Off-diagonal quantum holonomy along density operators

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Abstract

Uhlmann’s concept of quantum holonomy for paths of density operators is generalised to the off-diagonal case providing insight into the geometry of state space when the Uhlmann holonomy is undefined. Comparison with previous off-diagonal geometric phase definitions is carried out and an example comprising the transport of a Bell-state mixture is given.

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1 Introduction

Investigations in the polarisation of light have led Pancharatnam [1] in the mid-fifties to a notion of relative phase. Some thirty years later Berry [2] shed new light on the relative phase between two states by introducing a decomposition into a dynamical and a geometric part in the special case of adiabatically guided Hamiltonians. The geometric phase depends wholly on the shape of the curve in the subjacent parameter space representing the evolution of the system. These new findings encouraged further investigations leading towards more general notions, in particular the spectrum of Berry’s discovery has soon

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been enlarged to include nonadiabatic [3], noncyclic, and nonunitary [4] evolutions. Furthermore, a kinematic derivation has been given by Mukunda and Simon [5], and Pati defined the geometric phase via a reference section [6,7]. Since the special case of pure states in quantum mechanics is not sufficient for dealing with realistic problems, it is a legitimate question whether one can ascribe a geometric phase to mixed states. Uhlmann [8,9,10] proposed a phase holonomy for paths of density operators utilizing a purification scheme of mixed into pure states obtained via a certain parallelity condition. Based on Uhlmann’s definition there has been further investigations in the parallel transport of density matrices in mixed state space relating also to differential geometric techniques [11,12,13,14]. The experimental testability of the Uhlmann holonomy has been addressed recently in [15]. Another approach taken by Chaturvedi et al. [16] uses methods from differential geometry to obtain a mixed state geometric phase. In addition, Sjöqvist et al. [17] generalised the geometric phase to mixed states starting from an interferometry setup. This latter phase concept has recently been tested experimentally in nuclear magnetic resonance [18] and single photon interferometry [19]. The two approaches in Refs. [8,17] have been found out to be incompatible for arbitrary nondegenerate mixed states [20,21] fully coinciding only in the pure state limit.

From Pancharatnam’s relative phase concept it is easily deducible that one runs into problems while trying to calculate the relative phase between orthogonal states. This defect has been cured by Manini and Pistolesi [22] (see also [23] for a general framework in terms of Bargmann invariants) for pure states and by the current authors for mixed states [24] (see also Refs. [25,26]) by introducing off-diagonal geometric phases that may be well-defined when the phases discussed in Refs. [1,4,17] are not. In this paper, we follow this line of reasoning first in spotting nodal points of the Uhlmann quantum holonomy, i.e., configurations where the relative phase factor between the initial and final density operator turns out to be undefined, and second in proposing generalised holonomy quantities that may be well-defined in such situations. Furthermore we give examples to show the relevance of this extension.

2 Quantum holonomy and its nodal points

Let \( \mathcal{C} : t \in [0, \tau] \mapsto \rho(t) \) be a path of density operators. A lift of \( \mathcal{C} \) is a path \( \tilde{\mathcal{C}} : t \in [0, \tau] \mapsto W(t) \) such that \( \rho(t) = W(t)W^\dagger(t) \) with the amplitude \( W(t) = \rho^{1/2}(t)V(t) \), the one-parameter family of partial isometries \( V(t) \) being the phase factors of \( W(t) \) along the path \( \tilde{\mathcal{C}} \). If for any pair of amplitudes along the path the following condition is fulfilled

\[
W^\dagger(t)W(t') > 0,
\]
then \( W(t) \) and \( W(t') \) are said to be parallel. For infinitesimally close \( t \) and \( t' \) the parallelity condition reads

\[
W^\dagger(t) dW(t) = dW^\dagger(t) W(t) > 0, \tag{2}
\]

which, if valid for all \( t \in [0, \tau] \), defines a parallel lift of the path \( C \).

For an initial amplitude \( W(0) = \rho^{1/2}(0) \) with the phase factor \( V(0) \) chosen to be the identity operator on the support of \( \rho(0) \), the final amplitude \( W(\tau) \) is given by \( W(\tau) = \rho^{1/2}(\tau) \tilde{V}(\tau) \), if \( W(t) \) fulfils the parallel transport condition in Eq. (2). A gauge invariant quantity of the path \( C \) is given by the operator \( W(\tau)W^\dagger(0) \) [9] that can be written in terms of the initial and final state as

\[
W(\tau)W^\dagger(0) = \rho^{1/2}(\tau) \tilde{V}(\tau) \rho^{1/2}(0), \tag{3}
\]

which is only dependent on the path of states. That \( W(\tau)W^\dagger(0) \) and the relative phase factor \( \tilde{V}(\tau) \) restricted by the support of the initial density operator are indeed gauge invariant can be seen from the fact that a local gauge transformation \( W(t) \mapsto W'(t) = W(t)S(t) \) by a partial isometry \( S(t) \) has already been fixed by imposing the parallel transport condition on the path \( \tilde{C} \) [9]. Moreover, the remaining gauge freedom by a \( t \)-independent partial isometry \( S \) along the path, i.e., \( W(t) \mapsto W'(t) = W(t)S \) leaves Eq. (3) invariant. Note that the Uhlmann quantum holonomy invariant \( W(\tau)W^\dagger(0) \) is well-defined if the path \( C \) is sufficiently regular, in particular, the support of the density operators involved should change smoothly [9].

