Off-diagonal generalization of the mixed state geometric phase

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The concept of off-diagonal geometric phases for mixed quantal states in unitary evolution is developed. We show that these phases arise from three basic ideas: (1) fulfillment of quantum parallel transport of a complete basis, (2) a concept of mixed state orthogonality adapted to unitary evolution, and (3) a normalization condition. We provide a method for computing the off-diagonal mixed state phases to any order for unitarities that divide the parallel transported basis of Hilbert space into two parts: one part where each basis vector undergoes cyclic evolution and one part where all basis vectors are permuted among each other. We also demonstrate a purification based experimental procedure for the two lowest order mixed state phases and consider a physical scenario for a full characterization of the qubit mixed state geometric phases in terms of polarization-entangled photon pairs. An alternative second order off-diagonal mixed state geometric phase, which can be tested in single-particle experiments, is proposed.

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I. INTRODUCTION

The concept of geometric phase, anticipated by Pancharatnam, in his study of interference of classical light in distinct states of polarization and developed by Berry for cyclic adiabatic quantal evolution, has been generalized in several steps. Aharonov and Anandan considered the cyclic nonadiabatic case and pointed out that the geometric phase is due to the curvature of the space of pure quantal states. Samuel and Bhandari provided a general setting for the geometric phase so as to cover noncyclic evolution and sequential projection measurements. Another line of development has been the extension of the geometric phase to the mixed state case. Uhlmann was probably first to address this issue in the mathematical context of purification and Sjöqvist et al. discovered a mixed state geometric phase for nondegenerate density operators in noncyclic unitary evolution in interferometry. The parallel transport conditions in Refs. have been shown to lead to generically different interference effects and the mixed state concept in Ref. has been extended to the case of completely positive maps as well as to degenerate density operators. An experimental test of the proposed mixed state geometric phase in Ref. in the qubit case has been reported recently, using nuclear magnetic resonance technique.

The noncyclic geometric phases in Refs. become undefined when the interfering states are orthogonal and the interference visibility vanishes. This leads to an interesting nodal point structure in the experimental parameter space that could be monitored in a history-dependent manner. The existence of nodal points also led Manini and Pistolesi to introduce the off-diagonal geometric phases for pure states in adiabatic evolution. These phases may carry interference information at the nodal points of the standard geometric phase. The adiabaticity assumption of Ref. was subsequently removed by Mukunda et al. and the second order off-diagonal pure state geometric phase was verified by Hasegawa et al. for neutron spin. More recently, the off-diagonal generalization of the mixed state phase in Ref. for parallel transporting unitarities has been proposed and extended to general unitarities by the present authors.

In this paper, we wish to elaborate further on the concept in Ref. Our first concern is to develop systematically the off-diagonal mixed state geometric phase in unitary evolution, filling in some important conceptual gaps of Ref. The theory of parallel transport of a complete basis is considered. Under such a parallel transport, it is argued that the mixed state geometric phase follows naturally from a concept of orthogonality between density operators adapted to unitary evolution and a certain normalization condition. Our second concern is to provide a method for computing mixed state geometric phase factors to any order for the important class of unitarities under which the parallel transported basis of Hilbert space is divided into two parts: one part where each basis vector undergoes cyclic evolution and one part where all basis vectors are permuted among each other. The experimental realization of the two lowest order mixed state phases is discussed, using the idea of purification of the involved mixed states by attaching an ancilla system entangled to the considered system. We further develop the two-photon experiment proposed in Ref. so as to include also the lowest order mixed state phase. Finally, as an attempt to avoid the apparent need for an ancilla system, we consider an alternative off-diagonal mixed state geometric phase conceptually based upon the neutron experiment in Refs.
II. BASIC IDEAS

A. Quantum parallel transport

Consider a continuous one-parameter family \( \{ U(s), s \in [s_0, s_1] \} \) of unitarities that map any initial complete orthonormal basis \( \{|\psi_k\rangle\} \) of a Hilbert space \( \mathcal{H} \) of dimension \( N \) to a continuous set of complete orthonormal bases \( \{|\psi_k(s)\rangle, s \in [s_0, s_1]\} \) of the same \( \mathcal{H} \). In the context of off-diagonal phases, it proves useful to consider parallel transport of such a complete set of orthonormal pure state vectors.

Parallel transport in terms of the initial basis \( \{|\psi_k\rangle\} \) may be formulated as follows. Let \( J(s) \) be the Hamiltonian operator in the Heisenberg representation. For the corresponding evolution operator \( U(s) \) we have (\( \hbar = 1 \) from now on)

\[
iU(s) = U(s)J(s),
\]

the formal solution of which reads

\[
U(s) = \mathcal{P}^{-1} \exp \left( -i \int_{s_0}^{s} J(s') ds' \right).
\]

Here, \( \mathcal{P}^{-1} \) is inverse path ordering, i.e., ordering increasing \( s \) from left to right in each term of series expansion of the evolution operator. \( U(s) \) is said to parallel transport the initial basis \( \{|\psi_k\rangle\} \) if the local accumulation of phase along the unitary path vanishes for each \( |\psi_k\rangle \), which amounts to \( \langle \psi_k | U^\dagger(s) U(s) | \psi_k \rangle = 0 \), i.e.,

\[
\langle \psi_k | J(s) | \psi_k \rangle = 0, \quad \forall k.
\]

Thus, the one-parameter family of Hermitian generators \( J(s) \) has to be off-diagonal in the parallel transported initial basis and therefore traceless in any basis. In other words, \( U \in SU(N) \) is a necessary condition for \( U \) being parallel transporting a complete basis. The converse does not hold: there are \( SU(N) \) transformations that contain generators that have nonvanishing diagonal elements in the \( \{|\psi_k\rangle\} \) basis.

We may equally well formulate the parallel transport conditions in terms of the instantaneous basis \( \{|\psi_k(s)\rangle\} \). Here, we have \( \langle \psi_k(s) | \dot{U}(s) U^\dagger(s) | \psi_k(s) \rangle = 0 \), which entails

\[
\langle \psi_k(s) | H(s) | \psi_k(s) \rangle = 0, \quad \forall k,
\]

where \( H(s) = U(s)J(s)U^\dagger(s) \) is the Hamiltonian operator in the Schrödinger picture. Thus, \( H(s) \) has to be off-diagonal in the instantaneous parallel transported basis, which is consistent with \( U \in SU(N) \).

