Geometry of decomposition dependent evolutions of mixed states

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We examine evolutions where each component of a given decomposition of a mixed quantal state evolves independently in a unitary fashion. The geometric phase and parallel transport conditions for this type of decomposition dependent evolution are delineated. We compare this geometric phase with those previously defined for unitarily evolving mixed states, and mixed state evolutions governed by completely positive maps.

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I. INTRODUCTION

The concept of quantal geometric phase, first discovered for cyclic adiabatic evolutions by Berry [1], has been generalized in several steps. Aharonov and Anandan [2] removed the restriction of adiabaticity and pointed out that the pure state geometric phase is due to the curvature of projective Hilbert space. A general setting of the quantal geometric phase including noncyclic evolution and sequential projection measurements was put forward by Samuel and Bhandari [3], based upon Pancharatnam’s early work [4] on interference of classical light rays in distinct states of polarization. Extension of the geometric phase towards the mixed state case was first conceived by Uhlmann [5], who introduced parallel transport and concomitant geometric phase of density operators. Later, Sjöqvist et al. [6] discovered an operationally well-defined geometric phase for unitarily evolving nondegenerate density operators in the context of quantum interferometry. This latter phase concept has been generalized [7, 8, 9] and experimentally tested [10].

In brief, the mixed state geometric phase in Ref. [6] is basically an extension of Pancharatnam’s relative phase between distinct physical states, added to it the standard pure state parallel transport for each of the spectral basis states of the density operator. Explicitly, for a mixed state, initially described by the density operator $\rho(0)$, the quantity

$$\gamma = \arg \text{Tr}(\rho(0)U(\tau))$$ (1)

measures the Pancharatnam relative phase between the density operators $\rho(0)$ and $\rho(\tau) = U(\tau)\rho(0)U(\tau)\dagger$, $U(\tau)$ being unitary. Now, under the condition that $U(t)$, $t \in [0, \tau]$, continuously parallel transports the spectral basis of the density operator along some unitary path $C$ ending at $\rho(\tau)$, the Pancharatnam relative phase in Eq. (1) becomes the mixed state geometric phase $\gamma[C]$ associated with this unitary path. Mathematically, $\gamma[C]$ may be regarded the holonomy of a fiber bundle with structure group being the $N$ torus $T^N$.

Many properties of mixed states may be understood in terms of purifications of the considered system’s density operator $\rho$, i.e., by adding an ancilla system so that the whole system is in a pure state whose partial trace over the ancilla is $\rho$. From this perspective, the absence of unique concept of mixed state geometric phase may be considered a consequence of the fact that nonpure states can be purified in many ways. While the above described approach in Ref. [6] arises naturally in standard one-particle interferometry, Ref. [5] has been shown [11] to depend also upon operations on the ancilla.

In this paper, we propose another form of geometric phase that has a direct physical relation to the decomposition freedom of mixed states [12], and which reduces to Ref. [6] for one-term decompositions. We shall see that the associated gauge symmetry for such parallel transport has a fiber bundle interpretation and that it plays a role in a certain type of evolution, for which each component of the decomposition evolves independently in a unitary fashion. This kind of evolution, which we shall call decomposition dependent, is shown to have a natural interpretation in terms of conditional unitary dynamics [13] acting on separable mixed states in the space of the considered system and some additional ancilla.

As a preliminary, we briefly describe, in the next section, decompositions of density operators related to the freedom in the preparation of mixed states. Decomposition dependent parallel transport and mixed state geometric phase are introduced and analyzed in Sec. III. In Sec. IV, we examine particular instances of decomposition dependent evolution related to the unitary case and completely positive maps of the mixed state. The paper ends with the conclusions.

