\cos\frac{\chi}{2}(|01\rangle + |10\rangle) + \sin^2\frac{\chi}{2}|11\rangle$, $\Phi_{10} = \exp\{-\frac{i}{2}\chi J_y\}\frac{1}{\sqrt{2}}(|01\rangle + |10\rangle) = \frac{1}{\sqrt{2}}(-\sin\chi|00\rangle + \cos\chi(|01\rangle + |10\rangle) + \sin\chi|11\rangle)$ and $\Phi_{1-1} = \exp\{-\frac{i}{2}\chi J_y\}|11\rangle = \sin^2\frac{\chi}{2}|00\rangle - \sin\frac{\chi}{2}\cos\frac{\chi}{2}(|10\rangle + |01\rangle) + \cos^2\frac{\chi}{2}|11\rangle$. For $J = 0$, the eigenfunction is $\Phi_{00} = \exp\{-\frac{i}{2}\chi J_y\}\frac{1}{\sqrt{2}}(|01\rangle - |10\rangle) = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle))$. While $\{|00\rangle, |01\rangle, |10\rangle$ and $|11\rangle\}$ are the computational basis for the two-qubit system.

The evolution of wave function, under the cyclic condition with the period $T = 2\pi/\omega$, is given by

$$\begin{aligned}|\psi(T)\rangle = U(T)|\psi(0)\rangle &= \sum_{J,k} e^{-\frac{i}{2}\omega T J_z} e^{-iTH_{eff}}\Phi_{Jk} \\ &= \sum_{J,k} e^{-i\pi k} e^{-i\frac{\pi}{\omega}(-k\Omega + \lambda(J(J+1) - \frac{3}{2}))}\Phi_{Jk},\end{aligned} \tag{9}$$

where $U(T)=e^{-\frac{i}{2}\omega T J_z}e^{-iTH_{eff}}$. From (9), the total phase for the given J and k may be written as

$$\alpha_{Jk}=\pi k+\frac{\pi}{\omega}\left(-k\Omega+\lambda\left(J(J+1)-\frac{3}{2}\right)\right), \tag{10}$$

and the dynamic phase can be calculated by

$$\gamma^d_{Jk}=\int_0^T\langle\psi(t)|H(t)|\psi(t)\rangle dt=\frac{\pi}{\omega}\left(-\Omega k+\lambda\left(J(J+1)-\frac{3}{2}\right)\right)+k\pi\cos\chi. \tag{11}$$

Thus, the geometric phase is

$$\gamma^g_{Jk}=\alpha_{Jk}-\gamma^d_{Jk}=\pi k(1-\cos\chi)=k\gamma, \tag{12}$$

where $\gamma=\pi(1-\cos\chi)=\pi(1-(\Omega_1\cos\theta+\omega)/\Omega)$.

By analyzing (10)–(12), we find that when the following relation is satisfied,

$$(1+x)(\Omega_1\cos\theta+\omega)=(\Omega/\omega+x)\Omega, \tag{13}$$

the total, dynamic and geometric phases have the following relations,

$$\gamma^d_{Jk}=\frac{\pi\lambda}{\omega}\left(J(J+1)-\frac{3}{2}\right)+x\gamma^g_{Jk}, \tag{14}$$

and

$$\alpha_{Jk}=\frac{\pi\lambda}{\omega}\left(J(J+1)-\frac{3}{2}\right)+(1+x)\gamma^g_{Jk}. \tag{15}$$

It is noted that x may be either determined by (13), i.e.,

$$x=\frac{(\Omega_1\cos\theta+\omega)-\Omega^2/\omega}{\Omega-(\Omega_1\cos\theta+\omega)}, \tag{16}$$

where we do not need any choice of the parameters for the relations (14) and (15), or used as an arbitrary parameter by adjusting the initial physical quantities, such as Ω_0,Ω_1,θ and ω, according to requirements in experiment or in theory. By solving (13), we find

$$\Omega_0^2\sin^2\theta=(1+x)\omega(\Omega_1\cos\theta+\omega)-(\Omega_1\cos\theta+\omega)^2 \\ +\frac{1}{2}x^2\omega^2\pm x\omega^{3/2}\sqrt{(1+x)(\Omega_1\cos\theta+\omega)+\frac{1}{4}x^2\omega}, \tag{17}$$

