Geometric phases for mixed states in interferometry

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We provide a physical prescription based on interferometry for introducing the total phase of a mixed state undergoing unitary evolution, which has been an elusive concept in the past. We define the parallel transport condition that provides a connection-form for obtaining the geometric phase for mixed states. The expression for the geometric phase for mixed state reduces to well known formulas in the pure state case when a system undergoes noncyclic and unitary quantum evolution.

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When a pure quantal state undergoes cyclic evolution the system returns to its original state but may acquire a phase factor of purely geometric origin. Though this was realized in the adiabatic context [1], the nonadiabatic generalization was found in [2]. Based on Pancharatnam's [3] earlier work, this concept was generalized to noncyclic evolutions of quantum systems [4]. Subsequently, the kinematic approach [5] and gauge potential description [6,7] of geometric phases for noncyclic and non-Schrödinger evolutions were provided. The adiabatic Berry phase and Hannay angle for open paths were introduced [8] and discussed [9]. The noncyclic geometric phase has been generalized to non-Abelian cases [10]. Applications of geometric phase have been found in molecular dynamics [11], response function of many-body system [12,13], and geometric quantum computation [14,15]. Noncyclic geometric phase for entangled states has also been studied [16]. In all these developments the geometric phase has been discussed only for *pure* states. However, in some applications, in particular geometric fault tolerant quantum computation [14,15], we are primarily interested in mixed state cases. Uhlmann was probably the first to address the issue of mixed state holonomy, but as a purely mathematical problem [17,18]. In contrast, here we provide a new formalism of geometric phase for mixed states in the experimental context of quantum interferometry.

The purpose of this Letter is to provide an *operationally well defined* notion of phase for unitarily evolving mixed quantal states in interferometry, which has been an elusive concept in the past. This phase fulfills two central properties that makes it a natural generalization of the pure case: (i) it gives rise to a linear shift of the interference oscillations produced by a variable $U(1)$ phase, and (ii) it reduces to the Pancharatnam connection [3] for pure states. We introduce the notion of parallel transport based on our defintion of total phase. We moreover introduce a concept of geometric phase for unitarily evolving mixed quantal states. This geometric phase reduces to the standard geometric phase [5–7] for pure states undergoing noncyclic unitary evolution.

Mixed states, phases and interference: Consider a conventional Mach-Zehnder interferometer in which the beam-pair spans a two dimensional Hilbert space $\tilde{\mathcal{H}} = \{|\tilde{0}\rangle, |\tilde{1}\rangle\}$. The state vectors $|\tilde{0}\rangle$ and $|\tilde{1}\rangle$ can be taken as wave packets that move in two given directions defined by the geometry of the interferometer. In this basis, we may represent mirrors, beam-splitters and relative $U(1)$ phase shifts by the unitary operators

$$\tilde{U}_M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \tilde{U}_B = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$
$$\tilde{U}(1) = \begin{pmatrix} e^{i\chi} & 0 \\ 0 & 1 \end{pmatrix}, \quad (1)$$

respectively. An input pure state $\tilde{\rho}_{\rm in} = |\tilde{0}\rangle\langle\tilde{0}|$ of the interferometer transforms into the output state

$$\tilde{\rho}_{\rm out} = \tilde{U}_B \tilde{U}_M \tilde{U}(1) \tilde{U}_B \tilde{\rho}_{\rm in} \tilde{U}_B^\dagger \tilde{U}^\dagger(1) \tilde{U}_M^\dagger \tilde{U}_B^\dagger$$
$$= \frac{1}{2} \begin{pmatrix} 1+\cos\chi & i\sin\chi \\ -i\sin\chi & 1-\cos\chi \end{pmatrix} \quad (2)$$

that yields the intensity along $|\tilde{0}\rangle$ as $I \propto 1+\cos\chi$. Thus the relative $U(1)$ phase χ could be observed in the output signal of the interferometer.