II. DECOMPOSITION FREEDOM

Consider a preparation machine equipped with instructions to prepare a set of orthonormal pure states $\{|k\rangle\}$, each member of which with probability $w_k$. The resulting mixed state may then be represented by the density operator

$$\rho = \sum_{k=1}^{N} w_k |k\rangle\langle k|,$$ (2)
$N$ being the dimension of the considered system’s Hilbert space $\mathcal{H}$. Another, perhaps physically more feasible, preparation machine may instead prepare, with probabilities $\lambda_k$, the states $\rho_k$, yielding the density operator

$$\varrho = \sum_{k=1}^{M} \lambda_k \rho_k,$$

where the states $\rho_1, \ldots, \rho_M$ may be nonpure. If $\varrho = \rho$, then the two machines prepare the same mixed state, but in different ways. The different preparations of the same mixed state are called decompositions, and one can show that all mixed states (nonpure states) can be decomposed in infinitely many ways \[12\]. The decomposition displayed by Eq. $2$ into the eigenbasis of the density operator is called the spectral decomposition.

Given a mixed state represented by $\rho$ one cannot determine its decomposition, since the outcome of any measurement only depends on $\rho$, i.e., measurements are decomposition independent. Yet, we claim there is a subtle difference between the decomposition of a mixed state and the mixed state itself, because identifying the output of a given preparation procedure, with the density operator representing the state does not include any information about the details of the preparation procedure, whereas identifying the output with the corresponding decomposition does.

This latter observation makes it reasonable to introduce the set $S_\rho = \{ \varrho = \rho \}$ of all decompositions $\varrho$ of a density operator $\rho$ as being an equivalence set with projection map $\Pi : S_\rho \to \rho$. In the pure state case, each such equivalence set consist of a single element, as the decomposition is unique for such states. On the other hand, for any nonpure state $\rho$, there are infinitely many elements in $S_\rho$. We may envisage paths $\mathcal{D}$ in the space $S = \{ S_\rho \}$ of all decompositions of all mixed states. In the next section we discuss a concept of geometric phase for such paths, but let us first examine the space $S$ a little bit more thoroughly.

Consider the set $\mathcal{A}$ of separable states of the form

$$q_{sa} = \sum_{k=1}^{M} \lambda_k \rho_k \otimes |\psi_k^a\rangle \langle \psi_k^a|,$$

where $\langle \psi_k^a | \psi_l^a \rangle = \delta_{kl}$, $\delta_{kl}$ These states act on Hilbert space $\mathcal{H} \otimes \mathcal{H}_a$, $\mathcal{H}_a$ being Hilbert space of the considered system and $\mathcal{H}_a$ is some $M$-dimensional ancillary space. Further, let us introduce the equivalence relation

$$q_{sa} \sim (I \otimes U)q_{sa}(I \otimes U^\dagger),$$

$U$ being unitary, and $I$ the identity operator. The set $\mathcal{A}/ \sim$ of equivalent classes in $\mathcal{A}$ under $\sim$ is isomorphic to the set $S_M$ of decompositions into $M$ terms, where $M = \text{dim}(\mathcal{H}_a)$. Apparently $S_M$ is a subset of $S$, and in the following we focus on the space, rather than on $S$. Since $\mathcal{A}/ \sim$ is isomorphic to the set $S_M$ of $M$-term decompositions we may identify a decomposition of the form displayed by Eq. $3$ with a state of the form displayed by Eq. $4$, keeping the equivalence relation in mind.

## III. GEOMETRY OF DECOMPOSITION DEPENDENT EVOLUTIONS

Let $U(t), t \in [0, \tau]$, be a continuous one-parameter family of unitary operators with $U(0) = I$, $I$ being the identity operator on $\mathcal{H}$, and let $\{|k\rangle\}$ be the eigenbasis of the initial density operator $\rho(0)$, assumed to be nondegenerate \[14\]. Then, $U(t)$ is said to parallel transport the density operator if it fulfills the conditions

$$\langle k|U^\dagger(t)U(t)|k \rangle = 0, \forall k.$$

Any parallel transporting operator is denoted by $U||t\rangle$ in the following. For such an operator, we may write the mixed state geometric phase associated with the path $C : t \in [0, \tau] \to \rho(t) = U||t\rangle \rho(0)U||t\rangle^\dagger$ as

$$\gamma[C] = \text{arg} \text{Tr}(\rho(0)U||t\rangle^\dagger),$$

which is the total relative phase displayed by Eq. $4$ for parallel transported states. More generally, Singh et al. \[9\] have put forward a kinematic approach, akin to that of Ref. $15$, to the mixed state geometric phase in Ref. $6$. They demonstrated that for any unitarity $U(t)$ the mixed state geometric phase reads

$$\gamma[C] = \text{arg} \left( \sum_{l=1}^{N} w_l(|U(t)|l) e^{-\int_0^t dt' \langle [U(t)|l)|U(t)|l \rangle} \right).$$

The generalization lies in the fact that the phase is geometric even if $U(t)$ does not fulfill Eq. $4$ and that it includes the parallel transport condition, in the sense that the right-hand side of Eq. $3$ equals the total relative phase whenever Eq. $4$ is fulfilled.

