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Non-Markovian dynamics of the mixed-state geometric phase of dissipative qubits

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We investigate the geometric phase of a two-level atom (qubit) coupled to a bosonic reservoir with Lorentzian spectral density and find that for the non-Markovian dynamics in which the rotating-wave approximation (RWA) is performed, the geometric phase has a $\pi$-phase jump at the nodal point. However, the exact result without the RWA given by the hierarchical equations of motion method shows that there is no such phase jump or nodal structure in the geometric phase. Thus our results demonstrate that the counterrotating terms significantly contribute to the geometric phase in the multimode Hamiltonian under certain circumstances.

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I. INTRODUCTION

The geometric phase, originally defined in a quantum system that undergoes an adiabatic, unitary, and cyclic evolution [1], was later realized to be a holonomy effect in Hilbert space [2]. By relaxing superfluous assumptions such as periodicity and adiabatic evolution, the geometric phase was generalized to a much wider setting: For a cyclic but nonadiabatic evolution, Aharonov and Anandan proved the existence of a Hamiltonian-independent phase, which is called the Aharonov-Anandan phase [3]. The classical counterpart, the Pancharatnam phase, leads to the generalization of the geometric phase for almost arbitrary unitary evolution [4,5]. The geometric phase has been observed in more than one experiment [6–10] and is also closely related to Bargmann invariants [11]. However, when the initial state is orthogonal to the final state, the definition of geometric phase breaks down. Manini and Pistolesi introduced a complementary concept called the off-diagonal geometric phase [12] to recover the phase information, which was verified by Hasegawa et al. in the neutron interference experiment [13].

Another direction of generalization is to find the corresponding gauge-invariant phase of mixed states. Uhlmann [14] proposed a quantum holonomy for a given path of density matrices under certain parallel transport conditions. Sjöqvist et al. extended the geometric phase to mixed states under unitary evolution [15] by considering feeding a mixed state into a Mach-Zehnder interferometer, which was verified by Ericsson et al. by using single-photon interferometry [16]. For mixed states undergoing nonunitary evolution, Tong et al. generalized the geometric phase by applying the technique of purification [17]. Motivated by [15], Filipp and Sjöqvist [18] generalized the off-diagonal geometric phase of mixed states under unitary evolution. Using Uhlmann’s quantum holonomy, Filipp and Sjöqvist [19] generalized the off-diagonal geometric phase to nonunitary evolution. There is however some inconsistency between the two generalized off-diagonal geometric phases since the nonunitary one reduces to the unitary one only for density matrices with zero eigenvalues [19]; the inconsistency [20,21] also exists for the mixed-state geometric phase in Refs. [14,15].

The geometric phase is a promising concept [22] in quantum computation since it may provide a fault-tolerant way to perform a quantum operation [23]. One implementation of quantum computation is through cavity QED and the Jaynes-Cummings (JC) model [24] has served as a workhorse for cavity QED for decades. The JC model is successful in explaining various quantum optical phenomena and undergoes most experiments with satisfactory results [25]. However, the underlying rotating-wave approximation (RWA) may produce incorrect predictions. An example is the vacuum-induced Berry phase [26], in which a qubit can acquire a geometric phase even when there is no photon in the cavity. Later it is proved to be merely a result of the RWA and disappeared in the Rabi model [27], where the RWA is not performed. The JC model and Rabi model both suppose that the electromagnetic field inside the cavity is monochromatic (single mode), while in reality the imperfection of cavity mirrors will broaden the spectral line, which serves as a bosonic environment (bath), and there are already some works on how the geometric phase is affected by dephasing and a dissipative environment [28,29].

The description of decoherence is a difficult problem and only a few models can be solved analytically. The hierarchical equations of motion method (HEOM), established by Tanimura and co-workers [30,31], is an exact numerical method that goes beyond the Born and Markov approximations. This method was first developed for a system at finite temperature and described by the Drude spectrum. However, in quantum information processes, the qubits and devices are kept at very low temperature to protect entanglement. Ma et al. extended the HEOM to a system with a Lorentz-type system-bath coupling spectrum at zero temperature [32] and found it to be effective in computing physical properties such as quantum Fisher information [33].

