

Off-diagonal Geometric Phase of Two-Qubit System

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Abstract This paper focuses on the off-diagonal geometric phase of the thermal state of a two-qubit system under the external magnetic field. The properties of geometric phases of the state in critical and non-critical regions are discussed respectively. The sudden change of structure of degeneracy at the critical point do not affect the geometric phase of the model. Increasing temperature tends to suppress the off-diagonal geometric phase. The relationship between the geometric phase and external magnetic field is also discussed.

Keywords Geometric phase · Thermal state

1 Introduction

Panchartnam [1] was first to introduce the concept of geometric phase in his study of the interference of light in distinct states of polarization. Its quantal counterpart was discovered by Berry [2], who proved the existence of geometric phases in cyclic adiabatic evolution. Simon [3] subsequently recasted the mathematical formation of Berry phase with the language of differential geometry and fibre bundles. He observed that the origin of Berry phase is attributed to the holonomy in the parameter space. Due to its robustness to imperfections, such as decoherence and the random unitary perturbations, GP has many applications in the fields of quantum information processing and condensed matter physics. It has been pointed out that the non-Abelian holonomy may be used in the construction of universal sets of quantum gates for the purpose of achieving fault-tolerant quantum computation [4, 5]. On the other hand, GP, being a measure of the curvature of the Hilbert space, when associated with the energy crossing has a peculiar behavior near the degeneracy point, thus ground state GP may be considered as a good candidate for a universal order parameter for quantum phase transitions [6, 7].

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Another important development in this field was mixed-state GP. In realistic world, due to the effect of environment, the most states are mixed. Uhlmann was probably the first to introduce the notion of geometric phase for mixed quantal states [8, 9]. Later Sjöqvist et al. discussed the GP for non-degenerate mixed state under unitary evolution in Ref. [10], basing on the Mach-Zender interferometer. Singh et al. gave a kinematic description of the mixed-state GP in Ref. [11] and extended it to degenerate density operators. The generalization to nonunitary evolution has been addressed in Ref. [12].

The above definitions of GP are all diagonal. Diagonal GP was discovered not to exhaust all information contained in phases acquired when the quantal system undergoes an adiabatic evolution. The notions of GP break down in cases where the interference visibility between the initial and final states vanishes. This problem may be overcome by introducing the concept of off-diagonal geometric phases, as was first put forward for pure states in adiabatic evolutions [13]. Here, the concept of Berry phase was extended to the evolution of more than one state. A set of independent off-diagonal phase factors are defined to exhaust the geometrical phase information carried by the basis of eigenstates along the path. The off-diagonal pure-state GP has been verified in the neutron interferometer experiments [14, 15]. Soon the concept of off-diagonal GP was extended to the mixed-state cases [16, 17].

The off-diagonal geometric phase factor of degenerate mixed states is defined in Ref. [17],

$$\gamma^{(l)} = \Phi \left[\text{Tr} \left(\prod_{\alpha=1}^l U(\tau) V_{j_\alpha}^{\parallel}(\tau) \sqrt{\rho_{j_\alpha}} \right) \right], \tag{1}$$

where $\Phi[z] \equiv z/|z|$ for any nonzero complex number z . $U(\tau) = \exp(-i\tau H/\hbar)$ is the unitary evolution operator and H is the total Hamiltonian. Throughout this paper, Planck’s constant \hbar is set to unity for simplicity. One can define a set of noninterfering density operators,

$$\rho_n = \lambda_1 P_{n;1}^{(m_1)} + \dots + \lambda_K P_{n;K}^{(m_K)}, \quad n = 1, \dots, N, \tag{2}$$

where $P_{n;k}^{(m_k)} = W^{n-1} P_{1;k}^{(m_k)} (W^\dagger)^{n-1}$ and $P_{n;k}^{(m_k)}$ is the projector of rank m_k onto the m_k -fold degenerate eigenspace. W is a permutation unitarity as $W = |\psi_1\rangle\langle\psi_N| + |\psi_N\rangle\langle\psi_{N-1}| + \dots + |\psi_2\rangle\langle\psi_1|$. The parallel transport unitary operator for ρ_n may be expressed as $U_n^{\parallel}(t) = U(t) V_n^{\parallel}(t)$ with supplementary operators $V_n^{\parallel}(t) = \alpha_{n;1}^{\parallel}(t) + \dots + \alpha_{n;k}^{\parallel}(t)$, where

$$\alpha_{n;k}^{\parallel} = P_{n;k}^{(m_k)} \mathbf{T} \exp \left(- \int_0^t P_{n;k}^{(m_k)} U^\dagger(t') \dot{U}(t') P_{n;k}^{(m_k)} dt' \right) P_{n;k}^{(m_k)}. \tag{3}$$

\mathbf{T} denotes time ordering. The phase is manifestly gauge invariant.