Any parallel transporting unitarity is denoted by \( U^\parallel \) in the following. Moreover, an initial (instantaneous) nondegenerate density operator whose eigenvectors coincide with the basis \( \{|\psi_k\rangle\} \) \( \{|\psi_k(s)\rangle\} \) is said to be the parallel transported by \( U^\parallel \) fulfilling Eqs. (4) and (6).

For \( \dim \mathcal{H} = N \), any \( J(s) \) fulfilling the parallel transport conditions may be written in terms of \( N^2 - N \) linearly independent off-diagonal generators in the basis \( \{|\psi_k\rangle\} \). As an example, consider the qubit case \( N = 2 \). Here, we expect \( J(s) \) to be dependent upon two of the Pauli operators. Let \( \{|\psi_1\rangle, |\psi_2\rangle\} \) be a parallel transported basis. Then \( J(s) = a(s)\sigma_x + b(s)\sigma_y \) with \( \sigma_x = |\psi_1\rangle \langle \psi_2| + |\psi_2\rangle \langle \psi_1|, \quad \sigma_y = -i|\psi_1\rangle \langle \psi_2| + i|\psi_2\rangle \langle \psi_1| \), and \( a(s), b(s) \) being scalar functions of \( s \). Any density operator \( \rho \) of the form \( \rho = \lambda_1|\psi_1\rangle \langle \psi_1| + \lambda_2|\psi_2\rangle \langle \psi_2| \), \( \lambda_1 \neq \lambda_2 \) is parallel transported by the corresponding unitarity. The same holds true for \( H(s) \) by making the replacement \( \{|\psi_1\rangle, |\psi_2\rangle\} \rightarrow \{|\psi_1(s)\rangle, |\psi_2(s)\rangle\} \).

B. Orthogonality

Two pure state vectors are orthogonal if their scalar product vanishes. On the other hand, any useful scalar product between density operators does not have this simple property and the concept of orthogonality becomes less straightforward in the mixed state case. Instead, for a given density operator \( \rho \), one may take another density operator \( \rho' \) to be orthogonal to \( \rho \) if it yields minimum of the Hilbert-Schmidt product \( Tr[\rho \rho'] \) or the Bures fidelity [20] \( F_B[\rho, \rho'] = [Tr\sqrt{\rho \rho'}]^2 \), the latter being a worst case measure of distinguishability between \( \rho \) and \( \rho' \) [21]. Here, we take a third approach to the concept of orthogonality adapted to unitarily connected density operators. The idea is to say that \( \rho \) and \( \rho' = U \rho U^\dagger \) are orthogonal whenever they cannot interfere in the sense of Ref. [26].

To develop this idea in detail, let us first suppose \( |\psi\rangle \) and \( |\varphi\rangle \) are Hilbert space representatives of two arbitrary pure quantal states \( \psi \) and \( \varphi \), and assume further that \( |\psi\rangle \) is exposed to the variable \( U(1) \) shift \( e^{i\chi} \). The resulting interference pattern obtained in superposition is determined by the intensity profile [22]

\[
\mathcal{I} \propto |e^{i\chi}|^2 = 2 + 2 |\langle \psi | \varphi \rangle| \cos \left[ \chi - \arg(\psi|\varphi\rangle) \right] \tag{5}
\]

that oscillates as a function of \( \chi \). The key point here is to note that \( \psi \) and \( \varphi \) are orthogonal if and only if \( \mathcal{I} \) is independent of \( \chi \) so that the interference oscillations disappear.

This feature translates naturally to the mixed state case. Consider a pair of isospectral nondegenerate density operators

\[
\rho_{\psi} = \sum_k \lambda_k |\psi_k\rangle \langle \psi_k|, \quad \rho_{\varphi} = \sum_k \lambda_k |\varphi_k\rangle \langle \varphi_k|, \tag{6}
\]

where each \( |\varphi_k\rangle = U(|\psi_k\rangle \) for some unitarity \( U \). Each such orthonormal pure state component of the density operator contributes to the interference according to Eq. (5). Thus, the total intensity profile becomes [30]

\[
\mathcal{I} \propto \sum_k \lambda_k |e^{i\chi}|^2 = 2 + 2 \sum_k \lambda_k |\langle \psi_k | \varphi_k \rangle| \cos \left[ \chi - \arg(\psi_k|\varphi_k\rangle) \right], \tag{7}
\]
where we have used that the \(\lambda\)'s sum up to unity. Following the above pure state case, we say that \(\rho_\phi\) and \(\rho_\varphi\) are orthogonal if and only if \(I\) is independent of \(\chi\) for all Hilbert space representatives \(|\psi_k\rangle\) and \(|\varphi_k\rangle\) of the eigenstates of \(\rho_\phi\) and \(\rho_\varphi\), respectively. It follows that \(\rho_\phi\) and \(\rho_\varphi\) are orthogonal if and only if \(|\psi_k\rangle\langle \varphi_k| = 0\), \(\forall k\).

For an \(N\) dimensional Hilbert space \(H\), we may generate a set of \(N\) mutually orthogonal density operators as follows. Assume \(\rho_l|\psi_k\rangle = \lambda_k|\psi_k\rangle\) is nondegenerate and introduce a unitary operator \(U_g\) such that

\[
|\psi_n\rangle = (U_g)^{n-1}|\psi_1\rangle, \quad n = 1, \ldots, N.
\]

Thus, we may write

\[
U_g = |\psi_1\rangle\langle \psi_N| + |\psi_N\rangle\langle \psi_{N-1}| + \ldots + |\psi_2\rangle\langle \psi_1|\]

and it follows that

\[
\rho_n = (U_g)^{n-1} \rho_1 (U_g)^{n-1}, \quad n = 1, \ldots, N
\]

is a set of mutually orthogonal density operators. Explicitly, this entails that

\[
\rho_1 = \lambda_1|\psi_1\rangle\langle \psi_1| + \lambda_2|\psi_2\rangle\langle \psi_2| + \ldots + \lambda_N|\psi_N\rangle\langle \psi_N|,
\]

\[
\rho_2 = \lambda_1|\psi_2\rangle\langle \psi_2| + \lambda_2|\psi_3\rangle\langle \psi_3| + \ldots + \lambda_N|\psi_1\rangle\langle \psi_1|,
\]

\[
\rho_N = \lambda_1|\psi_N\rangle\langle \psi_N| + \lambda_2|\psi_1\rangle\langle \psi_1| + \ldots + \lambda_N|\psi_{N-1}\rangle\langle \psi_{N-1}|.
\]

Notice here that different sets of mutually orthogonal mixed states may be generated by permuting the \(\psi_n\)'s in \(U_g\).

