

Kinematic Approach to the Mixed State Geometric Phase in Nonunitary Evolution

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A kinematic approach to the geometric phase for mixed quantal states in nonunitary evolution is proposed. This phase is manifestly gauge invariant and can be experimentally tested in interferometry. It leads to well-known results when the evolution is unitary.

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The concept of geometric phase was first introduced by Pancharatnam [1] in his study of interference of classical light in distinct states of polarization. Berry [2] discovered the quantal counterpart of Pancharatnam's phase in the case of cyclic adiabatic evolution. Since then there has been an immense interest in holonomy effects in quantum mechanics, which has led to many generalizations of the notion of geometric phase. The extension to nonadiabatic cyclic evolution was developed by Aharonov and Anandan [3]. Samuel and Bhandari [4] generalized the pure state geometric phase further by extending it to noncyclic evolution and sequential projection measurements. The geometric phase is a consequence of quantum kinematics and is thus independent of the detailed nature of the dynamical origin of the path in state space. This led Mukunda and Simon [5] to put forward a kinematic approach by taking the path traversed in state space as the primary concept for the geometric phase. Further generalizations and refinements, by relaxing the conditions of adiabaticity, unitarity, and cyclicity of the evolution, have since been carried out [6].

Another line of development has been towards extending the geometric phase to mixed states. This was first addressed by Uhlmann [7] within the mathematical context of purification. Sjöqvist *et al.* [8] introduced an alternative definition of geometric phase for nondegenerate density operators based upon quantum interferometry. Singh *et al.* [9] gave a kinematic description of the mixed state geometric phase in Ref. [8] and extended it to degenerate density operators. The relation between phases of an entangled system and its subsystems has been investigated [10]. The concept of off-diagonal geometric phases in Ref. [11] for pure states has also been generalized to mixed states undergoing unitary evolution [12]. Recently, the mixed state geometric phase in Ref. [8] has been verified experimentally using the nuclear magnetic resonance technique [13].

The generalization of the mixed state geometric phase to nonunitary evolution has been addressed [14,15]. The concept proposed in Ref. [14] for completely positive maps (CPMs) is operationally well-defined but may yield

different values of geometric phase for a given CPM when using different Kraus representations. The approach in [15] also concerns the mixed state geometric phase for CPMs but is based upon a weaker form of parallel transport condition than [14], which makes it unclear whether [15] reduces to expected results [8,9] in the limit of unitary evolution. Related to these research efforts has been the effort to analyze the effect of nonunitary processes on the pure state geometric phase [16,17]. The lack of a clear consensus regarding the mixed state geometric phase in the nonunitary case makes it important to pursue further studies on this issue.

Geometric phases are useful in the context of quantum computing as a tool to achieve fault tolerance [18]. However, practical implementations of quantum computing are always done in the presence of decoherence. Thus, a proper generalization of the geometric phase for unitary evolution to that for nonunitary evolution is central in the evaluation of the robustness of geometric quantum computation. In this Letter, we propose a quantum kinematic approach to the geometric phase for mixed states in nonunitary evolution. We also propose a scheme to realize nonunitary paths in the space of density operators in the sense of purification, which could be of use in experimental tests of the mixed state geometric phase.

Consider a quantum system s with N dimensional Hilbert space \mathcal{H}_s . An evolution of the state of s may be described as the path

$$\mathcal{P} : t \in [0, \tau] \rightarrow \rho(t) = \sum_{k=1}^N \omega_k(t) |\phi_k(t)\rangle \langle \phi_k(t)|, \quad (1)$$

where $\omega_k(t) \geq 0$ and $|\phi_k(t)\rangle$ are the eigenvalues and eigenvectors, respectively, of the system's density operator $\rho(t)$. All the nonzero $\omega_k(t)$ are assumed to be nondegenerate functions of $t \in [0, \tau]$, leaving the extension to the degenerate case to the end of this Letter.