By introducing the functional

\[
\nu_C(A) \equiv \arg \text{Tr}[AW(\tau)W^\dagger(0)] \tag{4}
\]

on the observables \( A \in \mathcal{B}(\mathcal{H}) \), where \( \mathcal{B}(\mathcal{H}) \) denotes the algebra of linear operators acting on the Hilbert space \( \mathcal{H} \) under consideration, we obtain the well-known Berry phase [2,3,4] for pure states as follows.

Consider the initial state \( |0\rangle \in \mathcal{H} \) and its standard purification \( W(0) = |0\rangle\langle a| \in \mathcal{H} \otimes \mathcal{H}^* \), where \( \langle a| \) can be any element of the dual Hilbert space \( \mathcal{H}^* \) and the unitary evolution operator \( U(t) \in \mathcal{B}(\mathcal{H}) \). Then the amplitude at time \( t \) is given by \( W(t) = U(t)|0\rangle\langle a| \). The Uhlmann holonomy invariant \( W(\tau)W^\dagger(0) \) is then \( U(\tau)|0\rangle\langle 0| \) and by setting \( A = 1 \) in Eq. (4) we obtain the usual geometric phase \( \nu_C(1) = \arg\langle 0|U(\tau)|0\rangle \) for \( U(t) \) fulfilling the parallel transport condition \( \langle 0|U^\dagger(t)U(t)|0\rangle = 0 \).

In the pure state limit above, \( \nu_C(1) \) has nodal points (i.e., is undefined) for orthogonal initial and final states. In general, let \( \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \ldots \oplus \mathcal{H}_n \) be an orthogonal sum decomposition of the Hilbert space \( \mathcal{H} \) of the system, where \( n \leq \dim \mathcal{H} \) with equality for the case discussed by Manini and Pistolesi [22]. Then, if the initial state \( \rho(0) \) with support in \( \mathcal{H}_k \) (\( \rho(0) \in \mathcal{B}(\mathcal{H}_k) \)) evolves to the state...
\( \rho(\tau) \) with support in \( \mathcal{H}_l \) \((l \neq k)\), \( \nu_C(1) \) is undefined since the trace vanishes as is apparent from Eq. (3). If this happens \( \rho(0) \) and \( \rho(\tau) \) are said to be orthogonal. Analogous to the mixed state generalization [24] of the off-diagonal geometric phase defined in [22] based on the interferometric approach to mixed state geometric phases taken in [17] an off-diagonal quantum holonomy based on Uhlmann’s idea [8] of a relative phase factor accompanying the parallel transport of mixed states can be constructed to cover such situations.

3 Off-diagonal generalisation of quantum holonomies

The criteria imposed on such a generalising quantity are: (a) the reducibility to the off-diagonal pure state geometric phase, (b) the inclusion of Uhlmann’s relative phase as a special instance, in the same manner as the geometric phase for mixed states in [17] is included in its generalisation [24], (c) the invariance under a gauge transformation \( \rho_k \mapsto \rho'_k = S_k \rho_k S_k^\dagger \) of the initial mixed states \( \rho_k \) by partial isometries \( S_k \) on the support of \( \rho_k \), and (d) it should potentially be well-defined for orthogonal initial and final states.

The latter is evidently the main motivation in constructing an off-diagonal quantum holonomy for mixed states in order to obtain geometric information whenever the Uhlmann holonomy shows nodal points. To this end we assume a set of initial density operators \( \rho_k(0) \), \( k = 1, \ldots, n \), each of which with support in the corresponding Hilbert space \( \mathcal{H}_k \). For a given evolution one obtains the final set of density operators \( \rho_k(\tau) \), \( k = 1, \ldots, n \), and one can associate a path \( C_k \) to each \( \rho_k \) giving rise to the holonomies \( \mathcal{V}_k(C_k) \). Instead of regarding the latter separately one can consider gauge invariant quantities depending on some or all of the paths revealing insight into the geometric properties of state space in case of one or more vanishing \( \mathcal{V}_k(C_k) \)’s.

As in Uhlmanns original construction the basic elements are the purifications \( W_k(0) \) and \( W_k(\tau) \) of the initial and the final states represented by \( \rho_k(0) \) and \( \rho_k(\tau) \) and their Hermitian conjugates to guarantee the reduction to Uhlmann’s definition. The only issue left is the correct order to ensure the validity of criteria (a)-(d) from above. As we will see there is essentially just one possibility.