In this work we reanalyze the behavior of the geometric phase in Ref. [34], where a qubit was coupled to a cavity at zero temperature with a Lorentzian spectrum and a dipole interaction was assumed. We show that their analysis is incomplete because singularities or nodal structures [35] are left out and we give an upper bound to the existence of the nodal structure. Moreover, by using the HEOM to obtain the exact dynamics, we find that the nodal structures disappear and the geometric phase is well defined in the whole parameter space.

The structure of this article is as follows. In Sec. II we introduce the geometric phase under nonunitary evolution...
and explain how Bargmann invariants are connected to the geometric phase. In Sec. III we introduce the model of a qubit interacting with the environment described by the Lorentzian spectrum and we derive the explicit expression of the geometric phase under the RWA, where nodal structures are analyzed with special attention. In Sec. III B the HEOM is introduced and numerical results are shown and analyzed. A brief discussion and summary are given in Sec. IV.

II. GEOMETRIC PHASE AND BARGMANN INVARIANTS

In this section we briefly review the definition of a geometric phase for mixed states under nonunitary evolution [17]. When the evolution is unitary, cyclic, and adiabatic, the geometric phase for a pure state is defined as

$$\Phi_g = \arg \left[ \langle \psi(0)|\psi(T) \rangle \exp \left( - \int_0^T \langle \psi(t)|\frac{\partial}{\partial t}|\psi(t)\rangle dt \right) \right]$$

where $\langle \psi(0)|\psi(T) \rangle$ can be viewed as the total phase accumulated after $T$, with the geometric phase part and dynamic phase part together, which is also called $\Phi_{tot}$. Multiplying $\Phi_{tot}$ by $\exp[-\int_0^T \langle \psi(t)|\frac{\partial}{\partial t}|\psi(t)\rangle dt]$ offsets the dynamic phase and leaves only the geometric phase. When the evolution is unitary only, Eq. (3) reduces to the Berry phase under general settings [4].

The definition of the geometric phase for mixed states under nonunitary evolution [17] is

$$\Phi_g = \arg \left[ \sum_i \sqrt{\epsilon_i(0)\epsilon_i(T)} |i(0)\rangle \langle i(T)| \right. \times \exp \left( \int_0^T -\langle i|\frac{\partial}{\partial t}|i\rangle dt \right)$$

where $\epsilon_i(t)$ and $\langle i(t)|$ are the $ith$ eigenvalue and $ith$ eigenvector of the system’s density matrix $\rho_S(t)$ and $T$ is the total time of evolution. Equation (2) can be explained as the geometric phase of a state under nonunitary evolution being the weighted sum of the geometric phase accumulated on each eigenstate of the initial state. When evolution is unitary, Eq. (2) reduces to the expression of the geometric phase for mixed states under unitary evolution [15]. If the system is prepared in a pure state, then without loss of generality, we can assume that $\epsilon_1(0) = 1$, while the rest of the eigenvalues are all zero. Then Eq. (2) reduces to

$$\Phi_g = \arg \left[ \langle \psi(0)|\psi(T) \rangle \exp \left( - \int_0^T \langle \psi(t)|\frac{\partial}{\partial t}|\psi(t)\rangle dt \right) \right]$$

which looks exactly the same as Eq. (1) except that the evolution here is nonunitary and noncyclic. In Eq. (3) $\langle \psi(t)|$ is the eigenvector of $\rho_S(t)$, corresponding to the eigenvalue $\epsilon_1(t)$; $\sqrt{\epsilon_1(0)\epsilon_1(T)}$ is omitted because it is real and larger than 0 and thus has no effect under the operation of taking out the phase.

