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]. 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 [16,17]. In contrast, here we provide a simple discussion 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 definition 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 quantum evolution.

Pure states, phases and interference: Consider a conventional Mach-Zehnder interferometer in which the beam-pair spans a two dimensional Hilbert space $\mathcal{H} = \{|0\rangle, |1\rangle\}$. The state vectors $|0\rangle$ and $|1\rangle$ 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

$$\hat{U}_M = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{U}_B = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix},$$

$$\hat{U}(1) = \begin{pmatrix} e^{i\chi} & 0 \\ 0 & 1 \end{pmatrix},$$

(1)

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

$$\tilde{\rho}_{out} = \hat{U}_B \hat{U}_M \hat{U}(1) \hat{U}_B \tilde{\rho}_{in} \hat{U}_B \hat{U}(1) \hat{U}_M \hat{U}_B$$

$$= \frac{1}{2} \begin{pmatrix} 1 + \cos \chi & i \sin \chi \\ -i \sin \chi & 1 - \cos \chi \end{pmatrix}$$

(2)

that yields the intensity along $|0\rangle$ as

$$I \propto 1 + \cos \chi.$$

(3)

Thus the relative $U(1)$ phase $\chi$ 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 $\mathcal{H}_s$ is spanned by the vectors $|k\rangle$ chosen so that the associated density operator is initially diagonal

$$\rho_0 = \sum_k w_k |k\rangle\langle k|$$

(4)

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

$$\rho_0 \longrightarrow U_i \rho_0 U_i^\dagger$$

(5)

with $U_i$ 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 $\hat{U}_M$ and $\hat{U}_B$ by $\hat{U}_M = \hat{U}_M \otimes 1_i$ and $\hat{U}_B = \hat{U}_B \otimes 1_i$, respectively, $1_i$ being the internal unit operator. Furthermore, we introduce the transformation
\[
\hat{U} = \left( \begin{array}{cc} 0 & 0 \\ 0 & 1 \end{array} \right) \otimes \hat{I}_1 + \left( \begin{array}{cc} e^{i\chi} & 0 \\ 0 & 0 \end{array} \right) \otimes \hat{I}_1. \tag{6}
\]
The operators $\hat{U}_M$, $\hat{U}_B$, and $\hat{U}$ act on the full Hilbert space $\mathcal{H} \otimes \mathcal{H}_i$. $\hat{U}$ corresponds to the application of $U_i$ along the $|1\rangle$ path and the $U(1)$ phase $\chi$ similarly along $|0\rangle$. We shall use $\hat{U}$ to generalize the notion of phase to unitarily evolving mixed states.