which implies that there exist, indeed, some solutions with the physical meaning in (13). In other words, by adjusting the magnetic field parameter Ω_1 in z-direction and angle θ in x–y plane for given x and frequency ω, we can find a positive value of magnetic field parameter Ω_0 in the x–y plane. For example, for $x=0$, if $\sin\theta>0$ and $\cos\theta<0$ are chosen, $\Omega_0=\sqrt{\omega(\Omega_1\cos\theta+\omega)-(\Omega_1\cos\theta+\omega)^2}/\sin\theta$ will be determined. If $\sin\theta<0$ and $\cos\theta<0$ are chosen, $\Omega_0=-\sqrt{\omega(\Omega_1\cos\theta+\omega)-(\Omega_1\cos\theta+\omega)^2}/\sin\theta$ will be determined. For $x=1$, similarly, by choosing $-(9/8)\omega<\Omega_1\cos\theta<\sqrt{3/2}\omega$, we can get a group of positive Ω_0 at least. These choices may be easy to be realized for both experiment and theory.

It is noted in (14) and (15) that our approach for two-qubit system is neither different from the conventional nor unconventional approaches, where the total, dynamic and geometric phases satisfy the mathematic expressions. There doesn't exist, especially, solution of the dark state because of the spin-spin interaction.

From (9), we know that the eigenstates of the effective Hamiltonian H_{eff} can evolve cyclically. The system may be separated two subspace with $J = +1$ and $J = 0$. For subsystem $J = 1$, the input states are Φ_{1+1}, Φ_{1+0} and Φ_{1-1} in quantum gate. After a cyclic evolution, the output state is

$$\begin{aligned}|\psi_1(f)\rangle = \exp\left\{-i\frac{\pi\lambda}{\omega}\left(J(J+1)-\frac{3}{2}\right)\right\}(b_{1+1}\exp\{-i(1+x)\gamma\}\Phi_{1+1}+b_{10}\Phi_{10}\\ + b_{1-1}\exp\{i(1+x)\gamma\}\Phi_{1-1}),\end{aligned} \tag{18}$$

where b_{Jk} $(j = 1, k = 1, 0, -1)$, decided by the initial states, are constant independent of the evolving time. It is noted that $|\psi_1(f)\rangle$ is an entangled state.

For subsystem with $J = 0$, similarly, the input state is Φ_{00} and the output one is

$$|\psi_0(f)\rangle = b_{00}\exp\left\{i\frac{3\pi\lambda}{2\omega}\right\}\Phi_{00}, \tag{19}$$

which is a unentangled state.

We see that the phase factors $\exp\{-i\frac{\pi\lambda}{\omega}(J(J+1)-\frac{3}{2})\}$ and $\exp\{i\frac{3\pi\lambda}{2\omega}\}$ can be regarded as overall phase factors for spin $J = 1$ subsystem and spin $J = 0$ subsystem respectively, which are not important and may be dropped in quantum computation under the condition that the control qubit is far away from the resonance condition for the operation of the target qubit so that the strength λ of the interaction between two qubits is very small.

Geometric phases are important in both a fundamental point of physical view and their applications. On the one hand, the physical system retains a memory of its evolution in terms of the geometric phase. On the other hand, the geometric quantum computation is a scheme intrinsically fault-tolerant and therefore resilient to certain types of computational errors. Therefore, it is very interesting to introducing the geometric phase as a basically physical degree of freedom. According to (12), we find

$$\cos\chi = 1-\frac{\gamma}{\pi}, \qquad \sin\chi = \sqrt{1-\left(1-\frac{\gamma}{\pi}\right)^2}. \tag{20}$$

Thus the wave function $|\psi_1(f)\rangle$ may be expressed by the geometric phase as

$$\begin{aligned}|\psi_1(f)\rangle = {} & \left(b_{1+1}e^{-i(1+x)\gamma}\left(1-\frac{\gamma}{2\pi}\right)-\frac{1}{\sqrt{2}}b_{10}\sqrt{1-\left(1-\frac{\gamma}{\pi}\right)^2}+b_{1-1}e^{i(1+x)\gamma}\frac{\gamma}{2\pi}\right)|00\rangle\\ & + \left(\frac{1}{2}b_{1+1}e^{-i(1+x)\gamma}\sqrt{1-\left(1-\frac{\gamma}{\pi}\right)^2}+\frac{1}{\sqrt{2}}b_{10}\left(1-\frac{\gamma}{\pi}\right)\right.\\ & \left. - \frac{1}{\sqrt{2}}b_{1-1}e^{i(1+x)\gamma}\sqrt{1-\left(1-\frac{\gamma}{\pi}\right)^2}\right)|01\rangle\\ & + \left(\frac{1}{2}b_{1+1}e^{-i(1+x)\gamma}\sqrt{1-\left(1-\frac{\gamma}{\pi}\right)^2}+\frac{1}{\sqrt{2}}b_{10}\left(1-\frac{\gamma}{\pi}\right)\right.\end{aligned}$$