### C. Consistency and normalization

The final step towards the concept of off-diagonal mixed state geometric phase, is to determine how the mutually orthogonal density operators should appear in the trace. This may be resolved as follows. We take the simplest nontrivial choice fulfilling this requirement, which is

\[
\gamma_{\rho_1\rho_2\ldots\rho_l}^{(1)} \equiv \Phi \left[ \text{Tr}(U^\| P_{j_1} U^\| P_{j_2} \ldots U^\| P_{j_l}) \right],
\]

where \(\Phi[z] = z/|z|\) for any complex number \(z\). We propose to replace each of these projectors with \(F^{(l)}(\rho_{j_k})\), where, for reason of permutation symmetry of the indexes \(j_1, j_2, \ldots, j_l\), the form of the function \(F^{(l)}\) may only depend on \(l\). To assure consistency with Ref. [13] we further require that \(F^{(l)}(\rho_{j_k}) \rightarrow \rho_{j_k}\) in the pure state limit. We take the simplest nontrivial choice fulfilling this requirement, which is

\[
F^{(l)}(\rho_{j_k}) = \rho_{j_k}^{p/q}, \quad p = p(l) \text{ and } q = q(l) \text{ integers}.
\]

Next, from \(P_k U^\| = P_k\), we obtain the normalization condition

\[
\text{Tr}(U_g^\| P_k U_g^\| P_{(k+1)} \mod N \cdots U_g^\| P_{(k+l)} \mod N) = \text{Tr}((U_g^\|)^l P_k) = \delta_{lN}, \quad \forall k \in [1, N],
\]

where we have used \(U_g^\|\) defined in Eq. [5]. \(P_{(k+l)} \mod N = (U_g^\|)^{-(k+l)} P_k (U_g^\|)^{-(k+l)} \mod N = I\). We propose to demand that this normalization structure is preserved in the mixed state case. After the replacement \(P_{j_k} \rightarrow \rho_{j_k}\), we similarly have

\[
\text{Tr}(U_g^\| \rho_{j_k}^{p/q} U_g^\| \rho_{j_{k+1}}^{p/q} \cdots U_g^\| \rho_{j_{k+l}}^{p/q}) = \text{Tr}((U_g^\| \rho_{j_k}^{p/q})^l), \quad \forall k \in [1, N],
\]

where we have used that \((U_g \rho U_g^\|)^{p/q} = U_g \rho^{p/q} U_g^\|.\)

This may be resolved as follows. We propose experimental realization of this general framework if we put \(l = 1\) and second order \((l=2)\) phases, the latter being defined by

\[
\gamma_{\rho_1\rho_2}^{(2)} = \Phi \left[ \text{Tr}(U^\| \rho_{j_1} U^\| \rho_{j_2}) \right],
\]

in polarization-entangled two-photon interferometry.

### III. OFF-DIAGONAL MIXED STATE GEOMETRIC PHASE

We are now ready to state our main result. The off-diagonal mixed state phase for an ordered set of \(l \leq N\) mutually orthogonal nondegenerate density operators \(\rho_{j_k}, k = 1, \ldots, l\), parallel transported by \(U^\|\) is naturally given by

\[
\gamma_{\rho_1\rho_2\ldots\rho_l}^{(1)} = \Phi \left[ \text{Tr}(U^\| \rho_{j_1} U^\| \rho_{j_2} \ldots U^\| \rho_{j_l}) \right].
\]

This is manifestly gauge invariant and independent of cyclic permutations of the indexes \(j_1, j_2, \ldots, j_l\). By construction it reduces to Eq. [13] in the limit of pure states. The mixed state geometric phase factor

\[
\gamma_{\rho_1\rho_2}^{(2)} = \Phi \left[ \text{Tr}(U^\| \rho_{j_1} U^\| \rho_{j_2}) \right],
\]

proposed in Ref. [5] may be seen as a natural consequence of this general framework if we put \(l = 1\). In Sec. V we propose experimental realization of this first \((l = 1)\) and second order \((l = 2)\) phases, the latter being defined by

\[
\gamma_{\rho_1\rho_2}^{(2)} = \Phi \left[ \text{Tr}(U^\| \rho_{j_1} U^\| \rho_{j_2}) \right],
\]

in polarization-entangled two-photon interferometry.

### IV. COMPUTATION OF OFF-DIAGONAL MIXED STATE PHASES

In the qubit case \(N = 2\), consider the unitarity

\[
U^\| = U^\|_{11}|\psi_1\rangle\langle \psi_1| + U^\|_{12}|\psi_1\rangle\langle \psi_2| + U^\|_{21}|\psi_2\rangle\langle \psi_1| + U^\|_{22}|\psi_2\rangle\langle \psi_2|
\]

(17)
that parallel transport some orthonormal basis \( \{ |\psi_1\rangle, |\psi_2\rangle \} \). The matrix elements of \( U^\parallel \) fulfill \( U^\parallel_{11} = \langle U^\parallel_{22} \rangle = \eta e^{-i\Omega/2} \) and \( U^\parallel_{12} = -\eta e^{-i\Omega/2} \). Here, \( \eta = \langle \psi_1 | U^\parallel | \psi_1 \rangle \) is the pure state visibility and \( \Omega \) is the solid angle enclosed by the path traced out by the basis vectors \( \{ |\psi_1\rangle, |\psi_2\rangle \} \) and the shortest geodesic connecting its end points on the Bloch sphere.

Now, \( U^\parallel \) in Eq. 18 parallel transports the mutually orthogonal density operators \( \rho_1 = \lambda_1 |\psi_1\rangle\langle\psi_1| + \lambda_2 |\psi_2\rangle\langle\psi_2| \) and \( \rho_2 = \lambda_1 |\psi_2\rangle\langle\psi_2| + \lambda_2 |\psi_1\rangle\langle\psi_1| \), for which we obtain

\[
\text{Tr}(U^\parallel \rho_1) = \text{Tr}(U^\parallel \rho_2)^* = \eta (\lambda_1 e^{-i\Omega/2} + \lambda_2 e^{i\Omega/2}),
\]

where we have used the Bures fidelity \( F_B[\rho_1, \rho_2] = \left[ \text{Tr}(\sqrt{\rho_1 \rho_2 \sqrt{\rho_1}}) \right]^2 = 4\lambda_1 \lambda_2 \). Notice that \( F_B[\rho_1, \rho_2] = 0 \) for pure states and \( F_B[\rho_1, \rho_2] = 1 \) in the maximally mixed state case.