Mixed states, phases and interference: An incoming state given by the density matrix
\[
\hat{\rho}_{in} = \hat{\rho}_{in} \otimes \rho_0 = |0\rangle \langle 0| \otimes \rho_0 \tag{7}
\]
is split coherently by a beam-splitter and recombined at a second beam-splitter after being reflected by two mirrors. Suppose that $\hat{U}$ is applied between the first beam-splitter and the mirror pair. The incoming state transforms into the output state
\[
\hat{\rho}_{out} = \hat{U}_B \hat{U}_M \hat{U} \hat{\rho}_{in} \hat{U}_B^\dag \hat{U}_M^\dag. \tag{8}
\]
Inserting Eqs. (1), (6), and (7) into Eq. (8) yields
\[
\hat{\rho}_{out} = \frac{1}{4} \left[ \left( \begin{array}{cc} 1 & 1 \\ 1 & 1 \end{array} \right) \otimes \hat{U}_i \rho_0 \hat{U}_i^\dag + \left( \begin{array}{cc} 1 & -1 \\ -1 & 1 \end{array} \right) \otimes \rho_0 \right] \\
+ e^{i\chi} \left( \begin{array}{cc} 1 & 1 \\ 1 & -1 \end{array} \right) \otimes \rho_0 \hat{U}_i^\dag \\
+ e^{-i\chi} \left( \begin{array}{cc} 1 & -1 \\ 1 & 1 \end{array} \right) \otimes \hat{U}_i \rho_0. \tag{9}
\]
The output intensity along $|0\rangle$ is
\[
I \propto \text{Tr} \left( \hat{U}_i \rho_0 \hat{U}_i^\dag + \rho_0 + e^{-i\chi} \hat{U}_i \rho_0 + e^{i\chi} \rho_0 \hat{U}_i^\dag \right) \\
\propto 1 + |\text{Tr} (\hat{U}_i \rho_0)| \cos [\chi - \arg \text{Tr} (\hat{U}_i \rho_0)], \tag{10}
\]
where we have used $\text{Tr}(\rho_0 \hat{U}_i^\dag) = [\text{Tr} (\hat{U}_i \rho_0)]^*$. The important observation from Eq. (10) is that the interference oscillations produced by the variable $U(1)$ phase $\chi$ is shifted by $\phi = \arg \text{Tr} (\hat{U}_i \rho_0)$ for any internal input state $\rho_0$, be it mixed or pure. This phase shift reduces to the Pancharatnam phase for pure states $\rho_0 = |\psi_0\rangle \langle \psi_0|$ as $\arg \text{Tr} (\hat{U}_i |\psi_0\rangle \langle \psi_0|) = \arg \langle \psi_0 |\hat{U}_i |\psi_0\rangle$. These two latter facts are the central properties for $\phi$ being a natural generalization of the pure state phase. Moreover the visibility of the interference pattern is $\nu = |\text{Tr} (\hat{U}_i \rho_0)| \geq 0$, which reduces to the expected $\nu = |\langle \psi_0 |\hat{U}_i |\psi_0\rangle|$ for pure states.

The output intensity in Eq. (10) may be understood as an incoherent weighted average of pure state interference profiles as follows. The state $k$ gives rise to the interference profile
\[
I_k \propto 1 + \nu_k \cos [\chi - \phi_k], \tag{11}
\]
where $\nu_k = |\langle k |\hat{U}_i |k\rangle|$ and $\phi_k = \arg \langle k |\hat{U}_i |k\rangle$. This yields the total output intensity
\[
I = \sum_k w_k I_k \propto 1 + \sum_k w_k \nu_k \cos [\chi - \phi_k], \tag{12}
\]
which is the incoherent classical average of the above single-state interference profiles weighted by the corresponding probabilities $w_k$. Eq. (12) may be written as $1 + \tilde{\nu} \cos (\chi - \tilde{\phi})$ by making the identifications
\[
\tilde{\phi} = \arctan \left( \frac{\sum_k w_k \nu_k \cos \phi_k}{\sum_k w_k \nu_k \sin \phi_k} \right), \\
\tilde{\nu} = \sqrt{\left( \sum_k w_k \nu_k \cos \phi_k \right)^2 + \left( \sum_k w_k \nu_k \sin \phi_k \right)^2}. \tag{13}
\]
On the other hand from Eq. (4) we have
\[
\text{Tr} (\hat{U}_i \rho_0) = \sum_k w_k \nu_k \cos \phi_k + i \sum_k w_k \nu_k \sin \phi_k. \tag{14}
\]
Thus $\nu = |\text{Tr} (\hat{U}_i \rho_0)| = \tilde{\nu}$ and $\phi = \arg \text{Tr} (\hat{U}_i \rho_0) = \tilde{\phi}$, which proves the above statement.

Parallel transport condition and geometric phase: Consider a continuous unitary transformation of the mixed state given by $\rho(t) = U(t) \rho_0 U(t)^\dag$. (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 $\rho_0$ if $\arg \text{Tr} [U(t) \rho_0]$ 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 $\rho(t + dt) = U(t + dt) U(t)^\dag \rho(t) U(t)^\dag (t + dt)$. Therefore, the phase difference between $\rho(t)$ and $\rho(t + dt)$ is $\arg \text{Tr} [\rho(t) U(t + dt) U(t)^\dag]$.