Using a Taylor expansion, the integral on the exponential function in (3) can be evaluated, to first order, as

$$\exp \left( - \int_0^T \langle \psi(t)|\frac{\partial}{\partial t}|\psi(t)\rangle dt \right)$$

$$\approx \prod_{i=1}^N \exp \left( - \langle \psi(t)|\frac{\partial}{\partial t}|\psi(t)\rangle \right)_{t=i \delta t}$$

$$\approx \prod_{i=1}^N \left[ 1 - \langle \psi(t)|\frac{\partial}{\partial t}|\psi(t)\rangle \right]_{t=i \delta t}$$

$$\approx \prod_{i=2}^N \langle \psi(t_i)|\psi(t_{i-1}) \rangle,$$

where $t_1 = 0$, $t_N = T$, $t_{i+1} = t_i + \delta t$, and $N = T/\delta t$. In the first line we approximate the integral using a summation of $N$ members, while the expression in second line is the result of the Taylor expansion and in third line we assume that $\langle \psi(t)|$ is continuous; both are accurate to first order of $\delta t$, thus we use the approximately equal sign. It is noted that in the last line, the range is changed from $[1, N]$ to $[2, N]$ due to the requirement of continuity. Then Eq. (3) can be rewritten as a consecutive inner product

$$\Phi_g \approx \arg[\langle \psi(T)|\psi(T - \delta t)| \cdots |\psi(t_1)|\psi(t_1) \rangle \times \cdots \langle \psi(\delta t)|\psi(0)|\psi(0)|\psi(T) \rangle],$$

where the consecutive inner product under the operation arg is the complex conjugate of $n$-vertex Bargmann invariants [36]. As $\delta t$ becomes infinitely small, the approximately equal sign in Eq. (5) can be replaced by an equal sign, hence the Bargmann invariants and the geometric phase are directly related in this limit [37,38].

Compared with Eq. (3), the numerical calculation of the Bargmann invariant expression is easy. When finding the eigenvectors for a matrix on a computer, an arbitrary phase factor $\chi (|\chi| = 1)$ is attached, which leads to anomalous behavior after the differential operation in Eq. (3). Instead, there is no differentiation and integration, only the basic inner product operation within the Bargmann invariant expression (5) and the eigenvector at different time $t$ come in pairs, so the phase factors cancel ($\chi \chi^* = 1$).

III. DYNAMICS AND GEOMETRIC PHASE OF A SINGLE QUBIT IN A LOSSY CAVITY

We consider a two-level atom coupled to a bosonic bath (cavity) at zero temperature, with the Hamiltonian [39]

$$H = H_S + H_B + H_I,$$

where

$$H_S = \omega_0 \sigma_+ \sigma_-$$

is the Hamiltonian of the two-level atom (with $\hbar = 1$),

$$H_B = \sum_k \omega_k a_k^\dagger a_k$$

(7)

(8)
is the Hamiltonian of the bath, and
\[ H_I = \sigma_k \sum_k g_k(a_k + a_k^\dagger) \] (9)
describes the interaction between the atom and bath. In Eq. (9),
g_k represents the coupling strength between the atom and the
kth mode of the bath and g_k is real. In the interaction picture,
\[ H_I(t) = \sum_k g_k(\sigma_k a_k + a_k^\dagger) e^{-i(o_k-a_k)t/\hbar} \]
(10)
By applying the rotation-wave approximation we ignore the rapid
oscillation terms, i.e., the terms with frequency \( o_k + \omega \),
which is equivalent to writing the Hamiltonian in Eq. (6) as
\[ H = H_S + H_B + \sum_k g_k(\sigma_k a_k + a_k^\dagger), \] (11)
which is exactly solvable by solving the Schrödinger equation
of the whole system. We suppose that the initial state is
\[ |\psi(0)\rangle = |c_0(0)|0\rangle_S + c_1(0)|1\rangle_S |0\rangle_k E, \] (12)
where |0\rangle and |1\rangle represent the spin-up and spin-down states
of the qubit and |0\rangle_k E represents the vacuum state, thus the
bath and system are at the product state initially.

Under the evolution of the Hamiltonian with the RWA, i.e.,
Eq. (11), the total state of the bath and qubit at time t takes the form
\[ |\psi(t)\rangle = \sum_k c_k(t)|0\rangle_S |0\ldots 1_k \ldots 0\rangle_E, \] (13)
The evolution of the initial state can be understood as follows:
|0\rangle_S |0\rangle_E does not evolve, while |1\rangle_S |0\rangle_E evolves into two
states: |1\rangle_S |0\rangle_E and |0\rangle_S |0\ldots 1_k \ldots 0\rangle_E.

