Off-diagonal geometric phase in composite systems

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The effect due to the inter-subsystem coupling on the off-diagonal geometric phase in a composite system is investigated. We analyze the case where the system undergo an adiabatic evolution. Two coupled qubits driven by time-dependent external magnetic fields are presented as an example, the off-diagonal geometric phase as well as the adiabatic condition are examined and discussed.

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A quantal system in a eigenstate $|\psi_j(\vec{s})\rangle$, adiabatically transport round a circuit by varying parameters $\vec{s} = (s_1, s_2, ...)$ in its Hamiltonian $H(\vec{s})$, will acquire a geometric phase $\Gamma_d$ in addition to the familiar dynamical phase $\Gamma_d$ given by $\Gamma_d = \text{arg} \langle \psi_j(\vec{s}_1) | \psi_j(\vec{s}_2) \rangle$; $\Gamma_d$ is the well known geometric phase (or Berry phase) when $\vec{s}_1 = \vec{s}_2$ and the state $|\psi_j(\vec{s})\rangle$ is transported adiabatically along a closed loop $[1]$. The geometric phase has been extended to mixed states $[2,3,4]$ and open systems $[5]$. Recent studies on the geometric phases found that the (diagonal) geometric phase itself could not exhaust all information containing in phases acquired when the quantum system undergo an adiabatic evolution, this can be understood as follows. Consider parallel transport generated by the operator $U(\vec{s})$ of the $j$th eigenstate $|\psi_j(\vec{s})\rangle$, in the case of $|\psi_k(\vec{s}_2)\rangle = U(\vec{s})|\psi_j(\vec{s}_1)\rangle$ ($j \neq k$) the scalar product $\langle \psi_k(\vec{s}_2) | U(\vec{s}) | \psi_j(\vec{s}_1) \rangle$ vanishes and the (diagonal) geometric phase becomes undefined. The only information left is the cross scalar product $\langle \psi_k(\vec{s}_2) | U(\vec{s}) | \psi_j(\vec{s}_1) \rangle$; this gives rise to the definition of the off-diagonal geometric phase factor $\tilde{\gamma}_{jk}$ ($j \neq k$)

$$
\tilde{\gamma}_{jk} = \sigma_{jk} \sigma_{kj},
$$
and $\phi_{jk} = z / |z|$. This definition satisfies the requirement of gauge and reparametrization invariant, hence it is solely a property of the geometry of Hilbert space and consequently is measurable. The adiabatic assumption in $[6]$ was subsequently removed $[11]$ and the second order off-diagonal pure state geometric phase was verified $[12]$. More recently, the study on the pure state off-diagonal geometric phase has been extended to mixed quantal states and an experiment to test the off-diagonal geometric phase was proposed $[13]$. All these studies are available for single particle systems or composite systems without intersubsystem couplings.

In this paper, we investigate the effect due to the inter-subsystem coupling on the off-diagonal phase in composite systems. This question arises when we examine the application of geometric phase in quantum information processing $[14,15,16,17,18]$, there all systems are composite and most subsystems interact with each other in order to store information and implement quantum logic gate. Besides, entanglement might be created among subsystems via interaction and it was proved to be a dominant factor in mixed state geometric phase $[19]$. Thus how inter-subsystem coupling may change the geometric phase of the system is of interest on its own. We will examine the off-diagonal geometric phase for a bipartite system consisting of two-coupled spin-1/2 (or quantum bit), both of them are driven by time-dependent magnetic fields. The Hamiltonian describing such a system reads $[10]$ (with $\hbar = 1$, hereafter).