To introduce the notion of mixed state geometric phase in nonunitary evolution, we begin by lifting the mixed state to a pure state in a larger system. Consider a combined system $s + a$, which consists of the considered system s and an ancilla a with $K \geq N$ dimensional

Hilbert space. Without loss of generality, we assume in the following that $K = N$. The mixed state $\rho(t)$ can be lifted to the purified state

$$|\Psi(t)\rangle = \sum_{k=1}^N \sqrt{\omega_k(t)} |\phi_k(t)\rangle \otimes |a_k\rangle, \quad t \in [0, \tau], \quad (2)$$

where $|\Psi(t)\rangle \in \mathcal{H}_s \otimes \mathcal{H}_a$ is a purification of the density operator of s in the sense that $\rho(t)$ is the partial trace of $|\Psi(t)\rangle\langle\Psi(t)|$ over the ancilla. The Pancharatnam relative phase between $|\Psi(\tau)\rangle$ and $|\Psi(0)\rangle$ reads

$$\begin{aligned} \alpha(\tau) &= \arg\langle\Psi(0)|\Psi(\tau)\rangle \\ &= \arg\left(\sum_{k=1}^N \sqrt{\omega_k(0)\omega_k(\tau)} \langle\phi_k(0)|\phi_k(\tau)\rangle\right). \end{aligned} \quad (3)$$

Since both $\{|\phi_k(0)\rangle\}$ and $\{|\phi_k(\tau)\rangle\}$ are orthonormal bases of the same Hilbert space \mathcal{H}_s , there exists, for each $t \in [0, \tau]$, a unitary operator $V(t)$ such that

$$|\phi_k(t)\rangle = V(t)|\phi_k(0)\rangle, \quad (4)$$

where $V(0) = I$, I being the identity operator on \mathcal{H}_s . Explicitly, we may take

$$V(t) = |\phi_1(t)\rangle\langle\phi_1(0)| + \dots + |\phi_N(t)\rangle\langle\phi_N(0)|. \quad (5)$$

Then, the relative phase can be recast as

$$\alpha(\tau) = \arg\left(\sum_{k=1}^N \sqrt{\omega_k(0)\omega_k(\tau)} \langle\phi_k(0)|V(\tau)|\phi_k(0)\rangle\right). \quad (6)$$

In order to arrive at the geometric phase associated with the path \mathcal{P} of the state of s , we need to remove the dependence of $\alpha(\tau)$ upon the purification of the type displayed by Eq. (2). To do this, we first notice that $\alpha(\tau)$ becomes the standard geometric phase of the pure en-

tangled state $|\Psi(t)\rangle$, $t \in [0, \tau]$ when the evolution satisfies the parallel transport condition $\langle\Psi(t)|\dot{\Psi}(t)\rangle = 0$. However, this single condition is insufficient for mixed states as it specifies only one of the N undetermined phases of $V(t)$, and the resulting pure state geometric phase remains strongly dependent upon the purification. Instead, the essential point to arrive at the geometric phase associated with \mathcal{P} is to realize that there is an equivalence set S of unitarities $\tilde{V}(t)$ that for $t \in [0, \tau]$ all realize \mathcal{P} , namely, those of the form

$$\tilde{V}(t) = V(t) \sum_{k=1}^N e^{i\theta_k(t)} |\phi_k(0)\rangle\langle\phi_k(0)|, \quad (7)$$

where $V(t) \in S$ fulfills $V(0) = I$, but is otherwise arbitrary, and $\theta_k(t)$ are real time-dependent parameters such that $\theta_k(0) = 0$. We may, in particular, identify $V^{\parallel}(t) \in S$, fulfilling the parallel transport conditions

$$\langle\phi_k(0)|V^{\parallel\dagger}(t)\dot{V}^{\parallel}(t)|\phi_k(0)\rangle = 0, \quad k = 1, \dots, N, \quad (8)$$

in terms of which the relative phase in Eq. (6) coincides with the geometric phase associated with the path \mathcal{P} . Substituting $V^{\parallel}(t) = \tilde{V}(t)$, with $\tilde{V}(t)$ given by Eq. (7), into Eq. (8), we obtain

$$\theta_k(t) = i \int_0^t \langle\phi_k(0)|V^{\dagger}(t')\dot{V}(t')|\phi_k(0)\rangle dt'. \quad (9)$$