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 $\text{Tr} [\rho(t) U(t)^\dag]$ is purely imaginary. Hence the above mixed state generalization of Pancharatnam’s connection can be met only when
\[
\text{Tr} [\rho(t) U(t)^\dag] = 0. \tag{15}
\]
This is the parallel transport condition for mixed states undergoing unitary evolution. On the projective Hilbert space $\mathcal{P}$ the above condition can be translated to $\text{Tr} \rho dU = 0$, where $d$ is the exterior derivative in $\mathcal{P}$. The parallel transport condition for a mixed state provides us a connection in the space of density operators which can be used to defined the geometric phase. As we will soon see a mixed state can acquire pure geometric phase if it undergoes parallel transport along an arbitrary
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. (15) reduces to $\langle\psi(t)|\psi(t)\rangle = 0$ as has been discussed in [2,4–7,20].

Now we can define a geometric phase for mixed state evolution. Let the state trace out an open unitary curve $\Gamma : t \in [0, \tau] \rightarrow \rho(t) = U(t)\rho_0 U(t)^\dagger$ in the space of density operators with “end-points” $\rho(0) = \rho_0$ and $\rho(\tau)$. The evolution need not be cyclic, i.e. $\rho(\tau) \neq \rho_0$. To this curve we may naturally assign a geometric phase $\gamma_g[\Gamma]$ by removing the dynamical contribution $\gamma_d$ from the total phase $\phi$, where the dynamical phase in Eq. (18) is naturally defined as

$$\gamma_d = -\frac{1}{\hbar} \int_0^\tau dt \text{Tr}[\rho(t)H(t)]$$

$$= -i \int_0^\tau dt \text{Tr}[\rho_0 U(t)\dot{U}(t)].$$

This may be interpreted as a weighted sum of pure state dynamical phases

$$\gamma_d = \sum_k w_k i \int_0^\tau dt \langle k(0)|U(t)^\dagger\dot{U}(t)|k(0)\rangle$$

$$= \sum_k w_k \gamma_{d,k},$$

which follows by inserting Eq. (4) into the definition of dynamical phase. Thus the geometric phase for a mixed state is defined as

$$\gamma_g[\Gamma] = \phi - \gamma_d = \text{Tr}[\rho_0 U(t)]$$

$$+ i \int_0^\tau dt \text{Tr}[\rho_0 U(t)^\dagger\dot{U}(t)].$$

We see that in the particular case where the parallel transport condition Eq. (15) is fulfilled along $\Gamma$ the dynamical component vanishes and the mixed state acquires a pure geometric phase.

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 in the space of density operators pertaining to the system. 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]

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

$$= \int_0^\tau dt i\langle\chi(t)|\dot{\chi}(t)\rangle$$

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

Next we ask, is there a gauge potential whose line integral will give the open path geometric phase for mixed state evolution? Indeed we find that the geometric phase can be expressed as

$$\gamma_g[\Gamma] = \int dt i\text{Tr}[\rho_0 W^\dagger(t)\dot{W}(t)]$$

$$= \int i\text{Tr}[\rho_0 W^\dagger dW],$$

where

$$W(t) = \frac{\text{Tr}[\rho_0 U^\dagger(t)]}{\text{Tr}[\rho_0 U(t)^\dagger]} U(t).$$

The quantity $\Omega = i\text{Tr}[\rho_0 W^\dagger dW]$ can be regarded as a gauge potential on the space of density operators pertaining to the system. In obtaining the above formula we have used the time derivative of the total phase for a mixed state and simplified it further.

**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

$$|\Psi\rangle = \sum_k \sqrt{w_k} |k_s\rangle |k_a\rangle,$$

where $|k_a\rangle$ 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 larger than that of the internal Hilbert space. If $|\Psi\rangle$ is transformed by a local unitary operator $U = U_s \otimes I_a$ then

$$|\Psi'\rangle = \sum_k \sqrt{w_k} U_s |k_s\rangle |k_a\rangle.$$

The inner-product of initial and final state

$$\langle\Psi|\Psi'\rangle = \sum_k w_k \langle k|U|k\rangle = \text{Tr}(U\rho_0)$$

gives the full description of the modified interference. Indeed by comparing Eqs. (10) and (24), we see that $\text{arg}(\Psi|\Psi')$ is the phase shift and $\langle\Psi|\Psi'\rangle$ is the visibility of the output intensity obtained in an interferometer.