It seems that the infinite number of modes k leads to an
unnormalizable state, while Eq. (13) is actually normalized. We
apply the Schrödinger equation to get the explicit expression of
the amplitude’s evolution in the interaction picture:
\[ c_0(t) = c_0, \]
\[ c_1(t) = -i \sum_{k=0}^{\infty} e^{i(o_k-a_k)t/\hbar} c_k(t), \] (14)
\[ c_k(t) = -i g_k e^{-i(o_k-a_k)t/\hbar} c_1(t). \]
With Eq. (14), we have
\[ \frac{d}{dt} \left( |c_0|^2 + |c_1|^2 + \sum_{k=0}^{\infty} |c_k|^2 \right) = c_1 \dot{c}_1^* + \sum_{k=0}^{\infty} c_k \dot{c}_k^* + \text{c.c.} \]
(15)
Since \( |c_0(0)|^2 + |c_1(0)|^2 + \sum |c_k(0)|^2 = 1 \), the state after evolution is also normalized.

In the calculation of the correlation function
\[ C(t - \tau) = \sum_k g_k g_k^* e^{i(o_k-a_k)(t-\tau)} \] (16)
assuming that the bath’s degree of freedom is large and modes
are closely spaced, we can replace the summation with the integral
\[ C(t - \tau) = \int_0^{+\infty} J(\omega) e^{i(o_0-a_0)(t-\tau)} d\omega, \] (17)
where \( J(\omega) \) is the spectral density. We assume here that the
spectral density is the Lorentzian shape [40]
\[ J(\omega) = \frac{1}{\pi} \frac{W^2}{(\omega_0 - \omega)^2 + \lambda^2}, \] (18)
where W reflects the coupling strength between the atom and
bath and is proportional to \( |g_k| \) and \( \lambda \) is the spectral width at
the resonance frequency \( \omega_0 \). The correlation function \( C \) under
the Lorentzian spectral density can be calculated as
\[ C(t - \tau) = W^2 \exp[-\lambda(t - \tau)], \] (19)
where we replace the lower limit of the integral from 0 to
\( -\infty \), which is known as the Weisskopf-Wigner approximation [39].
The parameter \( \lambda \) not only defines the spectral width, but is also connected to the bath correlation time with the relation \( \tau_c = \lambda^{-1} \).
Compared with the time scale of the system \( \tau_0 = 2\pi/\omega_0 \), when \( \tau_c \gg \tau_0 \), the dynamics is non-Markovian [34].

The explicit expression of \( c_1(t) \) is [40]
\[ c_1(t) = c_1(0)e^{-i\omega t} e^{-\lambda t/2} \left[ \cos \left( \frac{\Omega t}{2} \right) + \frac{\lambda}{\Omega} \sin \left( \frac{\Omega t}{2} \right) \right] \]
(20)
where
\[ f(t) = \begin{cases} e^{-\lambda t/2} \left[ \cos \left( \frac{\Omega t}{2} \right) + \frac{\lambda}{\Omega} \sin \left( \frac{\Omega t}{2} \right) \right], & \text{for } \lambda^2 > 4W^2 \\
\left[ \cos \left( \frac{\Omega t}{2} \right) + \frac{\lambda}{\Omega} \sin \left( \frac{\Omega t}{2} \right) \right], & \text{for } \lambda^2 < 4W^2, \end{cases} \]
(21)
with \( \Omega = \sqrt{\lambda^2 - 4W^2} \). When \( \lambda^2 \geq 4W^2 \), \( f(t) \) decreases from 1 to 0 monotonically; when \( \lambda^2 < 4W^2 \), \( f(t) \) decreases from 1 to 0 while oscillating, acting like an underdamped oscillator. Here \( f(t) \) is real regardless of \( \lambda \) and \( W \). As \( \lambda \) approaches zero, \( f(t) \) becomes \( \cos W t \).