Taking this expression for $\theta_k(t)$ into Eq. (6) for $V^{\parallel}(t)$, we finally obtain the geometric phase for the path \mathcal{P} as

$$\gamma[\mathcal{P}] = \arg\left(\sum_{k=1}^N \sqrt{\omega_k(0)\omega_k(\tau)} \langle\phi_k(0)|V^{\parallel}(\tau)|\phi_k(0)\rangle\right). \quad (10)$$

The explicit expression of it reads

$$\gamma[\mathcal{P}] = \arg\left(\sum_{k=1}^N \sqrt{\omega_k(0)\omega_k(\tau)} \langle\phi_k(0)|\phi_k(\tau)\rangle e^{-\int_0^\tau \langle\phi_k(t)|\dot{\phi}_k(t)\rangle dt}\right). \quad (11)$$

Now, a reasonable notion of mixed state geometric phase in the nonunitary case should satisfy the following conditions: (a) it must be gauge invariant, i.e., be dependent only upon the path traced out by the system's density operator $\rho(t)$; (b) it should reduce to well-known results in the limit of unitary evolution; (c) it should be experimentally testable. Let us verify that the geometric phase in Eq. (11) fulfills these conditions.

First, the phase $\gamma[\mathcal{P}]$ is manifestly gauge invariant in that it takes the same value for all $V(t) \in S$. One may check this point by directly substituting Eq. (7) into Eq. (11) and finding

$$\gamma[\mathcal{P}]|_{V(t)} = \gamma[\mathcal{P}]|_{\tilde{V}(t)}. \quad (12)$$

In particular, if we let $V(t) = V^{\parallel}(t)$, we have

$$\begin{aligned} \gamma[\mathcal{P}] &= \arg\left(\sum_{k=1}^N \sqrt{\omega_k(0)\omega_k(\tau)} \langle\phi_k(0)|V^{\parallel}(\tau)|\phi_k(0)\rangle\right) \\ &= \alpha(\tau), \end{aligned} \quad (13)$$

which verifies that the relative phase gives the geometric phase for $V(t) = V^{\parallel}(t)$. Thus, the geometric phase defined by Eq. (11) depends only upon the path \mathcal{P} traced out by $\rho(t)$.

Second, when the evolution is unitary, corresponding to the case where the eigenvalues ω_k are time independent and $V(t)$ is identified with the time evolution operator of the state, the geometric phase defined by Eq. (11) leads to well-known results [8,9].

Finally, we demonstrate that the phases $\alpha(\tau)$ and $\gamma[\mathcal{P}]$ are experimentally testable. The measurement can be done by using the scheme of purifying $\rho(t)$ described in Eq. (2). In fact, the interference profile between $|\Psi(0)\rangle$ and $|\Psi(\tau)\rangle$ reads

$$I(\chi) = |e^{i\chi}|\Psi(0)\rangle + |\Psi(\tau)\rangle|^2 \propto 1 + \nu(\tau) \cos[\chi - \alpha(\tau)], \quad (14)$$

where $\alpha(\tau)$ is the relative phase in Eq. (6), and

$$\nu(\tau) = \left| \sum_{k=1}^N \sqrt{\omega_k(0)\omega_k(\tau)} \langle \phi_k(0) | \phi_k(\tau) \rangle \right| \quad (15)$$

is the visibility of the interference fringes obtained by varying the additional U(1) shift χ . Using the Mach-Zehnder interferometer setup with $|\Psi(0)\rangle$ and $|\Psi(\tau)\rangle$ as internal states in each beam, the intensity modulation can be measured and the phase $\alpha(\tau)$ is obtained.

A construction of the purification Eq. (2) of the path \mathcal{P} is as follows. Let $U_{sa}(t)$ be a unitarity on $\mathcal{H}_s \otimes \mathcal{H}_a$ such that $|\Psi(t)\rangle = U_{sa}(t)|\Psi(0)\rangle$, $t \in [0, \tau]$, purifies the path $\mathcal{P} : t \rightarrow \rho(t)$. The purifications are obtained for all choices of $U_{sa}(t)$ for which the ancilla part of the Schmidt basis of the tensor product space $\mathcal{H}_s \otimes \mathcal{H}_a$ is kept fixed. Explicitly, $U_{sa}(t)$ may be expressed as