When the Hamiltonian is independent of the time t , $\alpha_{n;k}^{\parallel}$ will be reduced to

$$\alpha_{n;k}^{\parallel} = P_{n;k}^{(m_k)} \mathbf{T} \exp(it P_{n;k}^{(m_k)} H P_{n;k}^{(m_k)}) P_{n;k}^{(m_k)}. \tag{4}$$

Apparently $\gamma^{(1)}$ is the standard mixed-state geometric phase factor associated with the unitary paths in state space. The off-diagonal mixed-state GP contains information about the geometry of state space along the path connecting pairs of density operators, when the standard mixed-state GPs are undefined. The uncontained information can be shown via high-order off-diagonal GP.

The off-diagonal GP for some quantum models has been discussed. For example, The $l = 2$ case has been discussed in terms of two-particle interferometry [18, 19]. X.X. Yi et al. [20]

investigated the effect of the intersubsystem coupling on the off-diagonal geometric phase in a composite system, where the system undergoes an adiabatic evolution.

In the following sections, the off-diagonal GP of a two-qubit system will be considered.

2 Model

This paper focus on the thermal state of hydrogen atom. As we know, in the hydrogen atom, the electron spin is coupled to the nuclear spin by the hyperfine interaction. The hyperfine line for the hydrogen atom has a measured magnitude of 1420 MHz in frequency. Some calculation on the basis of first-order perturbation for the magnetic dipole interaction between the electron and nucleus gives contribution to the coupling strength of $\mathbf{I} \cdot \mathbf{S}$ term. Here \mathbf{I} denotes nuclear spin and \mathbf{S} nuclear spin. The Hamiltonian can be described by [21]

$$H_0 = J(I_x \otimes S_x + I_y \otimes S_y + \Delta I_z \otimes S_z) \quad (5)$$

where J is the coupling constant and Δ is the anisotropy factor. Here the electronic orbital angular momentum L is assumed to be zero. With Δ is varied, the ground state of the model can show different structures. Especially when $\Delta = 1$, the Hamiltonian is isotropic and the ground state has particular degeneracy structure.

As we know, for a hydrogen atom, the nucleus and electron have both spin-1/2, $\mathbf{I} = \mathbf{S} = \sigma/2$. The eigenvalues of H_0 are $E_1 = E_3 = \Delta J/4$, $E_2 = (2 - \Delta)J/4$, $E_4 = -(2 + \Delta)J/4$ for general cases. The four eigenvectors $|\phi_i\rangle$ are independent of the anisotropy factor Δ :

$$\begin{aligned} |\phi_1\rangle &= |00\rangle, \\ |\phi_2\rangle &= \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle), \\ |\phi_3\rangle &= |11\rangle, \\ |\phi_4\rangle &= \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle). \end{aligned}$$

For the isotropic case $\Delta = 1$, the Hamiltonian equation (5) has 2 distinct eigen-energies: $J/4$ and $-3J/4$ and the former is 3-fold degenerate with eigenvectors: $|\phi_i\rangle$, $i = 1, 2, 3$ and the latter is non-degenerate with eigenvector $|\phi_4\rangle$. When $\Delta = -1$, the eigenvalue $-J/4$ is 3-fold degenerate corresponding to eigenvectors $|\phi_i\rangle$, $i = 1, 3, 4$ and eigenvalue $3J/4$ corresponds to $|\phi_2\rangle$. From above, one can see the anisotropic factor Δ can dominate the degeneracy structure of the state.

Now suppose the atom is under the temperature T . The density matrix ρ can be written in terms of partition function $\rho = e^{-\beta H} / \text{tr} e^{-\beta H}$, where $\beta = 1/kT$ and k is Boltzmann's constant and it is set to unity throughout this paper. T denotes the temperature. Due to the effect of thermal fluctuation, the system is highly mixed. At the initial time $t = 0$, it is assumed that no magnetic field is imposed so the density matrix of the initial state can be described as

$$\rho_0 = \frac{e^{-\beta H_0}}{\text{tr} e^{-\beta H_0}}. \quad (6)$$

It is obvious the above 4 eigenvectors are also the eigenvectors of ρ_0 . After the initial time $t = 0$, the external magnetic field \mathbf{B} is imposed upon the system and the total Hamiltonian