In the nondegenerate mixed state case \( \lambda_1 \neq \lambda_2 \), the \( l = 1 \) phases are indeterminate only for \( \eta = 0 \), for which the \( l = 2 \) phase is well-defined since \( \text{Tr}(U^\parallel \sqrt{\rho_1 U^\parallel \rho_2}) = -1 \). In the degenerate case \( \lambda_1 = \lambda_2 \), the density operators \( \rho_1 \) and \( \rho_2 \) become identical and spherically symmetric, so that no specific basis is singled out by the parallel transport condition and the mixed state geometric phase factors \( \gamma^{(1)} \) and \( \gamma^{(2)} \) therefore become undefined. Still, there is a unique notion of relative phase in this case with additional nodal points, as discussed in Ref. 12. For a generic \( U = e^{-i\theta} \sigma \), \( \sigma = (\sigma_x, \sigma_y, \sigma_z) \) being the standard Pauli operators and \( |n| = 1 \), we obtain for \( l = 1 \) nodal points at \( \text{Tr}(U^\parallel \rho_1) = \text{Tr}(U^\parallel \rho_2) = \text{Tr}(U^\parallel) = \cos \delta = 0 \) at which \( \delta \) we have \( \text{Tr}(U^\parallel \sqrt{\rho_1 U^\parallel \rho_2}) = \cos 2\delta = -1 \). This shows that the \( l = 1 \) and \( l = 2 \) phases never become indeterminate simultaneously and thus provide a complete phase characterization of the qubit case.

The off-diagonal mixed state geometric phase in the qubit case has a nontrivial nodal structure that arises due to the nonvanishing Bures fidelity. This can be seen by putting the left-hand side of Eq. 18 to zero and solving for \( \eta^2 \) yielding

\[
\eta^2 = \left( 1 + \sqrt{F_B[\rho_1, \rho_2]} \cos \Omega \right)^{-1},
\]

which has solutions at \( \eta < 1 \) for \( F_B[\rho_1, \rho_2] \cos \Omega > 0 \). Thus, the off-diagonal mixed state geometric phase factor may change sign across the nodal surfaces in the parameter space \( (F_B[\rho_1, \rho_2], \eta, \Omega) \) defined by the solutions of Eq. 19, as shown in Fig. 1. Thus, the corresponding off-diagonal mixed state geometric phase can take both values 0 and \( \pi \), contrary to the corresponding pure state phase, which can only be \( \pi \).

To generalize the discussion we proceed to arbitrary Hilbert space dimensions \( N \) and provide a method for computing mixed state geometric phases to any order \( l \leq N \) for unitaries under which the parallel transported eigenbasis \( \{ |\psi_1\rangle, ..., |\psi_N\rangle \} \) of the mutually orthogonal \( \rho \)'s is divided into two parts: one part where each basis vector undergoes cyclic evolution and one part where all basis vectors are permuted among each other. By appropriate labeling of the eigenvectors, such unitarities can always be decomposed into the direct sum

\[
U^\parallel = u_p^\parallel \oplus u_d^\parallel,
\]

where \( u_p^\parallel \) permutes \( |\psi_1\rangle \rightarrow |\psi_m\rangle \rightarrow ... \rightarrow |\psi_2\rangle \rightarrow |\psi_1\rangle \) and \( u_d^\parallel \) is diagonal in the remaining \( N - m \) cyclic eigenvectors. These terms do not mix so that one may write

\[
\text{Tr}(U^\parallel \sqrt{\rho_{j_1} \cdots U^\parallel \rho_{j_l}}) = D_{\rho_{j_1} \cdots \rho_{j_l}}^{(l)} + F_B[\rho_{j_1}, \rho_{j_1}],
\]

where \( D_{\rho_{j_1} \cdots \rho_{j_l}}^{(l)} = \text{Tr}(u_p^\parallel \sqrt{\rho_{j_1} \cdots u_p^\parallel \rho_{j_l}}) \) and \( F_B[\rho_{j_1}, \rho_{j_1}] = \text{Tr}(u_d^\parallel \sqrt{\rho_{j_1} \cdots u_d^\parallel \rho_{j_l}}) \).

Turning first to the contribution from the diagonal part of \( U^\parallel \), we have

\[
D_{\rho_{j_1} \cdots \rho_{j_l}}^{(l)} = \sum_{k=m+1}^{N} (U^\parallel_{kk})^l \lambda_{k_1} \cdots \lambda_{k_l},
\]

with \( U^\parallel_{kk} \) the matrix elements of \( u_d^\parallel \) in the eigenbasis of the \( \rho \)'s. As the density operators are nondegenerate, it follows that all \( \lambda_{k_i} \) are different in each term on the right-hand side of Eq. 22 and \( D_{\rho_{j_1} \cdots \rho_{j_l}}^{(l)} \) must vanish if \( l >
rank of the $\rho$’s. Notice here that $\arg U_{kk}^\| \,$ is the standard cyclic geometric phase for the pure state $\psi_k$. Considering the contribution from $u_p^\|$ we can establish the following. If $l = K \times m$, $K$ integer $\leq N/m$ and $m \geq 2$, then

$$P_{\rho_1, \ldots, \rho_l} = [(−1)^{m−1} \det u_p^\|]^K f^{(l)}_{\rho_1, \ldots, \rho_l} (\lambda_1, \ldots, \lambda_N),$$

(23)

where the $f^{(l)}$’s can be written as a sum of $m$ terms. For other $l$, the $P^{(l)}$’s vanish as there is $K \times m$ steps needed to connect $\sqrt{\rho_j^\|}$ and $\sqrt{\rho_j^\|}$ with $u_p^\|$. In the extreme case where all $N$ eigenvectors are permuted, only $P^{(N)}_{\rho_1, \ldots, \rho_N}$ may be nonvanishing. Here, $K = 1$ and $\det u_p^\| = \det U^\| = +1$ since $U^\| \in SU(N)$. It follows that

$$P^{(N)}_{\rho_1, \ldots, \rho_N} = (−1)^{N−1} f^{(N)}_{\rho_1, \ldots, \rho_N} (\lambda_1, \ldots, \lambda_N),$$

(24)

where each $f^{(N)}$ is determined by the sequence of $\rho$’s. These $f$’s have some interesting properties. First, it can be seen that

$$f^{(N)}_{\rho_1, \ldots, \rho_N} = 1, \forall N,$$

(25)

as a consequence of the normalization condition described in Sec. II.C. Thus, there exist at least one well-defined off-diagonal mixed state phases for $U^\| = u_p^\|$, independent of the rank of the $\rho$’s. Secondly, we have

$$f^{(N)}_{\rho_1, \ldots, \rho_N} \geq 0, \forall j, \ldots, J,$$

(26)

as each $f^{(N)}$ always can be written as a sum of positive functions of the $\lambda$’s. This implies that the off-diagonal mixed state phases for such unitarities are completely determined by the dimension of the Hilbert space $\mathcal{H}$. Indeed, for sequences where $f^{(N)} \neq 0$ we have

$$\gamma^{(N)} = −1, \text{ if } \dim(\mathcal{H}) \text{ even,}$$

$$\gamma^{(N)} = +1, \text{ if } \dim(\mathcal{H}) \text{ odd.}$$

(27)