A. Analytical result under the RWA
We choose the initial state of the qubit to be
\[ |\psi(0)\rangle = \cos \frac{\theta}{2} |1\rangle + \sin \frac{\theta}{2} |0\rangle \] (22)
with the bath in the vacuum state. After tracing out the bath and employing Eq. (20), the reduced density matrix at time \( t \) is
\[ \rho_3(t) = \begin{pmatrix} \cos^2 \frac{\theta}{2} f^2(t) & \sin^2 \frac{\theta}{2} f(t) e^{-i\omega t} \\ \sin^2 \frac{\theta}{2} f(t) e^{i\omega t} & 1 - \cos^2 \frac{\theta}{2} f^2(t) \end{pmatrix}. \] (23)
The eigenvalues of $\rho_5(t)$ are

$$
e_{\pm}(t) = \frac{1}{2} \pm \frac{1}{2} \sqrt{f^2(t) - \sin^2 \theta + [2 f^2(t) \cos^2(\theta/2) - 1]^2},$$

with the corresponding eigenvectors

$$|e_{\pm}(t)\rangle = e^{-i\alpha(t)} \cos \Theta_{\pm}|1\rangle + \sin \Theta_{\pm}|0\rangle,$$

$$\cos \Theta_{+} = \frac{\sin \theta f(t)}{N_{+}(t)},$$

$$\sin \Theta_{+} = \frac{2[\epsilon_{+} - \cos^2(\theta/2) f^2(t)]}{N_{+}(t)},$$

$$\cos \Theta_{-} = \frac{2[\epsilon_{-} - \cos^2(\theta/2) f^2(t)]}{N_{-}(t)},$$

$$\sin \Theta_{-} = \frac{\sin \theta f(t)}{N_{-}(t)},$$

where

$$N_{\pm}(t) = \sqrt{4[\epsilon_{\pm} - \cos^2(\theta/2) f^2(t)]^2 + f^2(t) \sin^2 \theta}$$

are normalizing factors.

Since the system and bath are prepared in the product state and the system alone is in the pure state initially, we apply Eq. (3) to calculate the geometric phase acquired during $T = 2\pi/\omega_0$:

$$\Phi_{g} = \arg \left[ \cos \left( \frac{\theta}{2} - \Theta_{+}(T) \right) \exp \left( i \int_{0}^{T} \omega_0 \cos^2 \Theta dt \right) \right].$$

Equation (28) differs from the geometric phase expression in Ref. [34] with a factor of $\cos[\theta/2 - \Theta_{+}(T)]$, which is simply $\arg(\psi(0)|\psi(T))$; this factor is crucial to the geometric phase and cannot be dropped. Actually, $\cos[\theta/2 - \Theta_{+}(T)]$ may be negative or zero here, leading to a discontinuous $\Phi_{g}$. It is noted that as $\lambda$ approaches zero, if we substitute $f(t) = \cos W t$ into Eq. (23), then we recover the density matrix under evolution of the JC model [24] and the phase jump still exists, as shown in Fig. 1.

A more explicit expression of the geometric phase is

$$\Phi_{g} = \begin{cases} \int_{0}^{T} \omega_0 \cos^2 \Theta_{+} dt, & \cos \left( \frac{\theta}{2} - \Theta(T) \right) > 0 \\ \text{undefined}, & \cos \left( \frac{\theta}{2} - \Theta(T) \right) = 0 \\ \pi + \int_{0}^{T} \omega_0 \cos^2 \Theta_{+} dt, & \cos \left( \frac{\theta}{2} - \Theta(T) \right) < 0. \end{cases}$$

When $\cos(\theta/2 - \Theta_{+})$ changes sign, the geometric phase has a sudden change of $\pi$; the point that $\cos(\theta/2 - \Theta_{+}) = 0$ is called the nodal point [18,35], where the geometric phase has no definition. The discontinuity originates from the definition of the geometric phase, e.g., $\arg(0.05) = 0$ and $\arg(-0.05) = \pi$. In experiment, interference visibility vanishes at the nodal point.