becomes $H = H_0 + H_i$. The interaction term H_i reads

$$H_i = C\mathbb{I} \otimes S_z + DI_z \otimes \mathbb{I}, \tag{7}$$

where \mathbb{I} stands for identity matrix. The parameters C and D are related to external magnetic field B and the nuclear spin I ,

$$C = g\mu_B B, \quad D = -\frac{\mu}{I} B.$$

The nuclear magnetic moment μ equals $2.793\mu_N$ where $\mu_N = e\hbar/(2m_p)$. In general C is much larger than D , $|C/D| \sim m_p/m_e \approx 2000$, so for most applications D may be neglected. At the same level of approximation the g factor of the electron may be put equal to 2. Therefore one has

$$H_i = g\mu_B B\mathbb{I} \otimes S_z.$$

It is obvious $[H_0, H_i] \neq 0$. The total Hamiltonian H becomes

$$H = H_0 + H_i = J(I_x \otimes S_x + I_y \otimes S_y + \Delta I_z \otimes S_z) + C\mathbb{I} \otimes S_z, \tag{8}$$

where $C = g\mu_B B$, which is the function of magnetic field B . It implies that the external magnetic field will drive the system to involve with the time. At time t , the state is

$$\rho(t) = U(t)\rho_0U^\dagger(t)$$

where the unitary matrix $U(t) = \exp\{-iHt\}$. The state is assumed to return to its initial state $\rho(0)$ after a period T , i.e., $\rho(0) = \rho(T)$, then one has

$$T = \frac{2n\pi}{\sqrt{C^2 + J^2}}. \tag{9}$$

Here we restrict ourselves to the case of $n = 1$. Note that the period is independent of the anisotropy factor Δ . Equation (9) suggests that the magnetic field B and coupling constant J can control the period T . During the evolution, a mixed-state GP can be observed. In the next sections, we will discuss this mixed-state GP.

3 Geometric Phase

As we have discussed, the initial mixed state mentioned above $\rho_0 = e^{-\beta H_0} / \text{tr} e^{-\beta H_0}$ is degenerate. In Ref. [22], A.T. Rezakhani and P. Zanardi studied the GP of an open quantum system interaction with a thermal environment by using the definition given in Ref. [12]. In Sect. 1, the drawbacks of the definition has been discussed. We will turn to use the definition of off-diagonal GP given in (1) to evaluate the GP to study the information which are not exhausted by diagonal GP. Because the dimension of the two-qubit system is 4, we only consider at most 4-order off-diagonal GP.

(1) $l = 1$

In the region $|\Delta| \neq 1$, only $E_1 = E_3 = J\Delta/4$. It is two-fold degenerate. Here the 1-order off-diagonal GP can be evaluated by the definition $\gamma^{(1)} = \Phi[\text{Tr}(U(T)V^{\parallel}\rho)]$ and for the model

$$\gamma^{(1)} = \Phi \left[i(e^{\beta J} - 1)e^{\frac{1}{2}\beta(\Delta-1)J} \sin\left(\frac{\pi J}{\sqrt{C^2 + J^2}}\right) - (e^{\frac{1}{2}\beta(\Delta-1)J} + e^{\frac{1}{2}\beta(\Delta+1)J}) \cos\left(\frac{\pi J}{\sqrt{C^2 + J^2}}\right) - 2 \right]. \quad (10)$$

From above, the 1-order off-diagonal phase factor $\gamma^{(1)} = \exp i\theta^{(1)}$ is obtained as

$$\tan \theta^{(1)} = \frac{\sinh \frac{\beta J}{2} e^{\beta \Delta J/2} \sin \frac{J\pi}{\sqrt{C^2 + J^2}}}{1 - e^{\beta \Delta J/2} \cosh \frac{\beta J}{2} \cos \frac{J\pi}{\sqrt{C^2 + J^2}}}. \quad (11)$$

One can study its asymptotic behavior in the vicinity of critical points. Let the anisotropy factor Δ approach 1, i.e., $\Delta \rightarrow 1$, the GP will approach to

$$\tan \theta^{(1)} \rightarrow \frac{(e^{\beta J} - 1) \sin\left(\frac{\pi J}{\sqrt{C^2 + J^2}}\right)}{2 - (e^{\beta J} + 1) \cos\left(\frac{\pi J}{\sqrt{C^2 + J^2}}\right)}. \quad (12)$$