$$U_{sa}(t) = (V(t) \otimes I)W(t)W^\dagger(0), \quad (16)$$

where $\{W(t)|t \in [0, \tau]\}$ is a one-parameter family of unitary operators on $\mathcal{H}_s \otimes \mathcal{H}_a$. These latter operators are restricted only by the requirement that the elements of the $k_0 l_0$ th column, say, of their matrix representation in the $|\phi_k(0)\rangle \otimes |a_l\rangle$ basis must obey

$$W_{kl, k_0 l_0}(t) = \delta_{kl} \sqrt{\omega_k(t)}, \quad (17)$$

where $k, l, k_0, l_0 = 1, \dots, N$. With $U_{sa}(t)$, the relative phase $\alpha(\tau)$ is measured via Eq. (14), and it gives the

$$\gamma[\mathcal{P}] = -\pi + \frac{\eta}{4\Lambda} \ln \left(\frac{(1 - \cos\theta_0)(\sqrt{\cos^2\theta_0 + \sin^2\theta_0 e^{-4\pi\Lambda/\eta}} + \cos\theta_0)}{(1 + \cos\theta_0)(\sqrt{\cos^2\theta_0 + \sin^2\theta_0 e^{-4\pi\Lambda/\eta}} - \cos\theta_0)} \right). \quad (21)$$

For small Λ/η , we may Taylor expand the right-hand side of Eq. (21) and obtain to first order

$$\gamma[\mathcal{P}] \approx -\pi(1 - \cos\theta_0) + \pi^2 \cos\theta_0 \sin^2\theta_0 \frac{\Lambda}{\eta}. \quad (22)$$

In Ref. [17], the effect of dephasing on the pure state geometric phase has been analyzed using a quantum-jump approach, leading to a dephasing independent geometric phase effect. From the perspective of the mixed state geometric phase, we have obtained a first order dependence on dephasing, which reduces only to that of Ref. [17] for nonunitary paths \mathcal{P} characterized by $\theta_0 =$

geometric phase either if $V(t) = V^{\parallel}(t)$ or if exposing the other beam by a compensating unitarity of the form

$$V_c(t) = \sum_{k=1}^N e^{i\int_0^t \langle \phi_k(0) | V^\dagger(t') \dot{V}(t') | \phi_k(0) \rangle dt'} |\phi_k(0)\rangle \langle \phi_k(0)|, \quad (18)$$

resulting in the relative unitarity $V(t)V_c^\dagger(t) = V^{\parallel}(t)$, acting on s . Thus, we have demonstrated that the present mixed state geometric phase is experimentally testable in principle [19].

To calculate the geometric phase for an explicit physical example, let us consider a qubit subjected to the free precession Hamiltonian $H = (\eta/2)\sigma_z$ and dephasing represented by the Lindblad operator [20] $\Gamma = \sqrt{(\Lambda/2)}\sigma_z$, where the real parameters η and Λ are the precession rate and strength of dephasing, respectively. For the qubit initially in a pure state characterized by the Bloch vector $\mathbf{r}(0) = (\sin\theta_0, 0, \cos\theta_0)$, the solution $\rho_{\text{dp}}(t)$ of the Lindblad equation [20] is characterized by

$$\begin{aligned} \omega_1(t) &= 1 - \omega_2(t) = \frac{1}{2}(1 + \sqrt{\cos^2\theta_0 + e^{-2\Lambda t} \sin^2\theta_0}), \\ |\phi_1(t)\rangle &= e^{-i\eta t/2} \cos\frac{\theta_t}{2} |0\rangle + \sin\frac{\theta_t}{2} e^{i\eta t/2} |1\rangle, \\ |\phi_2(t)\rangle &= -e^{-i\eta t/2} \sin\frac{\theta_t}{2} |0\rangle + \cos\frac{\theta_t}{2} e^{i\eta t/2} |1\rangle, \end{aligned} \quad (19)$$

where

$$\tan\theta_t = e^{-\Lambda t} \tan\theta_0 \quad (20)$$

and $\{|0\rangle, |1\rangle\}$ is the standard qubit basis. By inserting Eqs. (19) and (20) into Eq. (11), the geometric phase associated with the quasicyclic path $\mathcal{P} : t \in [0, 2\pi/\eta] \rightarrow \rho_{\text{dp}}(t)$ becomes (assuming $\cos\theta_0 \geq 0$)

$\pi/2$, corresponding to precession in the equatorial plane of the Bloch ball.