$$- \frac{1}{\sqrt{2}} b_{1-1} e^{i(1+x)\gamma} \sqrt{1 - \left(1 - \frac{\gamma}{\pi}\right)^2} \Bigg) |10\rangle$$

$$+ \left(b_{1+1} e^{-i(1+x)\gamma} \frac{\gamma}{2\pi} + \frac{1}{\sqrt{2}} b_{10} \sqrt{1 - \left(1 - \frac{\gamma}{\pi}\right)^2} + b_{1-1} e^{i(1+x)\gamma} \left(1 - \frac{\gamma}{2\pi}\right) \right) |11\rangle, \tag{21}$$

which means that the wave function may involve in terms of the geometric phase instead of the external parameters of NMR system. Differently from the conventional and unconventional approaches to the geometric quantum gate, we do not need any operations to cancel the dynamic phase.

3 Entangled Degree

From the point of view of a possible application, it is not only important to determine whether a given state is entangled, but also to quantify the degree of entanglement [22]. Among several such quantities, the entanglement of information introduced by Wootters al. [22] is often used for this purpose. Let $\rho(f) = |\psi_1(f)\rangle\langle\psi_1(f)|$ be the density matrix of a pair of qubits 1 and 2. The density matrix can be either pure or mixed. The entangle degree, called as concurrence, corresponding to density matrix will be defined according to the eigenvalues of the following operator,

$$\overline{\rho}(f) = \rho(f) \left(\sigma_1^y \otimes \sigma_2^y\right) \rho^*(f) \left(\sigma_1^y \otimes \sigma_2^y\right), \tag{22}$$

where $\rho^*(f)$ denotes the complex conjugation of $\rho(f)$ in the standard basis and σ^y is the well-known time reversal operator for spin-$\frac{1}{2}$ quantum systems. Thus, the concurrence for two entangled qubits can be calculated explicitly by

$$C = \mathbf{Max} \left\{0, \sqrt{\lambda_1} - \sqrt{\lambda_2} - \sqrt{\lambda_3} - \sqrt{\lambda_4}\right\}, \tag{23}$$

where the quantities λ_j $(j = 1, 2, 3, 4)$ are the eigenvalues arranged in decreasing order of the matrix. It is noted that the concurrence varies from $C = 0$ for a completely unentangled state to $C = 1$ for a maximally entangled state [23]. One finds that, furthermore, the entangled degree described by the concurrence with the wave function (18) may be expressed as

$$C = 2|a_1 a_2 - a_0 a_3|, \tag{24}$$

where

$$a_0 = b_{1+1} e^{-i(1+x)\gamma} \left(1 - \frac{\gamma}{2\pi}\right) - \frac{1}{\sqrt{2}} b_{10} \sqrt{1 - \left(1 - \frac{\gamma}{\pi}\right)^2} + b_{1-1} e^{i(1+x)\gamma} \frac{\gamma}{2\pi}, \tag{25}$$

$$a_1 = \frac{1}{2} b_{1+1} e^{-i(1+x)\gamma} \sqrt{1 - \left(1 - \frac{\gamma}{\pi}\right)^2} + \frac{1}{\sqrt{2}} b_{10} \left(1 - \frac{\gamma}{\pi}\right)$$

$$- \frac{1}{\sqrt{2}} b_{1-1} e^{i(1+x)\gamma} \sqrt{1 - \left(1 - \frac{\gamma}{\pi}\right)^2}, \tag{26}$$

$$a_2 = \frac{1}{2} b_{1+1} e^{-i(1+x)\gamma} \sqrt{1 - \left(1 - \frac{\gamma}{\pi}\right)^2} + \frac{1}{\sqrt{2}} b_{10} \left(1 - \frac{\gamma}{\pi}\right)$$
$$- \frac{1}{\sqrt{2}} b_{1-1} e^{i(1+x)\gamma} \sqrt{1 - \left(1 - \frac{\gamma}{\pi}\right)^2}, \tag{27}$$

$$a_3 = b_{1+1} e^{-i(1+x)\gamma} \frac{\gamma}{2\pi} + \frac{1}{\sqrt{2}} b_{10} \sqrt{1 - \left(1 - \frac{\gamma}{\pi}\right)^2} + b_{1-1} e^{i(1+x)\gamma} \left(1 - \frac{\gamma}{2\pi}\right). \tag{28}$$