Let us now focus on evolutions of decompositions. Such evolutions may be realized by starting from a state

$$q_{sa}(0) = \sum_{k=1}^{M} \lambda_k \rho_k \otimes |\psi_k^a\rangle \langle \psi_k^a|,$$

where $\langle \psi_k^a | \psi_l^a \rangle = \delta_{kl}$. Letting it evolve under $16$

$$U_{sa}(t) = \sum_{k=1}^{M} U_k(t) \otimes |\psi_k^a\rangle \langle \psi_k^a|,$$

where each $U_k(t), t \in [0, \tau]$, is a continuous one-parameter family of unitaries with $U_k(0) = I$. Since $U_{sa}(t)$ keeps the states $|\psi_k^a\rangle$ fixed, the evolution is well defined in the space $\mathcal{A}/ \sim$. Explicitly,

$$q_{sa}(t) = U_{sa}(t)q_{sa}(0)U_{sa}(t)^\dagger$$

$$= \sum_{k=1}^{M} \lambda_k U_k(t) \rho_k U_k^\dagger(t) \otimes |\psi_k^a\rangle \langle \psi_k^a|,$$

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$$= \sum_{k=1}^{M} \lambda_k U_k(t) \rho_k U_k^\dagger(t) \otimes |\psi_k^a\rangle \langle \psi_k^a|,$$
which defines the decomposition dependent evolution

\[ g(t) = \sum_{k=1}^{M} \lambda_k U_k(t) \rho_k U_k^\dagger(t). \]  

(12)

One can realize this type of decomposition dependent evolution using a type of preparation machine displayed by Fig. 1. Note that for \( M = 1 \), we obtain ordinary unitary evolution of a mixed state, while for \( M > 1 \) the evolution of the considered system is in general nonunitary.

FIG. 1: Realization of decomposition dependent evolution. A machine \( \mathbf{M} \) prepares outputs \( \rho_k \), \( k = 1, \ldots, M \), each of which with probability \( \lambda_k \) and conditionalized on the unitarity \( U_k \).

By using an approach similar to that of Singh et al. \[9\], we can define a geometric phase for this type of evolution. Let us first introduce a gauge transformation of the form

\[ \tilde{\varrho}(t) = \sum_{k=1}^{M} \tilde{U}_k(t) \rho_k \tilde{U}_k^\dagger(t), \]  

(13)

where

\[ \tilde{U}_k(t) = U_k(t) V_k(t), \]  

(14)

\[ V_k(t) \] being unitary and fulfilling \( V_k(0) = I \). This transformation may equivalently be expressed for the state \( \varrho_{sa}(t) \) as

\[ \tilde{\varrho}_{sa}(t) = \tilde{U}_{sa}(t) \varrho_{sa}(0) \tilde{U}_{sa}^\dagger(t), \]  

(15)

where

\[ \tilde{U}_{sa}(t) = U_{sa}(t) V_{sa}(t), \]  

\[ V_{sa}(t) = \sum_{k=1}^{M} V_k(t) \otimes |\psi_k^\rangle \langle \psi_k^|, \]  

(16)

\[ V_k(t) \] being unitary. The orbit of the decomposition remains unchanged under this transformation if \( [\varrho_{sa}(0), V_{sa}(t)] = 0 \), which is fulfilled only if

\[ [\rho_k, V_k(t)] = 0, \forall k. \]  

(17)

Let us now introduce a concept of relative phase \( \Gamma \) adapted to decomposition dependent evolutions. This is naturally given by considering the phase of the quantity \( \text{Tr} (\varrho_{sa}(0) U_{sa}(\tau)) \) yielding

\[ \Gamma = \arg \left( \sum_{k=1}^{M} \lambda_k \text{Tr} (\rho_k U_k(\tau)) \right). \]  

(18)

Note that for \( U_k(\tau) = U(\tau), \forall k \), this reduces to \( \gamma \) in Eq. (10).