Now assume that the particles carry additional internal degrees of freedom, e.g., spin. This internal spin space $\mathcal{H}_{\rm i} \cong \mathcal{C}^N$ is spanned by the vectors $|k\rangle$, $k = 1, 2, \ldots N$, chosen so that the associated density operator is initially diagonal

$$\rho_0 = \sum_k w_k |k\rangle\langle k| \quad (3)$$

with w_k the classical probability to find a member of the ensemble in the pure state $|k\rangle$. The density operator could be made to change inside the interferometer

$$\rho_0 \longrightarrow U_{\rm i} \rho_0 U_{\rm i}^\dagger \quad (4)$$

with $U_{\rm i}$ a unitary transformation acting only on the internal degrees of freedom. Mirrors and beam-splitters are assumed to leave the internal state unchanged so that we may replace $\tilde{U}_M$ and $\tilde{U}_B$ by $\mathbf{U}_M = \tilde{U}_M \otimes 1_{\rm i}$ and $\mathbf{U}_B = \tilde{U}_B \otimes 1_{\rm i}$, respectively, $1_{\rm i}$ being the internal unit operator. Furthermore, we introduce the unitary transformation

$$\mathbf{U} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \otimes U_{\rm i} + \begin{pmatrix} e^{i\chi} & 0 \\ 0 & 0 \end{pmatrix} \otimes 1_{\rm i}. \quad (5)$$

The operators $\mathbf{U}_M$, $\mathbf{U}_B$, and $\mathbf{U}$ act on the full Hilbert space $\tilde{\mathcal{H}} \otimes \mathcal{H}_{\rm i}$. $\mathbf{U}$ correponds to the application of $U_{\rm i}$ along the $|\tilde{1}\rangle$ path and the $U(1)$ phase χ similarly along $|\tilde{0}\rangle$. We shall use $\mathbf{U}$ to generalize the notion of phase to unitarily evolving mixed states.

Let an incoming state given by the density matrix $\varrho_{\rm in} = \tilde{\rho}_{\rm in} \otimes \rho_0 = |\tilde{0}\rangle\langle\tilde{0}| \otimes \rho_0$ be split coherently by a beam-splitter and recombine at a second beam-splitter after being reflected by two mirrors. Suppose that $\mathbf{U}$ is applied between the first beam-splitter and the mirror pair. The incoming state transforms into the output state

$$\varrho_{\rm out} = \mathbf{U}_B \mathbf{U}_M \mathbf{U} \mathbf{U}_B \varrho_{\rm in} \mathbf{U}_B^\dagger \mathbf{U}^\dagger \mathbf{U}_M^\dagger \mathbf{U}_B^\dagger. \quad (6)$$

Inserting Eqs. (1) and (5) into Eq. (6) yields

$$\varrho_{\rm out} = \frac{1}{4}\Bigg[\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \otimes U_{\rm i}\rho_0 U_{\rm i}^\dagger + \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \otimes \rho_0 + e^{i\chi}\begin{pmatrix} 1 & 1 \\ -1 & -1 \end{pmatrix} \otimes \rho_0 U_{\rm i}^\dagger + e^{-i\chi}\begin{pmatrix} 1 & -1 \\ 1 & -1 \end{pmatrix} \otimes U_{\rm i}\rho_0\Bigg]. \quad (7)$$

The output intensity along $|\tilde{0}\rangle$ is

$$I \propto {\rm Tr}\left(U_{\rm i}\rho_0 U_{\rm i}^\dagger + \rho_0 + e^{-i\chi}U_{\rm i}\rho_0 + e^{i\chi}\rho_0 U_{\rm i}^\dagger\right) \propto 1 + |{\rm Tr}\,(U_{\rm i}\rho_0)\,|\cos\left[\chi - \arg {\rm Tr}\,(U_{\rm i}\rho_0)\right], \quad (8)$$

where we have used ${\rm Tr}(\rho_0 U_{\rm i}^\dagger) = [{\rm Tr}\,(U_{\rm i}\rho_0)]^*$.

The important observation from Eq. (8) is that the interference oscillations produced by the variable $U(1)$ phase χ *is shifted by* $\phi = \arg Tr\,(U_i\rho_0)$ *for any internal input state* ρ_0, be it mixed or pure. This phase difference reduces for pure states $\rho_0 = |\psi_0\rangle\langle\psi_0|$ to the Pancharatnam phase difference between $U_{\rm i}|\psi_0\rangle$ and $|\psi_0\rangle$. These two latter facts are the central properties for ϕ being a natural generalization of the pure state phase. Moreover the visibility of the interference pattern is $\nu = |{\rm Tr}\,(U_{\rm i}\rho_0)\,| \geq 0$, which reduces to the expected $\nu = |\langle\psi_0|U_{\rm i}|\psi_0\rangle|$ for pure states.