First of all, we note that there are two alternatives stated in the literature for Uhlmann’s holonomies, either \( W(\tau)W^\dagger(0) \) [9,10] or \( W(0)W^\dagger(\tau) \) [8], both being invariants depending only on the path \( C : t \in [0,\tau] \mapsto \rho(t) \). We adopt the former since it reduces to Pancharatnam’s phase factor for pure states while the latter entails a phase with opposite sign. As for the ordering ensuring the reducibility to the pure state case the amplitudes of the initial and final states have to appear next to each other, i.e., the off-diagonal quantum holonomy is of the form \( W_1(\tau)W_1^\dagger(0)W_2(\tau)W_2^\dagger(0)\ldots W_k(\tau)W_k^\dagger(0) \).
We are now ready to define the off-diagonal quantum holonomy invariants as

\[
\mathcal{X}_{j_1 \ldots j_l}^{(l)}[C_{j_1} \ldots C_{j_l}] \\
= W_{j_1}(\tau)W_{j_1}^+(0)W_{j_2}(\tau)W_{j_2}^+(0) \ldots W_{j_l}(\tau)W_{j_l}^+(0) \\
= \mathcal{X}_{j_1}^{(1)}[C_{j_1}]\mathcal{X}_{j_2}^{(1)}[C_{j_2}] \ldots \mathcal{X}_{j_l}^{(1)}[C_{j_l}],
\]

where \( l = 1, \ldots, n \). Evidently, \( \mathcal{X}_{j_k}^{(1)}[C_{j_k}] \), \( k = 1, \ldots, n \), is the Uhlmann holonomy invariant for the path \( C_{j_k} : t \in [0, \tau] \rightarrow \rho_{j_k}(t) \) and each \( \mathcal{X}_{j_k}[C_{j_k}] \) comprises a relative phase factor \( \tilde{V}_{j_k} \) depending only on the path \( C_{j_k} \). Clearly, this definition comprises Uhlmann’s holonomy invariant for \( l = 1 \) fulfilling therefore criterion (b).

\( \mathcal{X} \equiv \mathcal{X}_{j_1 \ldots j_l}[C_{j_1} \ldots C_{j_l}] \) can be decomposed either as \( \mathcal{X} = (\mathcal{X}\mathcal{X}^\dagger)^{1/2}\mathcal{U}_r \) (right polar decomposition) or as \( \mathcal{X} = \mathcal{U}_l(\mathcal{X}^\dagger\mathcal{X})^{1/2} \) (left polar decomposition), where \( \mathcal{U}_r \) and \( \mathcal{U}_l \) are partial isometries on the right or left support of \( \mathcal{X} \) (denoted by r-sup \( \mathcal{X} \) or l-sup \( \mathcal{X} \), respectively). The polar decomposition theorem [27, p. 197] states that \( \mathcal{U}_l \) is unique under the condition that \( \text{Ker}\mathcal{U}_l = \text{Ker}\mathcal{X} \). Furthermore, l-sup \( \mathcal{U}_l = \text{l-sup} \mathcal{X} \). For \( \mathcal{U}_l \), the uniqueness condition is l-sup \( \mathcal{U}_r = \text{l-sup} \mathcal{X} \) and by using these restrictions of the supports of \( \mathcal{U}_{l,r} \), we can show the equality \( \mathcal{U}_l = \mathcal{U}_r \). Inserting the projection operator \( \mathcal{U}_r\mathcal{U}_l^\dagger \) onto the left support of \( \mathcal{U}_r \) (which is equal to the left support of \( \mathcal{X} \)) into the right polar decomposition of \( \mathcal{X} \) we obtain

\[
\mathcal{X} = (\mathcal{X}\mathcal{X}^\dagger)^{1/2}\mathcal{U}_r = \mathcal{U}_r\mathcal{U}_r^\dagger(\mathcal{X}\mathcal{X}^\dagger)^{1/2}\mathcal{U}_r = \mathcal{U}_l(\mathcal{X}^\dagger\mathcal{X})^{1/2}
\]

The last equality follows from the uniqueness of the polar decomposition and therefore we have

\[
\mathcal{U}_l = \mathcal{U}_r = \mathcal{U}.
\]

(7)

The holonomy \( \mathcal{U} \) is the Uhlmann analogue to the off-diagonal geometric phase factors defined in [22] for pure states and in [24] for mixed states.