With the relative phase at hand we may now introduce the quantity

\[ \Gamma[\mathcal{D}] = \arg \left( \sum_{k=1}^{M} \lambda_k \sum_{l=1}^{N} w_l^k \langle k_l | U_k(\tau) | k_l \rangle e^{-\int_0^\tau dt \langle k_l | U_k^\dagger(t) U_k(t) | k_l \rangle} \right), \]  

(19)

where \( \{ |k_i\rangle \}_{i=1}^N \) is the eigenbasis of \( \rho_k \) and \( \{ w_l^k \} \) are the corresponding eigenvalues. \( \Gamma[\mathcal{D}] \) is gauge invariant since each term in the sum is invariant under the corresponding transformation \( U_k(t) \rightarrow \tilde{U}_k(t) \) in Eq. (14) fulfilling Eq. (17). Moreover, since \( \Gamma[\mathcal{D}] \) is real-valued and reparametrization invariant, we may define it as the geometric phase for decomposition dependent evolutions. Demanding that the geometric phase equals the total phase for parallel transported states provides us the following \( N \times M \) parallel transport conditions

\[ \langle k_l | U_k^\dagger(t) \tilde{U}_k(t) | k_l \rangle = 0, \forall k, l. \]  

(20)

Apparently a given decomposition is parallel transported if each component \( \rho_k \) of the decomposition fulfills the parallel transport conditions given in Ref. \[11\], with respect to the unitary operator \( U_k(t) \) acting on that specific component.

The geometric phase \( \Gamma[\mathcal{D}] \) depends only on the path \( \mathcal{D} \) in the space \( \mathcal{S}_M \) of decompositions. Such a path may be lifted to that of a pure state \( |\Psi(t)\rangle \in \mathcal{H} \otimes \mathcal{H}_a \otimes \mathcal{H}_b \) by attaching yet another ancilla such that the projection map \( \pi : |\Psi(t)\rangle \rightarrow \text{Tr}_b |\Psi(t)\rangle \langle \Psi(t)| \) is \( \mathcal{D} \). This is fulfilled
by
\[ |\Psi(0)\rangle = \sum_{k=1}^{M} \sum_{l=1}^{N} \sqrt{\lambda_k} \sqrt{w_l^k} |k_l\rangle \otimes |\psi^a_k\rangle \otimes |\psi^b_k\rangle, \quad (21) \]
evolving as \( |\Psi(t)\rangle = U_{sa}(t)|\Psi(0)\rangle \), where
\[ U_{sa}(t) = \sum_{k=1}^{M} U_k(t) \otimes |\psi^a_k\rangle \langle \psi^a_k| \otimes I^b. \quad (22) \]

From this point of view, \( \Gamma[D] \) is the holonomy of the fiber bundle \( (S, \mathcal{H} \otimes \mathcal{H}_a \otimes \mathcal{H}_b, \pi, \mathcal{G}) \) with structure group \( \mathcal{G} \) being the \( N \times M \) torus \( T^N \times T^M \).

**IV. RELATION TO EVOLUTIONS OF MIXED STATES**

Consider the map
\[ \mathcal{F} : \varrho_{sa} \longrightarrow \text{Tr}_a \varrho_{sa}, \quad (23) \]
from the space \( \mathcal{A}/\sim \) to the space of mixed states. Using this map, and the fact that the space of decompositions is isomorphic to \( \mathcal{A}/\sim \), one can take a path \( D \) from the space of decompositions into a path \( \mathcal{C} \) in the space of mixed states. In this section we consider special cases of decomposition dependent evolutions producing paths \( D \), which corresponds to continuous sets of mappings \( \mathcal{C} \) in the space of mixed states.