On the other hand, if we let $\Delta \rightarrow -1$, the GP approaches to

$$\tan \theta^{(1)} \rightarrow \frac{(e^{\beta J} - 1) \sin\left(\frac{\pi J}{\sqrt{C^2 + J^2}}\right)}{2e^{\beta J} - (e^{\beta J} + 1) \cos\left(\frac{\pi J}{\sqrt{C^2 + J^2}}\right)}. \quad (13)$$

Now we can study the GP at the critical points $\Delta = \pm 1$. At the critical point, due to the level crossing, sudden change of degeneracy structure occurs, and many physical properties, such as ground state GP [6, 7] etc., can show some nonanalytical properties. GP at the critical points in our model will be evaluated. When $\Delta = 1$, the eigenvectors $|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle$ are degenerate. the corresponding eigen-energy is $E_1 = E_2 = E_3 = J/4$. The energy level crossing occurs. This is just like quantum phase transition although the concept of quantum phase transition is only valid for many-body system. In this case, one can obtain that at the critical point $\Delta = 1$, the 1-order off-diagonal GP is the same as the result in (12), which implies that the sudden change of structure of degeneracy at the critical point does not cause drastic change of the 1-order off-diagonal GP. When $\Delta = -1$, the degenerate eigenvectors are $|\phi_1\rangle, |\phi_3\rangle, |\phi_4\rangle$ and the corresponding eigen-energy is $-J/4$. The result is also as the same as the result in (13), despite of the sudden change of structure of degeneracy at the critical point.

From above, one can see at the critical point $\Delta = \pm 1$, the 1-order geometric phase do not show nonanalytical behavior although the structure of degeneracy is changed suddenly. Note that in this case GP is the function of anisotropy factor Δ , thus the 1-order off-diagonal GP varies smoothly with Δ . Figure 1 shows that the increasing temperature tends to suppress the 1-order off-diagonal GP. It can be verified directly from (11). Figure 2 shows the relationship between GP and magnetic field B .

(2) $l = 2$

Similarly, one can see at the non-critical region $\Delta \neq \pm 1$, the 2-order off-diagonal GP factor $\gamma^{(2)} = \exp i\theta^{(2)}$ can be obtained as

$$\tan \theta^{(2)} = \tanh \frac{\beta J}{4} \cot \frac{J\pi}{2\sqrt{C^2 + J^2}}. \quad (14)$$

Fig. 1 1-order off-diagonal GP $\gamma_g = \exp i\theta^{(1)}$ versus temperature T , when $C = g\mu_B B$ are 1, 2, 3 respectively

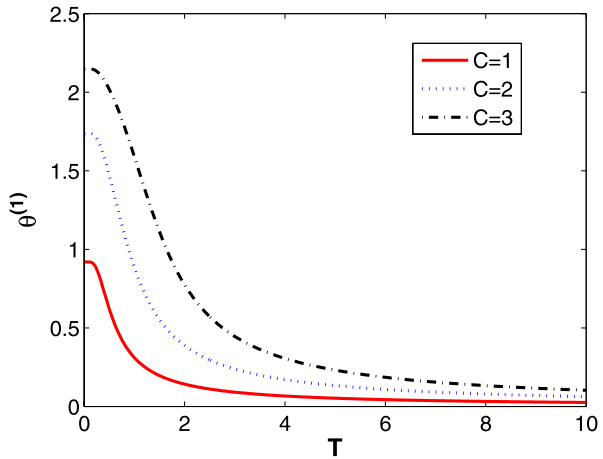
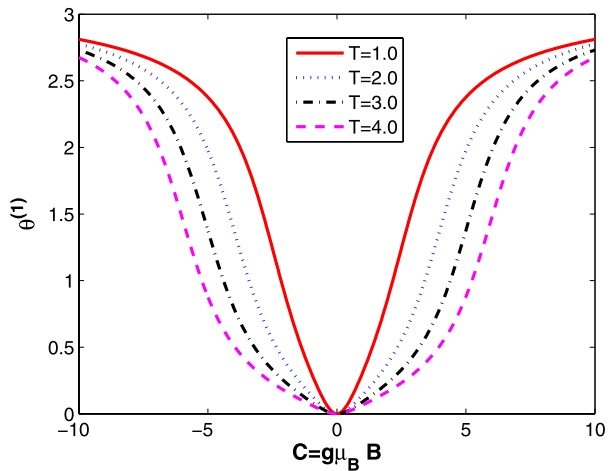


Fig. 2 1-order off-diagonal GP $\gamma_g = \exp i\theta^{(1)}$ versus external magnetic field $C = g\mu_B B$, when the temperature $T = 1.0, 2.0, 3.0, 4.0$ respectively



Note that the above result is independent of the anisotropic factor Δ . It is different from that of 1-order off-diagonal GP. It is clear that when the temperature is increased, i.e., $\beta \rightarrow 0$, the GP vanishes. This is displayed in Fig. 3. Figure 4 shows the effect of the external magnetic field $B = C/g\mu_B$ upon GP under different temperatures.