We shall now consider the nodal points of \( \mathcal{X} \). To this end we note that the nodal points of \( \mathcal{X}_{1}^{(1)}[C_1] \) has been located for vanishing \( \nu_C(1) \) in Section 2. Therefore, we introduce the generalised functional

\[
\nu_{C_{j_1} \ldots C_{j_l}}^{(l)}(A) \equiv \arg \text{Tr}[AW_{j_1}(\tau)W_{j_1}^+(0)W_{j_2}(\tau)W_{j_2}^+(0) \ldots W_{j_l}(\tau)W_{j_l}^+(0)] \\
= \arg \text{Tr}[AA^\dagger].
\]

(8)

Trivially, \( \nu_{C_{j_1} \ldots C_{j_l}}^{(l)}(1) \) is undefined for \( \mathcal{X} = 0 \). For \( \mathcal{X} \neq 0 \) a sufficient condition for a nodal point of \( \nu_{C_{j_1} \ldots C_{j_l}}^{(l)}(1) \) is orthogonal supports of the positive Hermitian parts of the left and right polar decomposition of \( \mathcal{X} \). This can be seen by
noting at first that the left and right support of the operator $\mathcal{X}$ is given by the support of $\mathcal{X}\mathcal{X}^\dagger$ and $\mathcal{X}^\dagger\mathcal{X}$, respectively, and in addition that the trace of $\mathcal{X}$ vanishes for nonoverlapping left and right support. Since $\mathcal{X}\mathcal{X}^\dagger$ and $\mathcal{X}^\dagger\mathcal{X}$ appear in the positive Hermitian parts of the polar decomposition the nodal points of $\tau_{C_{j_1}...C_{j_l}}(1)$ are necessary for orthogonal left and right supports of $\mathcal{X}$.

Let us have a detailed look at the right and left support of $\mathcal{X}$. The left support is given by

$$\mathcal{X}\mathcal{X}^\dagger = \rho_{j_1}^{1/2}(\tau)\tilde{V}_{j_1}(\tau)\rho_{j_1}^{1/2}(0) \times \rho_{j_2}^{1/2}(\tau)\tilde{V}_{j_2}(\tau)...\rho_{j_l}^{1/2}(\tau)\tilde{V}_{j_l}(\tau) \times \rho_{j_l}(0)\tilde{V}_{j_l}^\dagger(\tau)...\rho_{j_1}^{1/2}(0)\tilde{V}_{j_1}^\dagger(\tau)\rho_{j_1}^{1/2}(\tau)$$

and the right support

$$\mathcal{X}^\dagger\mathcal{X} = \rho_{j_1}^{1/2}(0)\tilde{V}_{j_1}^\dagger(\tau)\rho_{j_1}^{1/2}(\tau)...\rho_{j_l}^{1/2}(0) \times \tilde{V}_{j_1}^\dagger(\tau)\rho_{j_1}(\tau)\tilde{V}_{j_1}(\tau)\rho_{j_1}^{1/2}(0) \times \rho_{j_2}^{1/2}(\tau)\tilde{V}_{j_2}(\tau)...\rho_{j_l}^{1/2}(\tau)\tilde{V}_{j_l}(\tau)\rho_{j_l}^{1/2}(0).$$

These are apparently only orthogonal in the case where $\rho_{j_1}(\tau)$ and $\rho_{j_1}(0)$ have orthogonal support and this in turn can be avoided by a proper choice of initial states. These choices of the $\rho_{j_k}(0)$, $k = 1,...,l$ are evidently not unique, one can take any state $\rho_{j_l} \in \mathcal{B}(\mathcal{H}_{j_l})$ for a given $\rho_{j_1}$ with the minimal requirement that the $\rho_{j_k}(\tau)$ have overlapping supports at least with $\rho_{j_{k-1}}(0)$ where the indices $k$ have to be considered modulo $n$. This is equivalent to nonvanishing transition probability from $\rho_{j_k}(\tau)$ to $\rho_{j_{k-1}}(0)$ [28].

To assure that the off-diagonal quantum holonomy invariants $\mathcal{X}_{j_1...j_l}[C_{j_1}...C_{j_l}]$ fulfil all necessary criteria, we note that the $\mathcal{X}_{j_1...j_l}[C_{j_1}...C_{j_l}]$’s are only dependent on the paths $C_{j_k}$ by the same reasoning as for the $l = 1$ case. In fact, the final amplitude $W_{j_k}(t)$ of each initial state $\rho_{j_k}(0)$ is determined by the parallel transport condition in Eq. (2) up to a $t$-independent partial isometry $S$. This latter global gauge leaves $\mathcal{X}_{j_1...j_l}[C_{j_1}...C_{j_l}]$ invariant even for distinct choices $S = S_{j_k}$ for the different constituent initial states showing the validity of criterion (c). There is no need then to state a prescription for the relations between the $\rho_{j_k}$’s [29] and the reference states can be chosen arbitrarily taking into account that their supports belong to the correct subspaces.