Let us now turn our attention to partial permutations characterized by $m \neq N$, where we can use the following algorithm to determine $f^{(l)}_{\rho_1, \ldots, \rho_l}$. As in the $N = m$ case, each $f^{(l)}_{\rho_1, \ldots, \rho_l} (\lambda_1, \ldots, \lambda_N)$ decomposes into a sum of terms determined by the sequence of $\rho$’s. Explicitly, we can write $f^{(l)}_{\rho_1, \ldots, \rho_l} (\lambda_1, \ldots, \lambda_N)$ as a sum of $m$ terms

$$f^{(l)}_{\rho_1, \ldots, \rho_l} (\lambda_1, \ldots, \lambda_N) = \sum_{i=1}^m A_i (\lambda_1, \ldots, \lambda_N),$$

(28)

where $A_i$ is of the form $\sqrt{\lambda_1^{a_1^\prime} \cdots \lambda_l^{a_l^\prime}} \geq 0$ with $a_i$ integers ranging from 0 to $l$. Since we are not interested in the phase contributions from $u_p^\|$ that are already included in the factor $[(−1)^{m−1} \det u_p^\|]^K$, we replace $u_p^\|$ with the operator

$$U^{(m)}_g = |\psi_m⟩⟨\psi_1| + |\psi_1⟩⟨\psi_2| + \cdots |\psi_{m−1}⟩⟨\psi_m|,$$

(29)

being unitary on the permuted subspace. Thereafter, we compute $f^{(l)}_{\rho_1, \ldots, \rho_l} (\lambda_1, \ldots, \lambda_N) = \text{Tr}(W^{j_1} \cdots W^{j_l})$ with $W^{j_k} \equiv U^{(m)}_g \sqrt{\rho_j^\|}$. Applying ordinary matrix multiplication rules and noting that only one entry in each row and column of $W^{j_k}$ is nonvanishing, $A_i$ is in index notation given by

$$A_i = W^{j_i}_{i,(i+1) \mod m} W^{j_2}_{(i+1),(i+2) \mod m} \cdots W^{j_{i−1}}_{i−1,(i−1) \mod m}.$$ 

(30)

Each eigenvalue $\lambda_k$ of $\rho_1$ appears exactly once in each $W^{j_k}$, so our aim is to describe the correspondence between the components $W^{j_k}_{x,y}$ and $\lambda_k$ by appropriate index transformations.

To revert the off-diagonal matrices $W^{j_l}$ to diagonal form we apply $(U^{(m)}_g)^\dagger$ to each $W^{j_k}$, thus $W^{j_k} \rightarrow (\sqrt{\rho_j^\|}) = (U^{(m)}_g)^\dagger W^{j_k}$. This transforms the indexes according to

$$x \rightarrow x' = (x + 1) \mod m, \quad y \rightarrow y' = y,$$

(31)

leading to

$$W^{j_k}_{x,y} \rightarrow (\sqrt{\rho_j^\|}) (x+1) \mod m,g$$

(32)

in terms of components. Consequently we obtain

$$A_i = (\sqrt{\rho_{j_1}}_{i,(i+1) \mod m} m, (i+1) \mod m \cdots (\sqrt{\rho_{j_{i−1}}} i−1 \mod m, (i−1) \mod m \cdots m (\sqrt{\rho_{j_i}}), i,i).$$

(33)

The transformation back to the “unpermuted” $\rho_1$ can be achieved by applying $U_g$ described in Eq. 8 accomplishing $|\psi_n⟩ = (U_g)^{n−1} |\psi_1⟩$, $n = 1, \ldots, N$, thus $\sqrt{\rho_{j_k}} \rightarrow \sqrt{\rho_{j_k}} = (U_g)^{j_k−1} \sqrt{\rho_{j_k}} (U_g)^{j_k−1}$. Since $j_k − 1$ steps are needed to convert $\sqrt{\rho_{j_k}}$ to $\sqrt{\rho_{j_1}}$ we have to carry out the index transformation

$$x \rightarrow x' = (x − (j_k − 1)) \mod N$$

(34)

so that $(\sqrt{\rho_{j_k}})_{x,x} \rightarrow (\sqrt{\rho_{j}})_{x',x'}$. Since $\rho_1$ is diagonal with eigenvalues $\lambda_k$ in ascending order in $k$, the index $x'$ denotes the wanted eigenvalue $\lambda_{x'}$.

This algorithm traces the locations of the eigenvalues $\lambda_k$ from $W^n$ back to $\sqrt{\rho_n}$ when the unitary transformations along the path starting from $W^n$ are applied:

$$\sqrt{\rho_n} \rightarrow (U_g)^{n−1} \cdots (U_g)^{n−1} \rightarrow \sqrt{\rho_n}$$

(35)

$$\sqrt{\rho_n} \rightarrow (U_g)^{n−1} \cdots (U_g)^{n−1} \rightarrow \sqrt{\rho_n}$$

This analysis makes it possible to calculate the factor $f^{(l)}_{\rho_1, \ldots, \rho_l} (\lambda_1, \ldots, \lambda_N)$ more efficiently than performing a multiplication of the $l$ matrices involved.
Let us revisit the qubit \((N = 2)\) case using the above general theory. If \(m = 0\), both \(\gamma_1^{(1)}\) and \(\gamma_2^{(1)}\) exist. Moreover, we have

\[
D^{(2)}_{p_1p_2} = \sqrt{\lambda_1 \lambda_2} \left[ (U_{11}^\|)^2 + (U_{22}^\|)^2 \right],
\]
which is consistent with Eq. (18) for \(\eta = 1\). In the permutation case \(m = 2\), we may use \((-1)^{N-1} \det U = -1\) and, from Eq. (26), \(f^{(2)}_{p_1p_2} = 1\) for \(N = 2\), and obtain

\[
\mathcal{P}^{(2)}_{p_1p_2} = -1,
\]
in agreement with Eq. (18) for \(\eta = 0\).