The geometric phase with the RWA as a function of the initial angle $\theta$ and coupling strength $W$ is plotted in Fig. 2 for the Markovian case ($\tau_0/\tau_c = 5$) [Fig. 2(a)] and the non-Markovian case ($\tau_c/\tau_0 = 20$) [Fig. 2(b)]. A coupling strength as large as $0.1\omega_0$ is enough to invalidate the RWA, therefore the region $W \in (0,1.5\omega_0)$ we choose is adequate. When the dynamics are Markovian, $\Phi_{g}$ is continuous everywhere and decreases to 0 monotonically, which is believed to be caused by stronger dissipation and shorter decoherence time [34]. When the dynamics are non-Markovian, $\Phi_{g}$ becomes discontinuous and has a phase jump of $\pi$, which is also known as the nodal structure. We also observe that only if $\theta$ is smaller than $\pi/2$ will the phase jump occur; this initial-state-dependent phenomenon will be explained at the end of this section.

The intersection of Fig. 2 under non-Markovian dynamics is plotted in Fig. 3. It is clear that the phase jump of $\pi$ in the geometric phase is the direct result of the sign change of $\arg(\psi(0)|\psi(T))$. To restore the phase information at the nodal point requires the calculation of the off-diagonal geometric phase under nonunitary evolution [19]; however, this is not easy due to the lack of an explicit expression since the parallel
the explicit expression of $\theta$ argument in the previous paragraph that a phase jump must happen under non-Markovian dynamics and the main reason is the oscillation of $\langle \psi(0) | \psi(T) \rangle$ from a positive number to a negative one, as shown in Eq. (30). Now we derive the upper bound of the initial angle $\theta$ for $\Phi_\theta$ to become discontinuous, i.e., for $\langle \psi(0) | \psi(T) \rangle$ to become negative. Using Eq. (30) and ignoring $N_\tau(T)$ together with $\sin \theta T/2$ since it is always larger than 0 for $\theta \in (0, \pi)$, we have

$$\cos^2 \theta \left( -|f| + f^2 \right) + \varepsilon_+ \leq 0,$$

$$\cos^2 \theta \left( |f| + f^2 \right) \geq \frac{1}{2},$$

$$2 \cos^2 \theta \geq \frac{1}{2}$$

$$\Rightarrow \theta < \theta_C = \frac{2\pi}{3},$$

where in the first line we substitute $-|f|$ for $f$ since $f < 0$ is necessary for the nodal structure, in the second line we use the fact that $\varepsilon_+ \geq 1/2$, and in the third line $|f(T)| < 1$. Therefore, we conclude that $\theta < \theta_C = 2\pi/3$ is a necessary condition for the geometric phase to be discontinuous under the evolution of the Hamiltonian in Eq. (11); when $\theta > 2\pi/3$, the geometric phase must be continuous, regardless of $\lambda$ and $W$. The bound we derive in Eq. (32) covers the situation displayed in Fig. 2(b), where $\Phi_\theta$ is discontinuous for $\theta < \pi/2$ and becomes continuous afterward. It is noted that when $\theta = 0$, the geometric phase is ill defined regardless of $W$ and $\lambda$.

B. Hierarchical equations of motion method

The sudden change of geometric phase is interesting and puzzling, but it maybe a misuse of the RWA instead of a physical reality. In Figs. 3(c) and 3(d) $\Phi_\theta$ has a nonvanishing value even when $W \sim 1\omega_0$, which is not likely since a large coupling strength indicates a quick decoherence and $\Phi_\theta$ should decrease to zero, implying that the geometric phase under the RWA may go wrong. We also note that, in Fig. 2, the discontinuity lies in the strong-coupling strength area, which makes it suspicious. To answer these questions we need to know the exact dynamics of the system without the RWA.

The density matrix of the system in the interaction picture at time $t$ is

$$\rho_{\text{int}}(t) = \mathcal{T} \exp \left( -i \int_{0}^{t} H_{SB}(\tau) d\tau \right) \rho_{\text{tot}}(0),$$

where $H_{SB}(\tau) = e^{i(H_I + H_B)\tau} H_{SB} e^{-i(H_I + H_B)\tau}$ is the interaction term in the interaction picture. We also introduce the superscripts $\times$ and $\circ$ to denote superoperators $A^\times B \equiv [A, B]$ and $A^\circ B \equiv \{A, B\}$ and $\mathcal{T}$ stands for the time-ordering operator.