We now rewrite the parallel transport mechanism in the particular case of mixed states undergoing unitary evolution. The standard purification of a mixed state $\rho(0) = \sum \lambda_j |\psi_j\rangle\langle\psi_j|$ with $\sum_j \lambda_j = 1$ and $|\psi_j\rangle$ being a basis diagonalising $\rho(0)$ is $W(0) = \sum_j \sqrt{\lambda_j} |\psi_j\rangle \langle\phi_j|$, i.e., $\mathcal{H}$ is extended by an ancilla.
Hilbert space $\mathcal{H}' = \mathcal{H}^*$, where the $\langle \phi_j | \in \mathcal{H}^*$ form a basis in the ancilla part.

Subjected to the unitary evolution $\rho(0) \rightarrow \rho(t) = U(t)\rho(0)U^\dagger(t)$, $t \in [0, \tau]$, the path of the purifications $t \mapsto W(t)$ has to fulfil the parallelity condition (2).

This latter path can be described by applying a partial isometry $B(t) \in \mathcal{B}(\mathcal{H}')$ resulting in

$$W(t) = U(t)\rho^{1/2}(0)B(t),$$

where $B(t) = U^\dagger(t)V(t)$ and $U(t)$ are related via the parallel transport condition Eq. (2). Inserting (11) into (2) we obtain

$$2\rho^{1/2}(0)U^\dagger(t)\dot{U}(t)\rho^{1/2}(0) = B(t)\dot{B}^\dagger(t)\rho(0) - \rho(0)\dot{B}(t)B^\dagger(t),$$

where the dot denotes the derivative with respect to the parameter $t$. If $\rho(0)$ is pure, $\rho(0) = |\psi_j\rangle\langle \phi_j |$, Eq. (12) simplifies to

$$\langle \psi_j | U^\dagger(t)\dot{U}(t)|\psi_j \rangle = \langle \phi_j | B^\dagger(t)\dot{B}(t)|\phi_j \rangle.$$  

(13)

To verify that Eq. (5) is consistent with known results we consider the pure unitary case [22]. Having a set of initial pure states $|\psi_k\rangle$, $k = 1, \ldots, n$, the defining quantity from Eq. (5) can be written as

$$W_{j_1}(\tau)W^\dagger_{j_1}(0)W_{j_2}(\tau)W^\dagger_{j_2}(0)\ldots W_{j_l}(\tau)W^\dagger_{j_l}(0)$$

$$= U(\tau)|\psi_{j_1}\rangle\langle \phi_{j_1}|B(\tau)|\phi_{j_1}\rangle|\psi_{j_2}\rangle\langle \phi_{j_2}|B(\tau)|\phi_{j_2}\rangle|\psi_{j_3}\rangle\ldots|\psi_{j_{m-1}}\rangle\langle \phi_{j_{m-1}}|B(\tau)|\phi_{j_{m-1}}\rangle|\psi_{j_l}\rangle|\phi_{j_l}\rangle,$$

(14)

where we have used the purifed states $|\psi_k\rangle\langle \phi_k |$. If $U(t)$ is already parallel transporting the basis states, i.e., $\langle \psi_j | U^\dagger(t)U(t)|\psi_j \rangle = 0$, $B(t)$ may be chosen to be the identity and Eq. (14) simplifies to

$$W_{j_1}(\tau)W^\dagger_{j_1}(0)W_{j_2}(\tau)W^\dagger_{j_2}(0)\ldots W_{j_l}(\tau)W^\dagger_{j_l}(0)$$

$$= U(\tau)|\psi_{j_1}\rangle\langle \phi_{j_1}|U(\tau)|\psi_{j_2}\rangle|\phi_{j_2}\rangle\ldots|\psi_{j_{m-1}}\rangle\langle \phi_{j_{m-1}}|U(\tau)|\phi_{j_{m-1}}\rangle|\psi_{j_l}\rangle|\phi_{j_l}\rangle.$$  

(15)

It is straightforward to write down the off-diagonal phase factors corresponding to this quantity using $\nu^{(l)}_{C_{j_1}\ldots C_{j_l}}(1)$ to see the equivalence to those put forward by Manini and Pistolesi [22] in accordance with criterion (a).

What is even more noteworthy is the naturally arising generalisation of the latter to nonparallel transporting unitaries $U(t)$. A proper choice of $B(t)$ according to Eq. (13) yields a parallel lift and therefore a well-defined invariant of the paths $C_i$ of the $W_i$’s.