The output intensity in Eq. (8) may be understood as an incoherent weighted average of pure state interference profiles as follows. The state k gives rise to the interference profile

$$I_k \propto 1 + \nu_k \cos\left[\chi - \phi_k\right], \quad (9)$$

where $\nu_k = |\langle k|U_{\rm i}|k\rangle|$ and $\phi_k = \arg\langle k|U_{\rm i}|k\rangle$. This yields the total output intensity

$$I = \sum_k w_k I_k \propto 1 + \sum_k w_k \nu_k \cos\left[\chi - \phi_k\right], \quad (10)$$

which is the incoherent classical average of the above single-state interference profiles weighted by the corresponding probabilities w_k. Eq. (10) may be written in the desired form $1 + \tilde{\nu}\cos(\chi - \tilde{\phi})$ by making the identifications

$$\tilde{\phi} = \arg\left(\sum_k w_k \nu_k e^{i\phi_k}\right) = \arg {\rm Tr}\,(U_{\rm i}\rho_0) = \phi,$$
$$\tilde{\nu} = \left|\sum_k w_k \nu_k e^{i\phi_k}\right| = |{\rm Tr}\,(U_{\rm i}\rho_0)\,| = \nu. \quad (11)$$

Parallel transport condition and geometric phase: Consider a continuous unitary transformation of the mixed state given by $\rho(t) = U(t)\rho_0 U^\dagger(t)$. (From now on, we omit the subscript "i" of U.) We say that the state of the system $\rho(t)$ acquires a phase with respect to ρ_0 if $\arg {\rm Tr}[U(t)\rho_0]$ is nonvanishing. Now if we want to parallel transport a mixed state $\rho(t)$ along an arbitrary path, then at each instant of time the state must be *in-phase* with the state at an infinitesimal time. The state at time $t + dt$ is related to the state at time t as $\rho(t+dt) = U(t+dt)U^\dagger(t)\rho(t)U(t)U^\dagger(t+dt)$. Therefore, the phase difference between $\rho(t)$ and $\rho(t+dt)$ is $\arg {\rm Tr}[\rho(t)U(t+dt)U^\dagger(t)]$. We can say $\rho(t)$ and $\rho(t+dt)$ are in phase if ${\rm Tr}[\rho(t)U(t+dt)U^\dagger(t)]$ is *real and positive.* This condition can be regarded as a generalization of Pancharatnam's connection from pure to mixed states. However, from normalization and Hermiticity of $\rho(t)$ it follows that ${\rm Tr}[\rho(t)\dot{U}(t)U^\dagger(t)]$ is purely imaginary. Hence the above mixed state generalization of Pancharatnam's connection can be met only when

$${\rm Tr}[\rho(t)\dot{U}(t)U^\dagger(t)] = 0. \quad (12)$$

This is the parallel transport condition for mixed states undergoing unitary evolution. On the space of density matrices the above condition can be translated to ${\rm Tr}[\rho\ dU\ U^\dagger] = 0$, where d is the exterior derivative on the space of density operators. However, $\rho(t)$ determines the $N \times N$ matrix $U(t)$ (N being the dimension of the Hilbert space) up to N phase factors, and the single condition Eq. (12) while necessary is not sufficient to determine $U(t)$. These N phase factors are fixed by the N parallel transport conditions

$$\langle k(t)|\dot{U}(t)U^\dagger(t)|k(t)\rangle = 0, \;\; k = 1, 2, \ldots N, \quad (13)$$

where the $|k(t)\rangle$'s are orthonormal eigenstates of $\rho(t)$. These are sufficient to determine the parallel transport operator $U(t)$ if we are given a non-degenerate density matrix $\rho(t)$.

The parallel transport condition for a mixed state provides us a *connection* in the space of density operators which can be used to define the geometric phase. Thus a mixed state can acquire pure geometric phase if it undergoes parallel transport along an arbitrary curve. One can check that if we have a pure state density operator $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ then the parallel transport condition Eq. (12) reduces to $\langle\psi(t)|\dot{\psi}(t)\rangle = 0$ as has been discussed in [2,4–7,19,20] which is both necessary and sufficient.