$$
H(t) = 4\xi s_x^1 \otimes s_x^2 + \mu \vec{B}(t) \cdot (s_1 + s_2),
$$

where $\xi$ is the exchange interaction constant (assumed positive without loss of generality), $\mu$ is the gyromagnetic ratio, $s_j = (s_j^x, s_j^y, s_j^z)$ is the $k$th spin operator ($j = 1, 2$) composed of the pauli matrices. $\vec{B}(t) = (B_x(t), B_y(t), B_z(t))$ represents the time-dependent magnetic field $\vec{B}(t)$, and we will make use of notation $\vec{\beta} = (\beta_x, \beta_y, \beta_z) = \mu \vec{B}$ in latter discussions. The instantaneous eigenstates of $H(t)$ can be written as

$$
|\phi_j(t)\rangle = \frac{1}{\sqrt{N_j}}\beta_x + i\beta_y - (E_x - \xi + \beta_z)|\downarrow\rangle + (E_j - \xi + \beta_z)|\uparrow\rangle - \frac{(\beta_z - i\beta_y)(E_j - \xi + \beta_z)}{\sqrt{2}(\xi + \beta_z - E_j)}|\downarrow\rangle,
$$

and the corresponding eigenvalues satisfy

$$
E^3 - \xi E^2 - (\beta_x^2 + \beta_y^2 + \beta_z^2 + \xi^2)E
$$

and

$$
-\xi(\beta_x^2 - \beta_y^2 - \beta_z^2 - \xi^2) = 0,
$$

where $N_j$ is the number of eigenstates of $H(t)$ with energy $E_j$. The total system is investigated. We analyze the case where the system undergo an adiabatic evolution. Two coupled qubits driven by time-dependent external magnetic fields are presented as an example, the off-diagonal geometric phase as well as the adiabatic condition are examined and discussed.

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and taking fields. Clearly, the energies of the adiabatic states have avoided crossings. Indeed, a Gaussian pulse, centered at $t_{\Omega}(t)$ and set $\Omega_0 = 2.5\xi$, $\omega = 0.7\xi$, $A = 0.075\xi$ for this plot. The time $t$ was chosen in units of $1/(2\pi\xi)$.

where $|\psi_j^+\rangle = \frac{1}{\sqrt{2}}(|\downarrow\rangle_1|\uparrow\rangle_2 + |\uparrow\rangle_1|\downarrow\rangle_2)$ with $|\downarrow\rangle_k$ and $|\uparrow\rangle_k$ denoting, respectively, the spin-down ($m = -\frac{1}{2}$) and spin-up ($m = \frac{1}{2}$) states of the $k$th spin. This Hamiltonian is of relevance to NMR experiment where Carbon-13 labelled chloroform in $d_6$ acetone may be used as the sample. The single $^{13}C$ nucleus and the $^1H$ nucleus play the role of the two spin-$\frac{1}{2}$, the spin-spin coupling constant in this case is $4\xi \approx (2\pi)214.5$Hz. The quantum system initially in $|\psi_k(0)\rangle$ driven by the time-dependent magnetic field would acquire non-zero off-diagonal geometric phases when it evolves to the other instantaneous eigenstates $|\psi_j(t)\rangle$ ($j \neq k$), to see this is exactly the case in our discussion, we propose to use a magnetic field which rotates in the $xy$ plane at constant frequency $\omega$, $\beta_x(t) = \Omega(t)\cos \omega t$, $\beta_y(t) = \Omega(t)\sin \omega t$ and varies linearly in the $z$ direction, $\beta_z(t) = At$. As shown in Ref. [20], the energies of the bare (diabatic, or $\Omega(t) = 0$) states cross at two distinct times (for $\omega < 2\xi$) $t_a = (\omega + 2\xi)/A$ and $t_b = \omega/A$, this was illustrated in figure 1-(a), there the energies of the adiabatic states have avoided crossings due to the coupling of the system to the external driving fields. Clearly, state $|\downarrow\downarrow\rangle$ may undergo an adiabatic evolution ending in $|\psi_j^+\rangle$ by properly designing a pulse-shaped time dependence for the transverse-field envelope $\Omega(t)$, with such a choice the field-induced interaction is maximum at $t_a$ and can be made negligible at the other crossings. In deed, a Gaussian pulse, centered at $t_a$