Let us first consider unitary evolutions of mixed states, which corresponds to the special case of decomposition dependent evolutions where \( U_{k}(t) = U(t)V_k(t) \) and \( [V_k(t), \rho_k] = 0 \). In this case, the geometric phase \( \Gamma[D] \) in Eq. (19) becomes
\[ \Gamma[D] = \arg \left( \sum_{k=1}^{M} \lambda_k \sum_{l=1}^{N} w_l^k \langle k_l|U(\tau)|k_l\rangle \right) \times e^{-\int_{0}^{\tau} dt \langle k_l|U^{-1}(t)U(t)|k_l\rangle}, \quad (24) \]
which may in general be different from the geometric phase \( \gamma[C] \) introduced in Ref. 8. Hence, the additional information about the decomposition affects the geometric phase, as one could suspect. However, there exists a special case when the two geometric phases numerically coincide, namely when all terms in the decomposition have the same eigenbasis, i.e., \( \{|k_l\rangle \equiv |l\rangle \} \). Consequently, we obtain
\[ \Gamma[D] = \arg \left( \sum_{k=1}^{M} \lambda_k \sum_{l=1}^{N} w_l^k \langle l|U(\tau)|l\rangle \right) \times e^{-\int_{0}^{\tau} dt \langle l|U^{-1}(t)U(t)|l\rangle}, \quad (25) \]
i.e., \( \Gamma[D] = \gamma[C] \) in Eq. (22) by the identification \( w_l = \sum_k \lambda_k w_l^k \). This may be regarded a consequence of the fact that one can choose \( V_1(t) = \ldots = V_M(t) \equiv V(t) \) in this case, which precisely corresponds to the gauge symmetry \( T^N \) of the mixed state. On the other hand, if at least two of the \( \rho_k \)'s do not diagonalize in the same basis, the gauge group cannot be reduced to \( T^N \) and \( \Gamma[D] \) cannot be associated with the holonomy of the unitarily evolving mixed state.

One can further analyze the relation between decomposition dependent evolution and unitary mixed state evolution by considering the latter as decomposition dependent, where the decomposition contains a single term, i.e., \( \rho = \rho \). This entails that the path \( \mathcal{C} : t \rightarrow U(t)\rho U(t) \) in the space of mixed states corresponds to the path \( \tilde{\mathcal{C}} : t \rightarrow U(t)\rho U^\dagger(t) \otimes |\psi^a_k\rangle \langle \psi^b_k| \) in the space \( \mathcal{A}/\sim \). This seems to be a natural correspondence, and it is apparent that we have \( \Gamma[\tilde{\mathcal{C}}] = \gamma[C] \). However, the path \( \tilde{\mathcal{C}} \) can only be the same as a path \( D \) produced by a one-term decomposition. To see this, let us assume the opposite, i.e., paths \( D : t \rightarrow \sum_{k=1}^{M} \lambda_k U(t)\rho_k U^\dagger(t) \otimes |\psi^a_k\rangle \langle \psi^b_k| \).

Then \( D \) correspond to \( \mathcal{C} \) only if there exists a continuous one-parameter family of unitaries \( V(t) \), such that
\[ \sum_{k=1}^{M} \lambda_k U(t)\rho_k U^\dagger(t) \otimes |\psi^a_k\rangle \langle \psi^b_k| = U(t) \otimes V(t) \otimes |\psi^a_1\rangle \langle \psi^a_1| U^\dagger(t) \otimes V^\dagger(t). \quad (26) \]

Tracing over the system part on both sides gives us
\[ \sum_{k=1}^{M} \lambda_k |\psi^a_k\rangle \langle \psi^a_k| = V(t) |\psi^a_1\rangle \langle \psi^a_1| V^\dagger(t), \quad (27) \]
where the right-hand side is a pure state, whereas the left-hand side is a pure state only if all but one of the \( \lambda_k \)'s vanishes. Hence, the previously discussed numerical agreement between the geometric phase for a class of \( M \)-term decompositions and the mixed state geometric phase, cannot be explained as a correspondence between paths. Rather we have a situation where \( \Gamma[D] = \Gamma[\tilde{\mathcal{C}}] = \gamma[C] \), \( D \) and \( \tilde{\mathcal{C}} \) being distinct paths.