We end this section by noting that the quantity $\nu^{(l)}_{C_{j_1}\ldots C_{j_l}}(1)$ suggests the alternative ordering $\mathcal{Y} \equiv W^\dagger_{j_1}(0)W_{j_2}(\tau)W^\dagger_{j_2}(0)\ldots W^\dagger_{j_l}(0)W_{j_1}(\tau)$ by shifting $W_{j_1}(\tau)$ to the end, since the trace operation is invariant under cyclic permutations of the constituent operators. As for the gauge invariance of this alternative ordering, we observe that the global gauge transformation $W_{j_k}(t) \mapsto W^\prime_{j_k}(t) = W_{j_k}(t)S_{j_k}$
by a $t$ independent partial isometry $S_{jk}$ yields $\mathcal{Y} \mapsto S_{jk}^\dagger \mathcal{Y} S_{jk}$, i.e., $\mathcal{Y}$ is dependent on the choice of the initial amplitude. This neither changes the nodal point structure of $\mathcal{Y}$ nor does it appear when considering $\nu^{(l)}_{c_{j1} \cdots c_{jl}} (1)$. Thus, both definitions $\mathcal{X}$ and $\mathcal{Y}$ are suitable choices for a proper extension of Uhlmann’s relative phase, though we opt for the former of Eq. (5) in the course of this work since there is no need then to refer explicitly to the functional $\nu^{(l)}_{c_{j1} \cdots c_{jl}} (A)$ to obtain a gauge invariant also with respect to a global gauge.

4 Comparison to off-diagonal geometric phase for mixed states

Motivated by the mixed state geometric phase in [17], the present authors have recently introduced a concept of off-diagonal geometric phase factors for unitarily evolving mixed states [24]:

$$\gamma^{(l)}_{\rho_{j1} \rho_{j2} \cdots \rho_{jl}} \equiv \Phi \left[ \text{Tr} \left( U(\tau) \sqrt{\rho_{j1}} U(\tau) \sqrt{\rho_{j2}} \cdots U(\tau) \sqrt{\rho_{jl}} \right) \right]$$

with $\Phi[z] \equiv z/|z|$ for any complex number $z$, the $\rho_{jl}$’s only differing by permutations of their eigenstates, and $U(t)$, $t \in [0, \tau]$, fulfilling parallel transport for each common eigenstate of the $\rho_{jl}$’s. For $l = 1$ this reduces to the geometric mixed state phase in [17] that has in general been shown to be distinct from the trace of the $l = 1$ holonomy factor [21]. The question is therefore how the off-diagonal geometric phase definition in [24] relates to the off-diagonal generalisation of the Uhlmann phase factor introduced in the present treatise. Using the same scheme as above to compensate dynamical effects in the system by an appropriate choice of unitary operator $B(t) \in \mathcal{B}(\mathcal{H}')$, we get

$$W_{j1}(0) W_{j2}(\tau) W_{j2}^\dagger(0) \cdots W_{jl}(\tau) W_{jl}^\dagger(0) W_{j1}(\tau)$$

$$= \rho_{j1}^{1/2}(0) U(\tau) \rho_{j2}^{1/2}(0) B(\tau) \rho_{j2}^{1/2}(0) \cdots U(\tau) \rho_{jl}^{1/2}(0) B(\tau)$$

$$\times B(\tau) \rho_{jl}^{1/2}(0) U(\tau) \rho_{j1}^{1/2}(0) B(\tau),$$

(17)

where the $\rho_{jl}$’s are those of Eq. (16).

In a first guess one could think to obtain a similar form like $\gamma^{(l)}_{\rho_{j1} \rho_{j2} \cdots \rho_{jl}}$ with a unitarity $U(t)$ parallel transporting all eigenstates of the $\rho_{jl}$’s, so that the $B(t)$ can be chosen to be time-independent. But this procedure fails since the parallel transport condition behind the $\gamma^{(l)}_{\rho_{j1} \rho_{j2} \cdots \rho_{jl}}$’s is much weaker than the parallel transport condition in Eq. (12). In the former parallel transport is required for the state vectors $|\psi_k\rangle$ diagonalising the initial $\rho = \sum_k \lambda_k |\psi_k\rangle \langle \psi_k|$, i.e., $\langle \psi_k | U^\dagger(t) \dot{U}(t) | \psi_k \rangle = 0$, whereas in the latter case putting $B(t)$ constant amounts to vanishing matrix elements of $U^\dagger(t) \dot{U}(t)$ in the support of $\rho(0)$. For $\rho_{jl}$’s having only nonzero eigenvalues this means that the left-hand side...
of Eq. (12) can only vanish for unitarities $U(t)$ that leave all the $\rho_{jk}$’s appearing in $\mathcal{A}^{(l)}_{[C_{j_1} \ldots C_{j_l}]}$ unaffected or, in other words that the parallel transport condition is trivially fulfilled for no evolution at all. For a density operator $\rho$ with zero eigenvalues, however, the left-hand side of Eq. (12) vanishes, if $U(t)^\dagger \tilde{U}(t)$ maps the right support of all $\rho_{jk}$’s to their kernels, i.e. $U(t)^\dagger \tilde{U}(t) : r$-supp $\rho_{jk} \mapsto \text{Ker} \rho_{jk}$. In this case $B(t)$ can be set constant also for nonstationary density operators, as we will see in an example below. Furthermore, the two approaches are on equal footing in the limit of pure states.