Let us end by briefly delineating the degenerate case. Consider the path

$$\mathcal{P} : t \in [0, \tau] \rightarrow \rho(t) = \sum_{k=1}^K \sum_{\mu=1}^{n_k} \omega_k(t) |\phi_k^\mu(t)\rangle \langle \phi_k^\mu(t)|, \quad (23)$$

where $\omega_k(t)$, $k = 1, \dots, K \leq N$, are the eigenvalues of $\rho(t)$ each with degeneracy n_k , and $|\phi_k^\mu(t)\rangle$, $\mu = 1, \dots, n_k$, are the corresponding degenerate eigenvectors. The geometric phase of \mathcal{P} is

$$\gamma[\mathcal{P}] = \arg\left(\sum_{k=1}^K \sum_{\mu=1}^{n_k} \sqrt{\omega_k(0)\omega_k(\tau)} \langle \phi_k^\mu(0) | V^{\parallel}(\tau) | \phi_k^\mu(0) \rangle\right). \quad (24)$$

In the above expression, $V^{\parallel}(\tau)$ is defined by $V^{\parallel}(t) = V(t) \sum_k V_k(t)$ with $V(t) = \sum_{k,\mu} |\phi_k^\mu(t)\rangle \langle \phi_k^\mu(0)|$ and

$$V_k(t) = \sum_{\mu,\nu} |\phi_k^\mu(0)\rangle \langle \phi_k^\nu(0) | \alpha_k^{\mu\nu}(t), \quad (25)$$

where $\alpha_k^{\mu\nu}(t)$ are determined by the parallel transport condition

$$\langle \phi_k^\mu(0) | V^{\parallel\dagger}(t) \dot{V}^{\parallel}(t) | \phi_k^\nu(0) \rangle = 0, \quad \mu, \nu = 1, \dots, n_k, \quad (26)$$

with $\alpha_k(0) = I$, which leads to

$$\alpha_k^{\mu\nu}(t) = \langle \phi_k^\mu(0) | \mathbf{P} e^{-\int_0^t V^{\dagger}(t') \dot{V}^{\parallel}(t') dt'} | \phi_k^\nu(0) \rangle, \quad (27)$$

where \mathbf{P} denotes path ordering. The above may be generalized to the case where $\omega_k(t)$ is degenerate only on the time interval $[t_0, t_1] \subset [0, \tau]$ by noting that the eigenvectors in the corresponding subspace are, due to continuity, uniquely given at the end points $t = t_0$ and $t = t_1$.

In summary, we have proposed a kinematic approach to the mixed state geometric phase in nonunitary evolution. The proposed geometric phase is gauge invariant in that it depends only upon the path in state space of the considered system. We have demonstrated that the proposed geometric phase for nonunitarily evolving mixed states is experimentally testable in interferometry. Moreover, it leads to the well-known results when the evolution is unitary. As an example, we have used the present approach to calculate the geometric phase for nonunitarily evolving mixed states in the case of a qubit undergoing free precession around a fixed axis and affected by dephasing.

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$$W(t) = \sqrt{\omega_1(t)} \sigma_z \otimes I + \sqrt{\omega_2(t)} \sigma_x \otimes \sigma_x,$$

which is unitary and fulfills Eq. (17). It yields

$$U_{sa}(t) = (V(t) \otimes I)(\zeta I \otimes I + i\xi \sigma_y \otimes \sigma_x).$$

Here, $\sigma_x, \sigma_y, \sigma_z$ are the standard Pauli operators and

$$\zeta = \sqrt{\omega_1(0)\omega_1(t)} + \sqrt{\omega_2(0)\omega_2(t)},$$

$$\xi = \sqrt{\omega_1(t)\omega_2(0)} - \sqrt{\omega_2(t)\omega_1(0)}.$$

There are infinitely many other choices of $W(t)$, and thus also of $U_{sa}(t)$, to realize the evolution $|\Psi(t)\rangle$.

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