Another special case of decomposition dependent evolutions is
\[ \varrho(t) = \sum_{k=1}^{M} \lambda_k U_k(t)\varrho(0) U_k^\dagger(t), \quad (28) \]
i.e., when \( \rho_1 = \ldots = \rho_M = \varrho(0) \). The corresponding state \( \varrho_{sa}(0) \) takes the product form
\[ \varrho_{sa}(0) = \varrho(0) \otimes \left( \sum_{k=1}^{M} \lambda_k |\psi^a_k\rangle \langle \psi^a_k| \right). \quad (29) \]

Being a product state implies that this evolution corresponds to mixed state evolution governed by a continuous one-parameter family of completely positive (CP) maps
\[ \gamma[C] \]. This can also be seen by reexpressing Eq. (23) as
\[ \varrho(t) = \sum_{k=1}^{M} W_k(t) \varrho(0) W_k^\dagger(t), \quad (30) \]
which, for the mixed state, is the Kraus representation of a CP map, where \( W_k(t) = \sqrt{\Lambda_k} U_k(t) \), and 
\[
\sum_{k=1}^{M} W_k^\dagger(t) W_k(t) = I.
\]
Not all CP maps have a Kraus representation where \( W_k(t) = \sqrt{\Lambda_k} U_k(t) \), \( U_k(t) \) being unitary; only a fraction of all CP maps can be viewed as decomposition dependent evolutions \[18\], but for this class of maps we may define the geometric phase as

\[
\Gamma[\mathcal{D}] = \arg \left( \sum_{k=1}^{M} \lambda_k \sum_{l=1}^{N} w_l (\{ |l\rangle \}) |l\rangle e^{-\int_0^t dt (\{ |l\rangle U_k^\dagger(t) U_k(t) |l\rangle \})} \right),
\]

where \( \{ |l\rangle \} \) is the eigenbasis of \( \varrho(0) \), and \( w_l \) are the corresponding eigenvalues. The concomitant parallel transport conditions reads

\[
\langle |l\rangle U_k^\dagger(t) U_k(t) |l\rangle = 0, \forall k, l.
\]

The geometric phase for CP maps has previously been considered in Ref. \[8\]. In the special case of Kraus operators of the form \( W_k(t) = \sqrt{\Lambda_k} U_k(t), k = 1, \ldots, M \), this approach associates, at each \( t \), a relative phase \( \Gamma_k(t) \) to each \( W_k(t) \) by the expression

\[
v_k e^{i \Gamma_k(t)} = \sqrt{\Lambda_k} \text{Tr} [\varrho(0) U_k(t)].
\]

By introducing parallel transport conditions in Eq. \[32\], the \( M \) geometric phases are given by

\[
\tilde{\Gamma}_g^{(k)} = \arg \left( \sum_{l=1}^{N} w_l (\{ |l\rangle \}) |l\rangle e^{-\int_0^t dt (\{ |l\rangle U_k^\dagger(t) U_k(t) |l\rangle \})} \right).
\]

It follows that \( \Gamma_g \) and \( \tilde{\Gamma}_g^{(k)} \) are related as

\[
\Gamma[\mathcal{D}] = \arg \left( \sum_{k=1}^{M} \lambda_k r_k e^{i \tilde{\Gamma}_g^{(k)}} \right),
\]

where

\[
r_k \equiv \left| \sum_{l=1}^{N} w_l (\{ |l\rangle \}) e^{-\int_0^t dt (\{ |l\rangle U_k^\dagger(t) U_k(t) |l\rangle \})} \right|,
\]

is the mixed state visibility \( \tilde{\rho} \) for the unitary evolution \( \varrho(0) \rightarrow U_k(t) \varrho(0) U_k^\dagger(t) \).

\section{Conclusions}

We have introduced a concept of decomposition dependent evolution of quantal states and discussed the concomitant geometric phase and parallel transport. This geometric phase depends only upon the path in the space of all decompositions and is different, both conceptually and numerically, from the geometric phase of mixed states. It may even differ from the standard geometric phase for mixed states \[8\] in the case of unitary evolution of the decomposition. We have further demonstrated that the concept of geometric phase for decompositions and that of the corresponding mixed state in the unitary case, become identical if each component of the decomposition diagonalize in the same basis. We have also shown that the present approach leads to a notion of geometric phase for a special class of completely positive maps that essentially differs from previous suggestions \[8\] \[19\].

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