5 Spin Flip Operation on a Mixture of Bell States

One explicit example of an evolution that leads to orthogonal initial and final mixed states is a spin plus phase flip operation applied to a mixture of Bell states. For the initial state

$$\rho_1(0) = \frac{1}{1 + \varepsilon} \left( |\Psi^- \rangle \langle \Psi^- | + \varepsilon |\Psi^+ \rangle \langle \Psi^+ | \right), \quad \varepsilon \geq 0, \quad (18)$$

we obtain by spin- and phase-flipping the first qubit, i.e., $U_{sf} : (|0\rangle, |1\rangle) \mapsto (|1\rangle, -|0\rangle)$ or $U_{sf} = |\Phi^+ \rangle \langle \Phi^- | + |\Phi^- \rangle \langle \Phi^+ | - |\Psi^- \rangle \langle \Phi^+ | - |\Phi^- \rangle \langle \Psi^+ |$, the final state

$$\rho_1(\tau) = \frac{1}{1 + \varepsilon} \left( |\Phi^+ \rangle \langle \Phi^+ | + \varepsilon |\Phi^- \rangle \langle \Phi^- | \right), \quad (19)$$

where we have denoted the Bell states by $|\Psi^\pm \rangle = 2^{-1/2}(|01\rangle \pm |10\rangle)$ and $|\Phi^\pm \rangle = 2^{-1/2}(|00\rangle \pm |11\rangle)$. A simple implementation of such an operation is given by the time-independent Hamiltonian $H_s = \sigma_y \otimes I_2$ so that the path $\mathcal{C}_1 : t \in [0, \tau] \mapsto \rho_1(t) = U_s(t) \rho_1(0) U_s^\dagger(t)$ with $U_s(t) = e^{-itH_s}$ is traced out in state space. Inserting $U_s(t)$ into Eq. (12) yields a vanishing left-hand side, so that we can choose $B_{s_1}(t) = 1_1 \otimes 1_2$ to fulfil the parallel transport condition. For $t = \tau = \pi/2$ we obtain the amplitude $W_1(\tau) = U_s(\tau) \rho_1^{1/2}(0) = U_{sf} \rho_1^{1/2}(0)$ and the $l = 1$ holonomy invariant reads

$$\mathcal{A}_1^{(l)}[\mathcal{C}_1] = W_1(\tau) W_1^\dagger(0) = U_{sf} \rho_1(0)$$

$$= \frac{1}{1 + \varepsilon} \left( |\Phi^+ \rangle \langle \Psi^- | - \varepsilon |\Phi^- \rangle \langle \Psi^+ | \right), \quad (20)$$

which has nonoverlapping right and left support and is therefore undefined. In particular, the trace functional $\nu_C(1_1 \otimes 1_2) = \arg \text{Tr}[U_{sf} \rho_1(0)]$, which in this special case is the same expression as in [17,24,25], vanishes.

The $l = 2$ off-diagonal holonomy invariant can be formed by choosing the reference state $\rho_2(0) = \rho_1(\tau)$, which evolves to $\rho_2(\tau) = \rho_1(0)$ along the path $\mathcal{C}_2 : t \mapsto \rho_2(t) = U_s(t) \rho_2(0) U_s^\dagger(t)$. Again, we can set $B_{s_2}(t) = 1_1 \otimes 1_2$ and
obtain $\chi^{(1)}_2[\mathcal{C}_2] = W_2(\tau)W_2^\dagger(0) = U_{sf}\rho_2(0)$, which also has nonoverlapping left and right support. These considerations result in

$$
\chi^{(2)}_{12}[\mathcal{C}_1\mathcal{C}_2] = W_1(\tau)W_1^\dagger(0)W_2(\tau)W_2^\dagger(0) = U_{sf}\rho_1(0)U_{sf}\rho_2(0)
$$

$$
= -\frac{1}{(1 + \epsilon)^2} \left[ |\Phi^+\rangle\langle\Phi^+| + |\Phi^-\rangle\langle\Phi^-| \right],
$$

(21)

the left and right support of which are overlapping and $\chi^{(2)}_{12}$ is therefore well-defined at this particular nodal point of $\chi^{(1)}_i[\mathcal{C}_i]$.