As a further illustration, let us work out the \(N = 3\) case in detail. For \(m = 0\), all the \(\gamma^{(1)}\)'s are well-defined. The dependence upon the rank of the density operator is visible for higher \(l\), namely

\[
D^{(2)}_{p_1p_2} = \sqrt{\lambda_1 \lambda_2} \left[ (U_{11}^\|)^2 + \lambda_1 \lambda_2 (U_{22}^\|)^2 \right] + \sqrt{\lambda_2 \lambda_3} (U_{33}^\|)^2,
\]
\[
D^{(3)}_{p_1p_2p_3} = \sqrt{\lambda_1 \lambda_2 \lambda_3} \left[ (U_{11}^\|)^3 + (U_{22}^\|)^3 + (U_{33}^\|)^3 \right]
\]
with \(D^{(2)}_{p_1p_2}\) and \(D^{(2)}_{p_1p_2}\) obtained by permutations of the \(\lambda\)'s. In the \(m = 2\) case, \(|\psi_1\rangle \rightarrow |\psi_2\rangle \rightarrow |\psi_1\rangle\) while \(|\psi_3\rangle\) undergoes cyclic evolution. Explicitly we have

\[
\mathcal{D}^{(2)}_{p_1p_2} = \lambda_3 U_{33}^\|,
\]
\[
\mathcal{D}^{(2)}_{p_1p_2} = \lambda_2 \lambda_3 (U_{33}^\|)^2,
\]
\[
\mathcal{D}^{(3)}_{p_1p_2p_3} = \sqrt{\lambda_1 \lambda_2 \lambda_3} (U_{33}^\|)^3.
\]
\[\mathcal{P}^{(2)}_{p_1p_2p_3}\] can be calculated via the algorithm above as follows. Write \(f^{(2)}_{p_1p_2p_3} = A_1 + A_2\) with \(A_1 = W_{1,2}^2 W_{2,1}^2\) and \(A_2 = W_{2,1}^1 W_{1,2}^1\). Application of the rule in Eq. (31) yields

\[
A_1 = (\sqrt{\rho_1})_{2,2} (\sqrt{\rho_2})_{1,1},
\]
\[
A_2 = (\sqrt{\rho_1})_{1,1} (\sqrt{\rho_2})_{2,2},
\]
and after using the rule in Eq. (34) we obtain

\[
A_1 = (\sqrt{\rho_1})_{2,2} (\sqrt{\rho_2})_{3,3} = \sqrt{\lambda_2 \lambda_3},
\]
\[
A_2 = (\sqrt{\rho_1})_{1,1} (\sqrt{\rho_2})_{1,1} = \lambda_1.
\]
Thus, we obtain

\[
\mathcal{P}^{(2)}_{p_1p_2} = U_{12}^\| U_{21}^\| \left( \lambda_1 + \sqrt{\lambda_2 \lambda_3} \right),
\]
where we have used \((-1)^{N-1} \det U = +1\) and, again from Eq. (26), \(f^{(3)}_{p_1p_2p_3} = 1\) for \(N = 3\). The expression for \(\mathcal{P}^{(3)}_{p_1p_2p_3}\) follows from \(A_1 = A_2 = A_3 = \sqrt{\lambda_1 \lambda_2 \lambda_3}\) and requires full rank to be nonvanishing.

As an illustrative higher dimensional example we consider the case where \(N = 5\), \(l = 4\) and a partial permutation specified by \(m = 2\). The diagonal part can be calculated to

\[
\mathcal{D}^{(4)}_{p_1p_4p_5p_3} = U_{33}^\| \sqrt{\lambda_1 \lambda_3 \lambda_4 \lambda_5} + U_{44}^\| \sqrt{\lambda_1 \lambda_2 \lambda_4 \lambda_5} + U_{55}^\| \sqrt{\lambda_1 \lambda_2 \lambda_3 \lambda_5},
\]
and the permutation part is given by

\[
\mathcal{P}^{(4)}_{p_1p_4p_5p_3} = \left[ (-1)^1 \det u_p^\| \right]^2 f^{(4)}_{p_1p_4p_5p_3},
\]
where \(f^{(4)}_{p_1p_4p_5p_3} = A_1 (\lambda_1, \ldots, \lambda_5) + A_2 (\lambda_1, \ldots, \lambda_5)\). For a calculation of \(f^{(4)}_{p_1p_4p_5p_3}\) we use the algorithm described above. From Eq. (30) we know that

\[
A_1 = W_{1,2}^2 W_{2,1}^2 W_{1,2}^5 W_{2,1}^3 W_{1,2}^1,
\]
\[
A_2 = W_{2,1}^1 W_{1,2}^5 W_{1,2}^3 W_{2,1}^2.
\]
Applying rule (31) to the indices we obtain

\[
A_1 = \sqrt{\rho_1} \sqrt{\rho_2} \left( \sqrt{\rho_3} \right)_{2,2} \left( \sqrt{\rho_4} \right)_{1,1},
\]
\[
A_2 = \sqrt{\rho_1} \sqrt{\rho_2} \left( \sqrt{\rho_3} \right)_{1,1} \left( \sqrt{\rho_4} \right)_{2,2},
\]
After a transformation according to the rule (34) we have

\[
A_1 = \left( \sqrt{\rho_1} \right)_{2,2} \left( \sqrt{\rho_2} \right)_{3,3} \left( \sqrt{\rho_3} \right)_{4,4} = \sqrt{\lambda_2 \lambda_3 \lambda_4},
\]
\[
A_2 = \left( \sqrt{\rho_1} \right)_{1,1} \left( \sqrt{\rho_2} \right)_{1,1} \left( \sqrt{\rho_3} \right)_{2,2} = \sqrt{\lambda_1 \lambda_4 \lambda_5},
\]
and consequently

\[
f^{(4)}_{p_1p_4p_5p_3} = \sqrt{\lambda_1 \lambda_4 \lambda_5} + \sqrt{\lambda_1 \lambda_2 \lambda_4 \lambda_5},
\]
\[\mathcal{P}^{(4)}_{p_1p_4p_5p_3}\] can now be written as

\[
\mathcal{P}^{(4)}_{p_1p_4p_5p_3} = (U_{12}^\| U_{21}^\|)^2 \left( \sqrt{\lambda_2 \lambda_3 \lambda_4} + \sqrt{\lambda_1 \lambda_4 \lambda_5} \right),
\]
using \(\det u_p^\| = -U_{12}^\| U_{21}^\|\).