At the critical points $\Delta = \pm 1$, the structure of degeneracy of the thermal state is changed suddenly, but one can find the 2-order off-diagonal GPs at the critical points are not changed accordingly. It is the same as (14). From them, one can know the changes of structure of degeneracy at the critical point does not change the value of 2-order off-diagonal GP.

(3) $l = 3$ and $l = 4$

Now we turn to study the higher order off-diagonal GP. If $l = 3$, one can see in the non-critical region $|\Delta| \neq 1$, the 3-order off-diagonal GP is zero modula 2π , and the critical point $\Delta = \pm 1$, 3-order GP vanishes too. So that one can see that the change of structure of degeneracy does not affect the 3-order off-diagonal GP.

Fig. 3 2-order off-diagonal GP $\gamma_g = \exp i\theta^{(2)}$ versus temperature T , when $C = g\mu_B B$ are 1, 2, 3 respectively

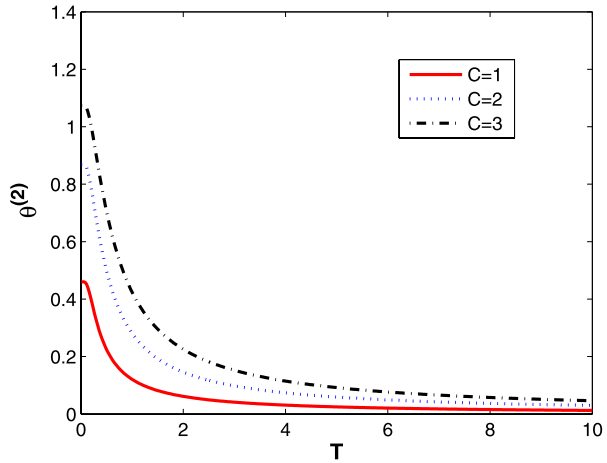
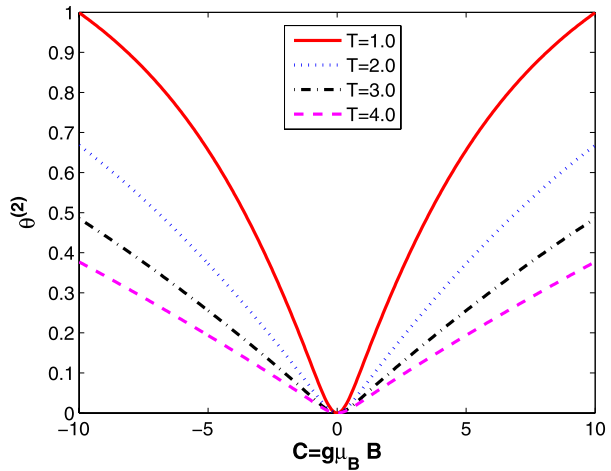


Fig. 4 2-order off-diagonal GP $\gamma_g = \exp i\theta^{(2)}$ versus external magnetic field $C = g\mu_B B$, when the temperature $T = 1.0, 2.0, 3.0, 4.0$ respectively



Let us study $l = 4$ case. Note that $l = 4$ corresponds to the highest-order off-diagonal GP for the model. Repeating same steps, one can discover that no matter in the noncritical regions or at the critical point, the 4-order off-diagonal GP are both zero modulo 2π .

From the above, one can see for our model, only 1-order and 2-order off-diagonal GP can be observed experimentally.

4 Summary

We have obtained the different-order off-diagonal GP respectively. We also have demonstrated the effect of temperature and anisotropy factor Δ upon the off-diagonal GP of a thermal state. It shows that increasing temperature tends to suppress the off-diagonal GP. As the temperature is increased, the thermal fluctuation will dominate the behavior of the particles and it will suppress the off-diagonal GP. If we want to detect the GP or realize some quantum information processing by using diagonal or off-diagonal GP, e.g., geometric

quantum computation, the environment temperature should be very low. On the other hand, we demonstrate the effect of the structure of degeneracy upon different-order off-diagonal GP. It seems that in our model, in the vicinity of critical points, the off-diagonal GP of the thermal state does not show nonanalytical behavior in spite of the sudden change of the structure of degeneracy caused by level crossing. It is different from the ground state GP.

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