$$\Omega(t) = \Omega_0 e^{-(t-t_a)^2/T^2}$$  

is one of the choices that satisfies the requirements, and the solid lines in figure 1-(a) are plotted for the instantaneous eigenvalues with this choice. The time $t_a$ at which the adiabatic states have avoided crossings depends on $\xi$ and can be made negligible at the other crossings. So, the inter-subsystem coupling would affect the adiabaticity of the system. Mathematically, the adiabatic condition can be given by

$$\frac{1}{\sqrt{2}}|\Omega\Delta - \Omega\Delta| << (2\Omega^2 + \Delta^2)^{\frac{3}{2}}$$  

with $\Delta = 2\xi + \omega - At$.

To proceed further, we introduce new notations $|1\rangle \equiv |\downarrow\rangle$, $|2\rangle \equiv |\psi_1^+\rangle$ and $|3\rangle \equiv |\uparrow\uparrow\rangle$ to simplify the representation. With these notations, the off-diagonal geometric phase factor can be expressed as $\gamma_{12}(t) = \sigma_{12}(t)\sigma_{21}(t)$ with

$$\sigma_{12}(t) = \Phi[|1\rangle|\phi_2(t)\rangle]$$

$$\sigma_{21}(t) = \Phi[|2\rangle|\phi_1(t)\rangle].$$  

Here $|\phi_j(t)\rangle = U^{\dagger}|j\rangle$ ($j = 1, 2$) denotes the parallel transported state starting from $|j\rangle$, for an adiabatic evolution it would coincide with the instantaneous eigenstate of the Hamiltonian except a dynamical phase factor difference. In the qubit (two-level) case, it is proved that the off-diagonal geometric phase factor $\gamma_{ij}$ becomes $-1$ for any
path on the Bloch sphere. The situation under consideration is quite different from the qubit case, it represents coupled two qubits driven by a varying magnetic field, since the singlet state $\langle \psi_t^{-} \rangle = \frac{1}{\sqrt{2}}(|\downarrow \downarrow \rangle - |\uparrow \uparrow \rangle)$ is isolated from the triplet in this model, it also describes a three-level system precessing in a magnetic field for the special inter-subsystem coupling $s_1^z \otimes s_2^z$. The numerical results for the off-diagonal geometric phase $\Gamma_{12} = arg(\gamma_{12})$ were shown in figure 2, where we plotted $\Gamma_{12}$ as a function of time (figure 2-(b), dotted line), the diagonal geometric phase $\Gamma_3 = arg(\gamma_3) = arg(\Phi(|\uparrow \uparrow \rangle,|\psi_3(t)\rangle))$ was also illustrated for making a contrast with $\Gamma_{12}$. It is clear that, the system starts acquiring off-diagonal geometric phases from $t \approx 10\left(\frac{1}{2\pi\xi}\right)$, when the population begin changing dramatically, and stops gaining it at $t \approx 30\left(\frac{1}{2\pi\xi}\right)$, from that instant of time the populations of the three involved levels remain constant. As figure 2-(a) shows, the two eigenstates, $|1\rangle$ and $|2\rangle$, at the final point of the path are a permutation of the initial states, i.e., $|1(\tilde{s}_2)\rangle = |2(\tilde{s}_1)\rangle$, $|2(\tilde{s}_2)\rangle = |1(\tilde{s}_1)\rangle$, where $\tilde{s}_1$ and $\tilde{s}_2$ denote the initial and the final point on the path, respectively. This permutation properties lead to $\Gamma_{12}\Gamma_3 = -1$ (figure 3-(b)) as predicted in [10].