The hierarchical equations of motion method has two requirements: One is that the system and bath are initially separable $\rho_{\text{tot}}(0) = \rho_S(0) \otimes \rho_B(0)$ and the other is that the system-bath interaction should be bilinear $H_{SB}(\tau) = B(\tau) V(\tau)$, where $B(\tau)$ and $V(\tau)$ are the bath and system operators, respectively. Both conditions are satisfied, as shown in Eqs. (6) and (12). If
we trace out the bath, then we obtain
\[ \rho_S^{(1)}(t) = T \exp \left( -i \int_0^t dt_1 \int_0^{t_1} dt_2 V(t_2)x(C^R(t_2 - t_1)V(t_1))^x + iC^I(t_2 - t_1)V(t_1)f \right) \rho_S(0). \] (34)

In Eq. (34), \( V(0) = \sigma_x \) is the operator of the qubit in \( H_{SB} \) and \( C^I \) and \( C^R \) are the imaginary and real parts of the bath’s time correlation function \( (B(t)B(0)) \), respectively, where \( B(0) = \sum_k g_k(a_k^d + a_k) \) is the operator of the bath in \( H_{SB} \).

The principle of the HEOM is to transform the operator-related integral (34) to a set of ordinary differential equations [31–33]
\[ \frac{\partial}{\partial t} \omega_{\bar{n}}(t) = -(iH_s^x + \bar{n} \cdot \bar{v})\omega_{\bar{n}}(t) - i \sum_{k=1}^{2} V^x \omega_{\bar{n}+\bar{e}}(t) - \frac{i}{2} \sum_{k=1}^{2} n_k[V^x + (-1)^k V^y] \omega_{\bar{n}+\bar{e}}(t), \] (35)
where \( \bar{n} = (n_1,n_2), \bar{e}_1 = (1,0), \bar{e}_2 = (0,1), \) and \( \bar{v} = (\lambda - i\omega_0, \lambda + i\omega_0) \) are auxiliary denotations. The initial condition for Eq. (35) is
\[ \omega_{\bar{n}}(0) = \rho_S(0) \text{ for } n_1 = n_2 = 0 \]
\[ 0 \text{ for } n_1 > 0, n_2 > 0. \]

The reduced density matrix \( \rho(t) \) under the evolution of the Hamiltonian (6) is obtained by solving Eq. (35) numerically. By calculating the evolution of \( \rho(t) \), its initial state is \( |\psi(0)\rangle = \sin \frac{\theta}{2} |1\rangle + \cos \frac{\theta}{2} |0\rangle \), we get an ordered series of eigenvectors \( |\psi(t)\rangle \) and then substitute them into the Bargamann invariants (5) to obtain the geometric phase without the RWA.

Figure 4(a) displays \( \Phi_\pi/\pi \) under Markovian dynamics without the RWA; it is qualitatively similar to that with the RWA, as shown in Fig. 2. A more interesting result is that \( \Phi_\pi \) within non-Markovian dynamics regimes without the RWA is continuous everywhere, which is completely different. In

\[ \Phi_{\pi/\pi} \text{ without the RWA as a function of coupling strength and initial angle: (a) } \lambda = 0.05\omega_0 \text{ and the geometric phase under the RWA decrease monotonically, just like in the RWA case, and (b) } \lambda = 0.05\omega_0 \text{ and the geometric phase is continuous in the whole parameter space, which is totally different from } \Phi_\pi \text{ under the RWA.} \]

In the non-Markovian regime, the deviation is not large, as shown in Figs. 6(a) and 6(b). We find that when the coupling strength becomes larger, decreases to 0.