From (24)–(28), we see that the concurrence is expressed as a function of the geometric phase and initial conditions. Therefore, it is called as geometrically entangled degree.

4 Results and Conclusions

At initial time $t = 0$, the physical states are input by Φ_{1+1}, Φ_{1+0} and Φ_{1-1} in our geometric quantum gate. It is obvious that these states are entangled. The degrees of entanglement depend on the external conditions.

Evolving curves of the concurrence are shown at Fig. 1 as a function of geometric phase for the different parameters x with the initial condition $b_{1+1} = b_{10} = b_{1-1} = \frac{1}{\sqrt{3}}$. We find that the entangled degree oscillates and depends strongly on the x. With the increasing of x, the maximum value of concurrence becomes larger and moves toward lower value of geometric phase at range of $0 < \gamma < 2\pi$. At the same time, the evolution of entanglement becomes complicated. The minimum value is larger than zero, which means that a universal entangling state is obtained under the case without including the environment coupling interaction.

We find that, furthermore, the evolving behavior of entanglement is very different for the different initial conditions with increasing of the geometric phase (see Figs. 2–5). In case of the same x, generally, there exists higher entangled degree for the initial conditions with the parameters $b_{1+1} = b_{10} = \frac{1}{\sqrt{3}}$, $b_{1-1} = -\frac{1}{\sqrt{3}}$ and $b_{1+1} = \frac{1}{\sqrt{3}}$, $b_{10} = \frac{\sqrt{5}}{\sqrt{12}}$, $b_{1-1} = -\frac{1}{2}$ in comparison with another two-group parameters $b_{1+1} = b_{10} = b_{1-1} = \frac{1}{\sqrt{3}}$ and $b_{1+1} = \frac{1}{\sqrt{3}}$, $b_{10} =$

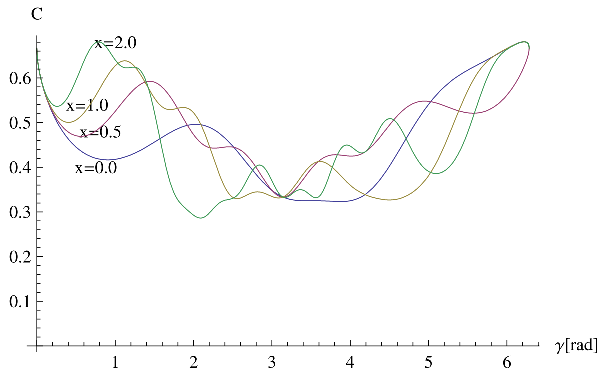

Fig. 1 Concurrence as a function of geometric phase for the different x with the initial conditions $b_{1+1} = b_{10} = b_{1-1} = \frac{1}{\sqrt{3}}$

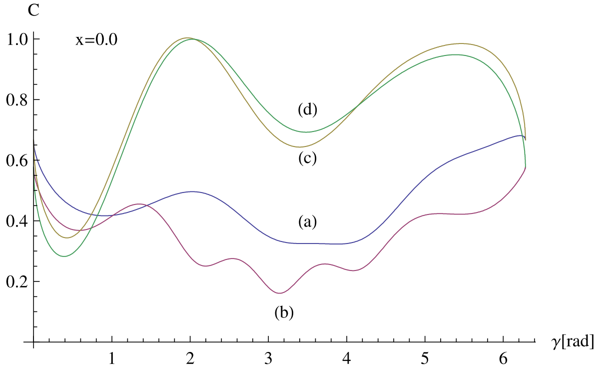

Fig. 2 Concurrence as a function of geometric phase for $x=0$ with the different initial conditions
(a) $b_{1+1}=b_{10}=b_{1-1}=\frac{1}{\sqrt{3}}$,
(b) $b_{1+1}=\frac{1}{\sqrt{3}}$, $b_{10}=\frac{\sqrt{5}}{\sqrt{12}}$, $b_{1-1}=\frac{1}{2}$,
(c) $b_{1+1}=b_{10}=\frac{1}{\sqrt{3}}$, $b_{1-1}=-\frac{1}{\sqrt{3}}$, (d) $b_{1+1}=\frac{1}{\sqrt{3}}$, $b_{10}=\frac{\sqrt{5}}{\sqrt{12}}$, $b_{1-1}=-\frac{1}{2}$