The Hamiltonian $H_s$ above is not a unique choice for a spin-flip implementation, this task can also be performed, e.g., by the time-dependent Hamiltonian $H_r(t) = [u_x\sigma_x + u_{xy}(\sigma_x \cos \omega t + \sigma_y \sin \omega t)] \otimes I_2$ similar to the Hamiltonian for a resonance spin-flipper (on the first particle) prevalent in NMR. The unitary time evolution operator corresponding to $H_r(t)$ can be written as $U_r(t) = U_{\text{tot}}U_{\text{eff}} = e^{-i\omega t\sigma_z/2}e^{-itH_{\text{eff}}} \otimes I_2$ with $H_{\text{eff}} = (u_z + \omega/2)\sigma_z + u_{xy}\sigma_x$. By the particular choice of the parameters $u_z = -u/2$ and $\omega = -2u_{xy} = -2u_z$, one can verify that for $t = \frac{\pi}{\omega} \equiv \tau$ we have the implemented the same spin-flipping unitary as in the static case, i.e., $U_r(\pi/\omega) = U_s(\pi/2) = U_{sf}$. Inserting $U_r$ on the left-hand side of Eq. (12) we obtain

$$
B_{r1}(t) = \cos \gamma(t) \left[ |\Psi^+\rangle\langle\Psi^+| + |\Psi^-\rangle\langle\Psi^-| \right]
$$

$$
- i \sin \gamma(t) \left[ |\Psi^+\rangle\langle\Psi^-| + |\Psi^-\rangle\langle\Psi^+| \right],
$$

$$
\gamma(t) = \frac{\sqrt{\epsilon}\omega t}{1 + \epsilon}.
$$

(22)

This gives us the $l = 1$ holonomy invariant for the path $\bar{C}_1 : t \in [0, \tau] \mapsto \rho_1(t) = U_r(t)\rho_1(0)U_r^\dagger(t)$ as

$$
\chi^{(1)}_1[\bar{C}_1] = W_1(\tau)W_1^\dagger(0) = U_{sf}\rho_1^{1/2}(0)B_{r1}(\tau)\rho_1^{1/2}(0)
$$

$$
= \frac{1}{1 + \epsilon} \left[ \cos \gamma(\tau) \left( |\Phi^+\rangle\langle\Phi^-| - \epsilon |\Phi^-\rangle\langle\Phi^+| \right)
$$

$$
+ i\sqrt{\epsilon}\sin \gamma(\tau) \left( -|\Phi^+\rangle\langle\Phi^+| + |\Phi^-\rangle\langle\Phi^-| \right) \right],
$$

(23)

which has nonoverlapping left and right supports and is therefore undefined. Similarly, by again taking $\rho_2(0) = \rho_1(\tau)$ from Eq. (19), the $l = 1$ holonomy invariant associated with the path $\bar{C}_2 : t \in [0, \tau] \mapsto \rho_2(t) = U_r(t)\rho_2(0)U_r^\dagger(t)$ becomes
with nonoverlapping left and right support.

We may use Eqs. (23) and (24) to obtain the $l = 2$ holonomy invariant

\[
\mathcal{X}^{(2)}_{12}[\tilde{C}_1 \tilde{C}_2] = W_1(\tau)W_1^\dagger(0)W_2(\tau)W_2^\dagger(0) = \frac{1}{1 + \epsilon} \left[ \cos \gamma(\tau) \left( \epsilon \langle \Psi^+ \rangle \langle \Phi^- \rangle - \langle \Psi^- \rangle \langle \Phi^+ \rangle \right) 
\right.
\]

\[
\left. + i \sqrt{\epsilon} \sin \gamma(\tau) \left( \langle \Psi^- \rangle \langle \Phi^- \rangle - \langle \Psi^+ \rangle \langle \Phi^+ \rangle \right) \right] \tag{25}
\]

which has overlapping right and left support and is therefore well-defined at this particular nodal point of $\mathcal{X}^{(2)}_{12}[\tilde{C}]$. The difference between $\mathcal{X}^{(2)}_{12}[\tilde{C}_1 \tilde{C}_2]$ from the Hamiltonian $H_s$ and $\mathcal{X}^{(2)}_{12}[\tilde{C}_1 \tilde{C}_2]$ from $H_r(t)$ reflects the path dependence of the off-diagonal holonomy.

6 Conclusions

We have introduced and discussed a concept of off-diagonal quantum holonomy in connection with the evolution of sets of density operators. Basically motivated by possible nodal points occurring in Uhlmann’s concept of relative phase [8,9,10] for some particular paths of mixed quantum states we have extended the original notion to off-diagonal quantum holonomy invariants. Utilizing these generalised quantities the problem of undefined relative Uhlmann phase for initial and final state with orthogonal supports can be overcome in line with the introduction of off-diagonal geometric phases for pure states [22]. The definition of the holonomy invariants is equivalent to the Manini-Pistolesi approach [22] in the pure state limit, moreover it provides us with a natural extension of the latter to nonparallel-transporting unitary evolutions. When comparing these holonomy invariants with the off-diagonal mixed state geometric phases in [24] we have detected a general discrepancy for these two approaches related to a fundamental difference in the treatment of parallel transport of quantum states. Finally, we have explicitly demonstrated by means of the evolution of a Bell state mixture the necessity to resort to off-diagonal quantum holonomies to obtain information about the geometry of state space.
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