From Sec. III A, we understand that with the RWA, the discontinuity in \( \Phi_\pi \) is the result of the sign change in \( |\psi(0)\rangle|\psi(T)\rangle \) and is natural to investigate how \( |\psi(0)\rangle|\psi(T)\rangle \) affects the \( \Phi_\pi \) without the RWA. The moduli of \( |\psi(0)\rangle|\psi(T)\rangle \) and \( \Phi_\pi \), obtained by the HEOM, are shown in Fig. 5, where \( W = 0.5\omega_0 \) and \( \lambda = 0.05\omega_0 \), i.e., within the strong-coupling and non-Markovian regimes. We find that the modulus never reaches 0, thus \( \Phi_\pi \) is continuous and defined for all initial states.

Fig. 4(b) counterrotating terms are included and nodal structures are gone. It is clear that under the evolution of the full Hamiltonian and within non-Markovian dynamics regimes, the geometric phase, as coupling strength becomes larger, decreases to 0.

The rotating-wave approximation affects the geometric phase not only in the non-Markovian regime, but also in the Markovian regime, which is not evident at first sight. From Figs. 6(a) and 6(b) we find that when the coupling strength is weak, the geometric phase is not affected by the rotating-wave approximation regardless of whether the dynamics are Markovian or non-Markovian. Now we can observe easily how counterrotating terms affect the geometric phase. In the Markovian regime, the deviation is not large, as shown in Fig. 6(c): however, in the non-Markovian regime, the geometric phase with the RWA deviates quantitatively and qualitatively from the geometric phase without the RWA. The sharp drop of the geometric phase without the RWA (blue line) in Fig. 6(d) is simply because we plot \( \Phi_\pi \text{ mod 2}\pi \text{ instead of } \Phi_\pi \) and this discontinuity of 2\pi can be removed by simply adding 2\pi back. Thus there is no nodal structure in the geometric phase without the RWA, while a discontinuity of \pi in the geometric phase with the RWA cannot be removed.

The reason that the behavior of the geometric phase in the non-Markovian regime is significantly affected by the RWA may be because the RWA is not justified in describing non-Markovian dynamics. Intravia et al. proved that for a harmonic oscillator the counterrotating terms contribute significantly to
non-Markovianity is affected by the RWA.

that the geometric phase may serve as an indicator of how the RWA is in agreement with previous work and we suggest that the counterrotating terms significantly contribute to the geometric phase disappears. Our results demonstrate that the counterrotating terms significantly contribute to the geometric phase in the multimode Hamiltonian when the coupling strength is strong and within the non-Markovian dynamics regime.

In summary, we have investigated the mixed-state geometric phase of a qubit, which is coupled to a bosonic bath with a Lorentzian spectrum, with and without the RWA. Under the RWA, we find that there is discontinuity (nodal structures) in the geometric phase when the coupling strength is strong and the dynamics are in the non-Markovian regime. This result was not reported in previous work [34] since the term $\arg \cos(\theta / 2 - \Theta_s(T))$ was missing. How the initial condition affects the nodal structure under non-Markovian dynamics was analyzed specifically and a bound for discontinuity to disappear was given.

Furthermore, with the hierarchical equations of motion method, we calculated numerically the geometric phase without the RWA. We found that, in the Markovian dynamics regime, the numerical result is in consonance with the analytical result under the RWA, thus the counterrotating wave terms under such circumstances are not important. However, within the non-Markovian dynamics regime, the behavior of the geometric phase without the RWA is quite different from the geometric phase with the RWA. After taking the counterrotating terms into consideration, the discontinuity in the geometric phase disappears. Our results demonstrate that the counterrotating terms significantly contribute to the geometric phase in the multimode Hamiltonian when the coupling strength is strong and within the non-Markovian dynamics regime.

IV. CONCLUSION

In summary, we have investigated the mixed-state geometric phase of a qubit, which is coupled to a bosonic bath with a Lorentzian spectrum, with and without the RWA. Under the RWA, we find that there is discontinuity (nodal structures) in the geometric phase when the coupling strength is strong and the dynamics are in the non-Markovian regime. This result was not reported in previous work [34] since the term $\arg \cos(\theta / 2 - \Theta_s(T))$ was missing. How the initial condition affects the nodal structure under non-Markovian dynamics was analyzed specifically and a bound for discontinuity to disappear was given.

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