The parallel transport condition, given by Eq. (15), follows immediately from the pure state case when applied to any purification of $\rho_0$

$$0 = \langle\Psi(t)|\dot{\Psi}(t)\rangle = \sum_k w_k \langle k|U^\dagger(t)\dot{U}(t)|k\rangle$$

$$= \text{Tr}[\rho_0 U^\dagger(t)\dot{U}(t)] = \text{Tr}[\rho(t)\dot{U}(t)U^\dagger(t)].$$

Thus a parallel transport of a density operator $\rho$ amounts to a parallel transport of any of its purifications.
where now \( r \cdot r \leq 1 \). The pure states \( r \cdot r = 1 \) define the unit Poincaré sphere containing the mixed states \( r \cdot r < 1 \). To calculate \( \phi \) it is convenient to introduce spherical polar coordinates \( r = r(\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \) and choose \( \mathbf{n} = \hat{z} \). Inserting Eqs. (26) and (27) into the expression of the phase \( \phi = \arg \text{Tr} (U \rho_0) \) and visibility \( \nu = |\text{Tr} (U \rho_0)| \) we obtain
\[
\phi = -\arctan \left( r \cos \theta \tan \frac{\alpha}{2} \right),
\nu = \sqrt{1 - (1 - r^2 \cos^2 \theta) \sin^2 \frac{\alpha}{2}},
\]
which reduce to the usual expressions for pure states \([18,19] \) by letting \( r = 1 \). In the case of maximally mixed states \( r = 0 \) we obtain \( \phi = \arg \cos(\alpha/2) \) and \( \nu = |\cos(\alpha/2)| \). Here \( \phi \) and \( \nu \) are independent of the angle \( \theta \), which may be understood from the fact that maximally mixed states are rotationally invariant. Thus the output intensity for such states is
\[
I \propto 1 + |\cos \frac{\alpha}{2}| \cos \left[ \chi - \arg \cos \frac{\alpha}{2} \right] = 1 + \cos \frac{\alpha}{2} \cos \chi.
\]

Early experiments \([21–23] \) to test the \( 4\pi \) symmetry of spinors utilized unpolarized neutrons. Eq. (29) show that in these experiments the sign change for \( \alpha = \omega t = 2\pi \) rotations of the neutrons is a consequence of the phase shift \( \phi = \arg \cos \pi = \pi \).

In order to calculate the geometric phase, let \( \alpha \) in \( U \) be a continuous function of some parameter. For simplicity \( \mathbf{n} \) is kept fixed in the \( z \) direction. The density operator follows the curve \( \Gamma : t \in [0, \tau] \rightarrow U(t) \rho_0 U^\dagger(t) \), where now \( U(t) = \exp \left( -\frac{i}{\hbar} \alpha(t) \mathbf{n} \cdot \sigma \right) \) and we have chosen \( \alpha(0) = 0 \). Using Eq. (18) we obtain the geometric phase for \( \Gamma \)
\[
\gamma_\rho[\Gamma] = -\arctan \left( r \cos \theta \tan \frac{\alpha(t)}{2} \right) + r \frac{\alpha(t)}{2} \cos \theta.
\]

This expression was obtained in \([24] \) for the case of two entangled spin-\( \frac{1}{2} \) particles, where one of the spins interacted with an external magnetic field in the \( z \) direction.

In the particular case of maximally mixed states \( r = 0 \) we see that the dynamical component of the phase vanishes so that the mixed state acquires a pure geometric phase. Note that \( \gamma_\rho[\Gamma] \) in Eq. (30) equals the geodesically closed solid angle on the Poincaré sphere iff \( r = 1 \); no simple relation to the solid angle traced out by the Bloch vector seems to exist for mixed states.

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 defined a condition for parallel transport of the mixed state and discussed a concept of geometric phase for mixed states. This reduces to known formulas for pure state case when the system follows a noncyclic unitary 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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