V. EXPERIMENTAL PROCEDURE

When we consider possible experimental realizations of the off-diagonal mixed state phases we immediately encounter a problem: how do we experimentally implement the \(l\)th root of density operators? Fortunately, this may be resolved in the \(l = 2\) case in the sense of purification, i.e., by adding an ancilla system in a certain way.
Here, we demonstrate this in general and propose a physical scenario for the qubit case in terms of polarization-entangled two-photon interferometry.

We first show how to realize the \( l = 1 \) and \( l = 2 \) phases via purification. For an \( N \) dimensional Hilbert space \( \mathcal{H} \), consider the nondegenerate density operator

\[
\rho_1 = \sum_{k=1}^{N} \lambda_k |\psi_k \rangle \langle \psi_k|.
\]

(51)

A purification of this \( \rho_1 \) is any pure state \( \Psi_1 \) obtained by adding an ancilla system \( a \) to the considered system \( s \) such that \( \rho_1 = \text{Tr}_a |\Psi_1 \rangle \langle \Psi_1| \). Thus, we may write

\[
|\Psi_1 \rangle = \sum_{k=1}^{N} \sqrt{\lambda_k} |\psi_k \rangle \otimes |\varphi_k \rangle,
\]

(52)

where \( \{ |\varphi_k \rangle \} \) is an orthonormal set of vectors in the ancilla Hilbert space \( \mathcal{H}_a \). Consequently, any orthogonal density operator \( \rho_n = (U_g)^{n-1} \rho_1 (U_g)^{n-1} \) has a purifications of the form

\[
|\Psi_n \rangle = (U_g)^{n-1} \otimes \tilde{U}_a |\Psi_1 \rangle
\]

(53)

for any unitarity \( \tilde{U}_a \) acting on \( \mathcal{H}_a \). In the following, we assume \( \dim \mathcal{H}_a = N \) and put \( |\varphi_k \rangle = |\psi_k \rangle \).

Let \( U_s \otimes U_a |\Psi_1 \rangle \) and \( V_s \otimes V_a |\Psi_1 \rangle \) be two Hilbert space representatives of a pair of purifications of \( U_s \rho_1 U_s^\dagger \) and \( V_s \rho_1 V_s^\dagger \). The coincidence interference pattern obtained in superposition is determined by the interference profile

\[
\mathcal{I} \propto \left| \text{Tr}(U_s \otimes U_a |\Psi_1 \rangle \langle \Psi_1| V_s \otimes V_a |\Psi_1 \rangle \langle \Psi_1|) \right|^2 - 2 + 2 \text{Re}[\text{Tr}(U_s \otimes U_a |\Psi_1 \rangle \langle \Psi_1| V_s \otimes V_a |\Psi_1 \rangle \langle \Psi_1|)]
\]

(54)

By choosing \( U_s = e^{i\chi} (U_g)^{j_1-1}, V_s = U|| (U_g)^{j_1-1} \) and \( U_a = V_a = I \), we obtain the \( l = 1 \) phase factors \( \gamma_{j_1}^{(1)} \) by variation of the U(1) phase \( \chi \) since

\[
\phi \left[ \text{Tr}((U_g)^{j_1-1} \otimes (U_g)^{j_1-1} \otimes |\Psi_1 \rangle \langle \Psi_1|) \right] = e^{-i\chi} \phi \left[ \text{Tr}((U_g)^{j_1-1} \otimes (U_g)^{j_1-1} \otimes |\Psi_1 \rangle \langle \Psi_1|) \right]
\]

(55)

where we have used that \( \text{Tr}_a [(U_g)^{j_1-1} |\Psi_1 \rangle \langle \Psi_1| (U_g)^{j_1-1}] = \rho_{j_1} \). Similarly, the \( l = 2 \) phase factors \( \gamma_{j_1, j_2}^{(2)} \) are obtained by letting \( U_s = e^{i\chi} (U_g)^{j_2-1}, V_s = U|| (U_g)^{j_2-1}, U_a = (U_g)^{j_2-1} \) and \( V_a = (U_g)^{j_2-1} \), \( T \) being transpose with respect to the ancilla basis \( \{|\psi_k \rangle\} \), since

\[
\phi \left[ \text{Tr}((U_g)^{j_1-1} \otimes (U_g)^{j_1-1} \otimes |\Psi_1 \rangle \langle \Psi_1|) \right] = e^{-i\chi} \phi \left[ \text{Tr}((U_g)^{j_1-1} \otimes (U_g)^{j_1-1} \otimes |\Psi_1 \rangle \langle \Psi_1|) \right]
\]

(56)

where the last equality may be obtained by explicit use of \( |\Psi_1 \rangle \) in Eq. (52) with \( |\varphi_k \rangle = |\psi_k \rangle \).

Let us discuss a physical purification scenario for the \( l = 1 \) and \( l = 2 \) phases in the qubit case. Consider the two-photon Franson-type setup in Fig. 2. A source that in the horizontal-vertical (\( h-v \)) basis produces polarization-entangled photon states of the form

\[
|\Psi_1 \rangle = \sqrt{\frac{1}{2}} (1+r) |h \rangle \otimes |h \rangle + \sqrt{\frac{1}{2}} (1-r) |v \rangle \otimes |v \rangle
\]

(57)

has been demonstrated in Ref. [26]. Considered as subsystems both photons are in a mixed linear polarization state \( \rho_1 \) with polarization degree \( r \). The desired superposition of \( U_s \otimes U_a |\Psi_1 \rangle \) and \( V_s \otimes V_a |\Psi_1 \rangle \) is obtained by requiring sufficiently short coincidence window so that detection occurs only when the photons both either took the shorter path or the longer path. A purification of the orthogonal density operator \( \rho_2 = U_s \rho_1 U_s^\dagger \) may be achieved by flipping the polarizations of the photons, yielding

\[
|\Psi_2 \rangle = U_g \otimes U_g |\Psi_1 \rangle = \sqrt{\frac{1}{2}} (1+r) |v \rangle \otimes |v \rangle + \sqrt{\frac{1}{2}} (1-r) |h \rangle \otimes |h \rangle.
\]

(58)

FIG. 2: Franson setup for polarization-entangled photon pairs. In the longer arms, the system and ancilla photons are exposed to the polarization affecting unitaries \( U_s \) and \( U_a \), respectively, and similarly \( V_s \) and \( V_a \) in the shorter arms.