Now, we turn to discuss the effect due to the inter-subsystem coupling on the off-diagonal geometric phase of the composite system, the inter-subsystem coupling is fixed for a specific sample in general, for instance, in NMR experiment the coupling constant $\xi = (2\pi)214.5Hz$, where $^{13}C$ and $^1H$ in $d_6$ acetone act as the two qubits. We might change the ratio of the inter-subsystem coupling $\xi$ to the external magnetic field driving $|\tilde{B}|$ via adjustable quantities $A$ and $\Omega_0$ in Eq. 5 and $\beta_a(t) = At$, this way we could get the effect of the inter-subsystem coupling on the off-diagonal geometric phase. Figure 3 shows the numerical results for $\Gamma_{12}$ and $\Gamma_{12}\Gamma_3$ as a function of $\Omega_0$ and $A$. For the system to undergo an adiabatic evolution, Eq. 6 must be satisfied, it would make constraints on $A$ and $\Omega_0$ when we choose Eq. 5 as the transverse-field envelope. An alternative constraint on $A$ and $\Omega_0$ to ensure the adiabatic evolution is whether $\Gamma_{12}\Gamma_3 = -\pi$, as it must be satisfied if the system remains in one of its instantaneous eigenstates in the evolution. The regime within which the system undergoes adiabatic evolutions was illustrated in figure 3-(b), while figure 3-(a) was plotted for $\Gamma_{12}$ versus $A$ and $\Omega_0$. It is clear that $\Gamma_{12}$ decreases with $\Omega_0$ and $A$ increasing; large $A$ leads to large slope in the eigenenergies and then results in the wide energy spacing between them. $\Omega_0$ characterizes the transition frequency among states $\{|\uparrow \uparrow\rangle,|\uparrow \downarrow\rangle,|\downarrow \downarrow\rangle\}$, consequently describes the energy gap between the two eigenenergies at time $t_a$. The off-diagonal geometric phase would depend upon (be proportional to) the transition frequency among the involved energy levels, the transition frequency would decrease with the energy spacing increasing, thus the off-diagonal geometric phase decrease with $A$ and $\Omega_0$ increasing as illustrated in figure 3-(a).

When there are more than two orthogonal eigenstates are involved in the permutations, the off-diagonal geometric phase depends on the decomposition of the permutation $\pi$. For instance, a permutation $P = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}$ can be decomposed as $1 \rightarrow 3 \rightarrow 2 \rightarrow 1$. In this case, the off-diagonal geometric phase factor was defined as $\gamma_{321} = \sigma_{32} \sigma_{21} \sigma_{13}$, and it would take value of 1 as proved in [10]. In our model, we may realize this process via designing the transverse-field envelope $\Omega(t)$. In fact, a twin Gaussian pulse centered at $t_a$ and $t_b$.

$$\Omega(t) = \Omega_{0a} e^{-(t-t_a)^2/T_a^2} + \Omega_{0b} e^{-(t-t_b)^2/T_b^2} \quad (8)$$

satisfies the requirement and would lead to the three-eigenstate involved permutation. Figure 4 shows the populations on states $|\uparrow \uparrow\rangle,|\psi_4^+(t)\rangle$ and $|\downarrow \downarrow\rangle$ with the system in $|\uparrow \uparrow\rangle$ initially. It is clear that the permutation among the involved three orthogonal eigenstates is completed with the properly chosen parameters.

Remarks and conclusion are in order. In this paper, we studied the off-diagonal geometric phase in the compos-
ite system with inter-subsystem couplings. Two cases are considered here (a) two states involved permutation and (b) three states involved permutations. The latter case yields +1 for the off-diagonal geometric phase factor while the off-diagonal geometric phase factors depend on the inter-subsystem coupling dramatically in the former case. These couplings usually can generated entanglement among the subsystems, then prior shared entanglement, as the couplings did, would affect the off-diagonal geometric phase of the composite system. For subsystems that compose a system with inter-subsystem coupling, there is no effective Hamiltonian available in general, so the generalization of the pure state off-diagonal geometric phase to the case of mixed states\cite{13} is not available for this case, it calls for further investigations.

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