Now we can define a geometric phase for mixed state evolution. Let the state trace out an open unitary curve $\Gamma : t \in [0,\tau] \longrightarrow \rho(t) = U(t)\rho_0 U^\dagger(t)$ in the space of density operators with "end-points" $\rho(0) = \rho_0$ and $\rho(\tau)$, where $U(t)$ satisfies Eq. (12). The evolution need not be cyclic, i.e. $\rho(\tau) \neq \rho_0$. We can naturally assign a geometric phase $\gamma_g[\Gamma]$ to this curve once we notice that the dynamical phase vanishes identically. The dynamical phase is the time integral of the average of Hamiltonian and can be defined as

$$\begin{aligned}\gamma_d &= -\frac{1}{\hbar}\int_0^\tau dt\ \mathrm{Tr}[\rho(t)H(t)] \\ &= -i\int_0^\tau dt\ \mathrm{Tr}[\rho_0 U^\dagger(t)\dot{U}(t)]. \qquad (14)\end{aligned}$$

Since the density matrix undergoes parallel transport evolution the dynamical phase vanishes identically. Moreover, the parallel transport operator $U(t)$ should fulfill the stronger condition Eq. (13). Thus the geometric phase for a mixed state is defined as

$$\gamma_g[\Gamma] = \phi = \arg \mathrm{Tr}[\rho_0 U(t)] = \arg\left(\sum_k w_k \nu_k e^{i\beta_k}\right), \quad (15)$$

where $\exp(i\beta_k)$ are geometric phase factors associated with the individual pure state paths in the given ensemble. The above geometric phase can be given a gauge potential description such that the line integral will give the open path geometric phase for mixed state evolution. Indeed the mixed state holonomy can be expressed as

$$\begin{aligned}\gamma_g[\Gamma] &= \int dt\ i\mathrm{Tr}[\rho_0 W^\dagger(t)\dot{W}(t)] \\ &= \int_\Gamma i\mathrm{Tr}\left[\rho_0 W^\dagger dW\right] = \int_\Gamma d\Omega, \qquad (16)\end{aligned}$$

where

$$W(t) = \frac{\mathrm{Tr}[\rho_0 U^\dagger(t)]}{|\mathrm{Tr}[\rho_0 U^\dagger(t)]|}U(t). \quad (17)$$

and $U(t)$ satisfies (13). The quantity $\Omega = i\mathrm{Tr}\left[\rho_0 W^\dagger dW\right]$ can be regarded as a gauge potential on the space of density operators pertaining to the system.

The geometric phase defined above is manifestly gauge invariant, does not depend explicitly on the dynamics but it depends only on the geometry of the open unitary path Γ in the space of density operators pertaining to the system. It is also independent of the rate at which the system is transported in the quantum state space. The geometric phase Eq. (16) can also be expressed in terms of an average connection form

$$\gamma_g[\Gamma] = \int_\Gamma \sum_k w_k i\langle\chi_k|d\chi_k\rangle = \int_\Gamma \sum_k w_k \Omega_k, \quad (18)$$

where Ω_k is connection-form and $|\chi_k(t)\rangle = W(t)|k\rangle$ is the "reference-section" for kth component in the ensemble. To be sure, what we have defined is consistent with known results, we can check that this expression reduces to the standard geometric phase [5–7]

$$\gamma_g[\Gamma] = \arg\langle\psi(0)|\psi(\tau)\rangle = \int_0^\tau dt\ i\langle\chi(t)|\dot{\chi}(t)\rangle \quad (19)$$

for a pure state $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$ when it satisfies parallel transport condition. Here, $|\chi(t)\rangle$ is a reference state, which gives the generalised connection one-form [6,7].

Purification: An alternative approach to the above results is given by lifting the mixed state into a purified state $|\Psi\rangle$ by attaching an ancilla. We can imagine that any mixed state can be obtained by tracing out some degrees of freedom of a larger system which was in a pure state

$$|\Psi\rangle = \sum_k \sqrt{w_k}|k\rangle_s|k\rangle_a, \quad (20)$$

where $|k\rangle_a$ is a basis in an auxiliary Hilbert space, describing everything else apart from the spatial and the spin degrees of freedom. The existence of the above purification requires that the dimensionality of the auxiliary Hilbert space is at least as large as that of the internal Hilbert space. If $|\Psi\rangle$ is the state at time $t = 0$ and it is transformed to $|\Psi(t)\rangle$ by a local unitary operator $U(t) = U_s(t) \otimes I_a$ then

$$|\Psi(t)\rangle = \sum_k \sqrt{w_k}U_s(t)|k\rangle_s|k\rangle_a. \quad (21)$$

The inner-product of initial and final state

$$\langle\Psi(0)|\Psi(t)\rangle = \sum_k w_k\langle k|U(t)|k\rangle = \mathrm{Tr}(U(t)\rho_0) \quad (22)$$

gives the full description of the modified interference. Indeed by comparing Eqs. (8) and (22), we see that $\arg\langle\Psi(0)|\Psi(t)\rangle$ is the phase shift and $|\langle\Psi(0)|\Psi(t)\rangle|$ is the visibility of the output intensity obtained in an interferometer.