To demonstrate the \( l = 1 \) and \( l = 2 \) geometric phases in this scenario, it is sufficient to consider unitaries that rotate linear polarization states along great circles at an angle \( \beta \) on the Poincaré sphere, see Fig. 3. This amounts to

\[
U(\beta, \theta) = \text{exp} \left( -i \frac{\beta}{2} \left[ \cos \theta (|h \rangle \langle v| + |v \rangle \langle h|) + \sin \theta (|-i| h \rangle \langle v| + i |v \rangle \langle h|) \right] \right)
\]

(59)

which fulfills the parallel transport conditions in Eqs. (50) and (51) with respect to the \( h-v \) basis. In practice, \( U(\beta, \theta) \) may be implemented by appropriate \( \lambda \)-plates, the thickness and orientation of which correspond to the
parameters \( \beta \) and \( \theta \), respectively. For example, \( U_s = U(\pi, \pi/2) \) acting on the linear polarization states as a polarization flip and thus connects \( \rho_1 \) and \( \rho_2 \), is achieved by a \( \lambda/2 \) plate with half axis making an angle 45° to the vertical \( (v) \) direction. Furthermore, \( \theta = 0 \) and \( \beta = \pi/2 \), corresponding to a \( \lambda/4 \) plate oriented along the vertical direction, takes \( h \) and \( v \) into the right \( (R) \) and left \( (L) \) circular polarization states, respectively.

VI. PROJECTION PHASE

Since the definition of the off-diagonal geometric mixed state phase claims to be reducible to the pure state off-diagonal geometric phase, the question arises if there is a connection to the experimental verification of the latter performed by Hasegawa et al. 13, 14. This has to be answered in the negative, since in this experiment the evolution of the orthogonal state is implemented as a projection operator, which is by definition equivalent to a pure state. On the other hand, by taking the impurity of the input state into account, the shift in the interference pattern in the Hasegawa et al. setup, given by the additional phase factor

\[
\gamma_{\rho P} \equiv \Phi[\text{Tr}(U \rho U P)],
\]

could be used as a definition of the off-diagonal geometric mixed state phase, if the unitarity \( U \) describing the evolution inside the interferometer is parallel transporting the eigenvectors of the nondegenerate \( \rho \). Here, \( P \) should project onto the eigenstate that corresponds to the smallest eigenvalue of \( \rho \). Parallel transport is for example fulfilled in the Hasegawa et al. experiment if the incident spinor is polarized in a plane perpendicular to the direction of the magnetic field. \( \gamma_{\rho P} \) is gauge invariant under a \( U(1) \) transformation of each of the basis vectors and it reduces to the corresponding off-diagonal geometric phase factor of Ref. 13, in the pure state limit when \( U = U^{\parallel} \).

In the two dimensional case relevant for the Hasegawa et al. experiment with input \( \rho = \lambda_1|\psi_1\rangle\langle\psi_1| + \lambda_2|\psi_2\rangle\langle\psi_2| \), \( \lambda_1 > \lambda_2 \), we can write Eq. 59 as

\[
\text{Tr}[U \rho U P] = \lambda_1(-1 + \eta^2) + \lambda_2 \eta^2 e^{-2i\alpha}.
\]

Here, \( U \in SU(2) \) with the diagonal matrix elements \( U_{11} = U_{22} = \eta e^{i\alpha} \) is not necessarily fulfilling the parallel transport condition with respect to \( \{ |\psi_1\rangle, |\psi_2\rangle \} \). In the pure state limit \( \lambda_1 = 1 \), \( \lambda_2 = 0 \) the off-diagonal phase is always \( \pi \) since \( \text{Tr}[U \rho U P]|_{\lambda_1=1} = -1 + \eta^2 \) is real and negative, irrespective of whether \( U \) parallel transports \( |\psi_1\rangle, |\psi_2\rangle \) or not. For a mixed input state \( \rho \) the \( \lambda_2 \)-term does not vanish and we obtain additional geometric and/or dynamical phase contributions. These can be considered to originate in the subjacent geometry only if \( U \) is a parallel transporting unitarity, but not for arbitrary \( U \).

To show the consistency with the experiment performed by Hasegawa et al. we calculate the phase \( \phi_{\rho P} = \arg \text{Tr}[U \rho U P] \). In the left panel of Fig. 2 we show \( \phi_{\rho P} \) for a mixed input state with \( \lambda_1 = 0.87, \lambda_2 = 0.13 \), in accordance with the experimental degree of polarization in Refs. 13, 14, and the spin polarization angle \( \theta = \pi/6 \) relative to the magnetic field in the upper arm of the interferometer (see Fig. 2 of Ref. 14). The calculated curve matches with the experimental and theoretical results presented in Fig. 5(d) of Ref. 14. Note that in this case \( U \) is not parallel transporting the incident spinor.
Another interesting fact is that due to the impurity of the input state we expect phase jumps for $\theta = \pi/2$ for $\delta = 2 \arccos \sqrt{\lambda_1}$ and $\delta = 2\pi - 2 \arccos \sqrt{\lambda_1}$, see right panel of Fig. 4, where $\delta$ is the precession angle of the incident spinor about the direction of the magnetic field. Here, we have a parallel transporting $U = U^\parallel$, thus these jumps have their origin in the subjacent geometry of state space.

Starting with a preliminary discussion about orthogonality of mixed states and quantum parallel transport we have provided a general treatment of the off-diagonal mixed state geometric phase comprising unitarities that can be decomposed into a diagonal part leaving the initial basis states unchanged and a permutation part reordering the initial states. An algorithm has been presented to calculate the appropriate phase factors efficiently for any dimension and for an arbitrary number of orthogonal density operators. Furthermore, we have discussed the projection off-diagonal geometric phase appearing in the neutron experiment by Hasegawa et al. [15, 16] as an alternative definition of off-diagonal mixed state phase.

In the qubit case the off-diagonal mixed state phase can be fully qualified both from the theoretical and from the experimental point of view. But it has to be mentioned that the measurement seems to require control and measurement of one or more ancilla systems although the off-diagonal mixed state phases are properties of the system alone, since the constituting set of density operators pertains solely to the system. Explicitly, a Franson interferometer setup for the qubit case has been presented illustrating the nontrivial sign change property of the off-diagonal phase connected to the mixed state case. The apparent need for control over an ancilla system seems to suggest that the proposed concept of off-diagonal mixed state geometric phase is a nonlocal and/or contextual property of the unitary evolution of a quantum system.

VII. CONCLUSIONS

Recent investigations in geometric phases in quantum systems have led to cases where the standard definitions breaks down. On one hand, such situations emerge for orthogonal initial and final pure states connected unitarily, on the other, unitary evolution of a system in a mixed state may lead to nodal points in parameter space. In search for a complementary geometric quantity defined in such cases, the off-diagonal mixed state geometric phase has been proposed [17] by the present authors as a generalization of the off-diagonal geometric phases for pure state put forward in Ref. [13].

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