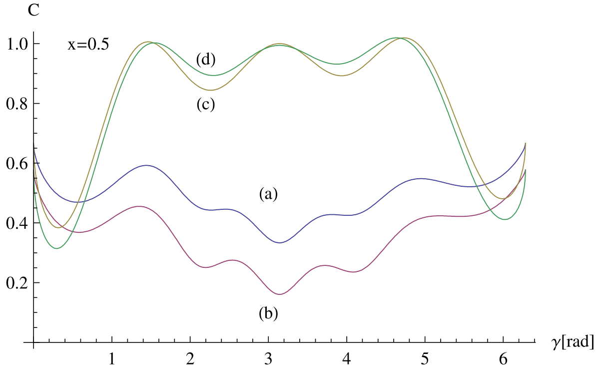

Fig. 3 Same with Fig. 2 with $x=0.5$

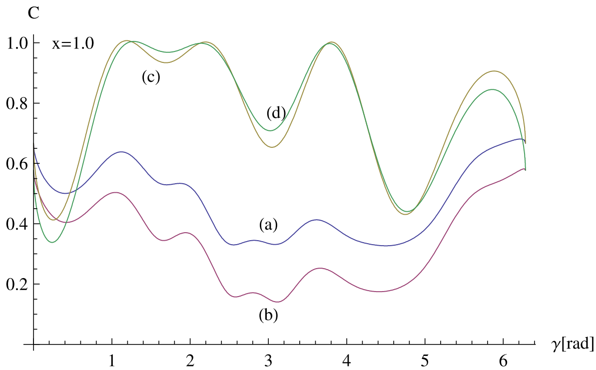

Fig. 4 Same with Figs. 2 and 3 with $x=1.0$

$\frac{\sqrt{5}}{\sqrt{12}}$, $b_{1-1}=\frac{1}{2}$. Especially, the maximum values trend to one, i.e., the maximum entangled state, for the larger x at some geometric phases. It is obvious that the concurrence is not a single-value function of the geometric phase. There exist several oscillated peaks in the evolving curve with the geometric phase. From Figs. 2–5, we see that the number of peaks become more with increasing of x. Therefore, it offers a wide choice between the maximum entangling state and the geometric phase.

In summary, the correlation between the entangled degree and geometric phase in NMR with two-qubit system is investigated, which may be helpful to effectively use both the geo-

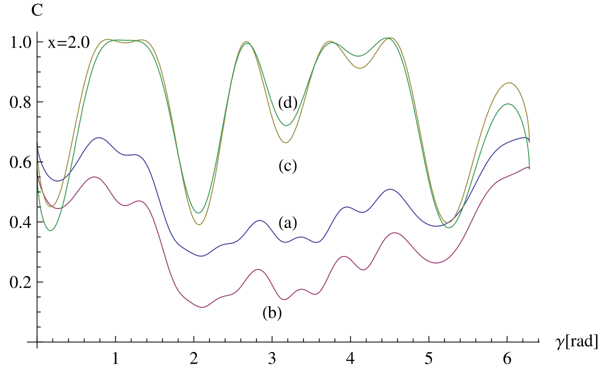

Fig. 5 Same with Figs. 2–4 with $x = 2.0$

metric and nonlocal properties of quantum system in the quantum computation. We show that, furthermore, the geometric phase may be taken as a basic degree of freedom in NMR system. By taking the geometric phase as an elementary degree of freedom, it may effectively decrease errors from the time manipulation. Especially, It also avoids the problems associated with types of errors that do not preserve cyclicity for the physical systems. Because the geometric phase has observable effect, the geometric phase and initial condition may be controlled by the external parameters. Thus, by choosing the suitable geometric phases and initial conditions, it may be realize a geometric quantum gate with higher entangled degree.

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