The parallel transport condition, given by Eq. (12), follows immediately from the pure state case when applied to any purification of ρ_0, i.e.

$$0 = \langle \Psi(t)|\dot{\Psi}(t)\rangle = \sum_k w_k \langle k|U^\dagger(t)\dot{U}(t)|k\rangle$$
$$= \mathrm{Tr}[\rho_0 U^\dagger(t)\dot{U}(t)] = \mathrm{Tr}[\rho(t)\dot{U}(t)U^\dagger(t)]. \quad (23)$$

Thus a parallel transport of a density operator $\rho(t)$ amounts to a parallel transport of any of its purifications.

Example: Consider a qubit (a spin-$\frac{1}{2}$ particle) whose density matrix can be written as

$$\rho = \frac{1}{2}(1 + r\hat{\mathbf{r}}\cdot\boldsymbol{\sigma}), \quad (24)$$

where $\hat{\mathbf{r}}$ is a unit vector and r is constant for unitary evolution. The pure states $r = 1$ define the unit Bloch sphere containing the mixed states $r < 1$. Suppose that during the time evolution $\hat{\mathbf{r}}$ traces out a curve on the Bloch sphere that subtends a geodesically closed solid angle Ω [19]. The two pure states $|\pm; \hat{\mathbf{r}}\cdot\boldsymbol{\sigma}\rangle$ acquire noncyclic geometric phase $\mp\Omega/2$ and identical visibility $\nu_+ = \nu_- \equiv \eta$. Using Eq. (15) we obtain the geometric phase for Γ

$$\phi = \gamma_g[\Gamma] = -\arctan\left(r\tan\frac{\Omega}{2}\right). \quad (25)$$

The visibility $\nu = |\mathrm{Tr}\,(U\rho_0)\,|$ is given by

$$\nu = \eta\sqrt{\cos^2\frac{\Omega}{2} + r^2\sin^2\frac{\Omega}{2}}. \quad (26)$$

For cyclic evolution we have $\eta = 1$ but the mixed state $\nu \neq 1$ due to the square root factor on the right-hand side of Eq. (26). Moreover Eqs. (25) and (26) reduce to the usual expressions for pure states $\phi = -\Omega/2$ and $\nu = \eta$ by letting $r = 1$.

In the case of maximally mixed states $r = 0$ we obtain $\phi = \arg\cos(\Omega/2)$ and $\nu = |\cos(\Omega/2)|$. Thus the output intensity for such states is

$$I \propto 1 + |\cos\frac{\Omega}{2}|\cos\left[\chi - \arg\cos\frac{\Omega}{2}\right]$$
$$= 1 + \cos\frac{\Omega}{2}\cos\chi. \quad (27)$$

Early experiments [23–25] to test the 4π symmetry of spinors utilized unpolarized neutrons. Eq. (27) show that in these experiments the sign change for $\Omega = 2\pi$ is a consequence of the phase shift $\phi = \arg\cos\pi = \pi$.

Note that $\gamma_g[\Gamma]$ in Eq. (25) equals the geodesically closed solid angle on the Poincaré sphere iff $r = 1$. In the mixed state case the geometric phase factor is weighted average of the solid angles subtended by the two pure state paths on the Bloch sphere.

In conclusion, we have provided a physical prescription based on interferometry for introducing a concept of total phase for mixed states undergoing unitary evolution. We have provided the necessary and sufficient condition for parallel transport of a mixed state and introduced a concept of geometric phase for mixed states when it undergoes parallel transport. This reduces to known formulas for pure state case when the system follows a noncyclic and unitary quantum evolutions. We have also provided a gauge potential for noncyclic evolutions of mixed states whose line integral gives the geometric phase. We hope this will lead to experimental test of geometric phases for mixed states and further generalization of it to nonunitary and nonlinear evolutions.

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