Kinematic approach to off-diagonal geometric phases of nondegenerate and degenerate mixed states

D.M. Tong\textsuperscript{1}, Erik Sjöqvist\textsuperscript{2}, Stefan Filipp\textsuperscript{3,4}, L.C. Kwek\textsuperscript{1,5}, and C.H. Oh\textsuperscript{1,6}

\textsuperscript{1}Department of Physics, National University of Singapore, 10 Kent Ridge Crescent, Singapore 119260, Singapore
\textsuperscript{2}Department of Quantum Chemistry, Uppsala University, Box 518, SE-751 20 Uppsala, Sweden
\textsuperscript{3}Atominstitut der Österreichischen Universität, Stadionallee 2, 1020 Vienna, Austria
\textsuperscript{4}Institut Laue Langevin, Boîte Postale 156, F-38042 Grenoble Cedex 9, France
\textsuperscript{5}National Institute of Education, Nanyang Technological University, 1 Nanyang Walk, Singapore 639798, Singapore

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Off-diagonal geometric phases have been developed in order to provide information of the geometry of paths that connect noninterfering quantal states. We propose a kinematic approach to off-diagonal geometric phases for pure and mixed states. We further extend the mixed state concept proposed in [Phys. Rev. Lett. \textbf{90}, 050403 (2003)] to degenerate density operators. The first and second order off-diagonal geometric phases are analyzed for unitarily evolving pairs of pseudopure states.

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I. INTRODUCTION

Pancharatnam’s work on the geometric phase in interference of light waves in distinct states of polarization plays a prominent role among early anticipations of the concept of geometric phase. It found its quantal counterpart when Berry discovered geometric phase factors accompanying cyclic adiabatic changes. Since then there has been an immense interest in holonomy effects in quantum mechanics, which has led to many generalizations of the notion of geometric phase. The extension to nonadiabatic cyclic evolution was developed by Aharonov and Anandan. Samuel and Bhandari generalized the pure state geometric phase further by extending it to noncyclic evolution and sequential projection measurements. Mukunda and Simon put forward a kinematic approach to the off-diagonal mixed state geometric phase by a neutron experiment. The concept of off-diagonal geometric phase has been extended to mixed states represented by nondegenerate density operators, as well as to the Uhlmann holonomy. These off-diagonal mixed state geometric phases contain information about the geometry of state space along the path connecting pairs of density operators, when the standard mixed state geometric phases in Refs. are undefined. In this paper, we propose a kinematic approach to the off-diagonal mixed state geometric phase in Refs. and further extend it to the degenerate case.

\begin{equation}
\langle \psi_k | U^R(t) U^R(t) \psi_k = 0, \ k = 1, \ldots, N \end{equation}

relative to the chosen basis. For any pair of basis vectors $| \psi_{j_1} \rangle$ and $| \psi_{j_2} \rangle$ such that $\langle \psi_{j_1} | U(t) \psi_{j_2} \rangle \neq 0$ and
where \( \langle \psi_j | U^\parallel(t) | \psi_j \rangle \neq 0 \), the quantity

\[
\gamma_{j_1j_2}^{(2)} = \Phi \left[ \langle \psi_j | U^\parallel(t) | \psi_j \rangle \langle \psi_j | U^\parallel(\tau) | \psi_j \rangle \right],
\]

(2)

where \( \Phi[z] \equiv z/|z| \) for any nonzero complex number \( z \), is gauge invariant and therefore a property of the pair of paths \( C_{j_1}, C_{j_2} : t \in [0, \tau] \rightarrow |\psi_j(t)\rangle\langle \psi_j(t) | \) in projective Hilbert space. The set \( \{ \gamma_{j_1j_2}^{(2)} \} \) constitutes the second order off-diagonal pure state geometric phase factors. It may be extended by considering \( l \leq N \) states yielding the \( l \)th order off-diagonal pure state geometric phase factors

\[
\gamma_{j_1...j_l}^{(l)} = \prod_{a=1}^{l} \Phi \left[ \langle \psi_j_a | U^\parallel(t) | \psi_{j_{a+1}} \rangle \right],
\]

(3)

where \( |\psi_{j_{a+1}} \rangle = |\psi_{j_a} \rangle \) and \( \langle \psi_{j_a} | U^\parallel(t) | \psi_{j_{a+1}} \rangle \neq 0 \) for all \( a = 1, ... l \).

Notice that there is an equivalence set \( S \) of unitaries \( \tilde{U}(t) \) that all realize \( \{ C_k \} \), namely those of the form

\[
\tilde{U}(t) = U(t) \sum_{k=1}^{N} e^{i\theta_k(t)} |\psi_k \rangle \langle \psi_k |,
\]

(4)

where \( U(t) \in S \) and \( \theta_k(t) \) are real time-dependent parameters such that \( \theta_k(0) = 0 \). We may in particular identify \( U^\parallel(t) \in S \) by substituting \( U^\parallel(t) = \tilde{U}(t) \) into Eq. (11), so that we obtain

\[
\theta_k(t) = \frac{\theta_k^\parallel(t)}{2} = i \int_{0}^{t} \langle \psi_k | U^\parallel(t') \tilde{U}(t') | \psi_k \rangle dt',
\]

(5)

and

\[
U^\parallel(t) = U(t) \sum_{k=1}^{N} e^{-\int_{0}^{t} \langle \psi_k | U^\parallel(t') \tilde{U}(t') | \psi_k \rangle dt'} |\psi_k \rangle \langle \psi_k |.
\]

(6)

Inserting this expression into Eq. (2) for \( U^\parallel(t) \), we obtain a kinematic expression for the \( l = 2 \) off-diagonal geometric phase factors as

\[
\gamma_{j_1j_2}^{(2)} = \Phi \left[ \langle \psi_j | U^\parallel(t) | \psi_j \rangle \langle \psi_j | U^\parallel(\tau) | \psi_j \rangle \right]
\times e^{-\int_{0}^{t} \langle \psi_j | U^\parallel(t') \tilde{U}(t') | \psi_j \rangle dt'}
\times e^{-\int_{0}^{\tau} \langle \psi_j | U^\parallel(t') \tilde{U}(t') | \psi_j \rangle dt'},
\]

(7)

In the above expression, the unitary operator \( U(t) \in S \) need not satisfy the parallel transport conditions. One may verify that \( \gamma_{j_1j_2}^{(2)} \tilde{U}(t) = \gamma_{j_1j_2}^{(2)} |\psi_j \rangle \langle \psi_j | \) for any choice of \( \theta_k(t) \).

An interesting aspect of Eq. (7) is that in the qubit case with \( |\psi_1 \rangle = |0 \rangle \) and \( |\psi_2 \rangle = |1 \rangle \), it follows that \( \langle 0 | U^\parallel(t) \tilde{U}(t) | 0 \rangle = -\langle 1 | U^\parallel(t) \tilde{U}(t) | 1 \rangle \) for any SU(2) operation, leading to

\[
\gamma_{01}^{(2)} = \Phi \left[ \langle 0 | U^\parallel(\tau) | 1 \rangle \langle 1 | U^\parallel(t) | 0 \rangle \right] = -1,
\]

(8)

whenever \( \langle 0 | U^\parallel(\tau) | 1 \rangle \neq 0 \) and \( \langle 1 | U^\parallel(t) | 0 \rangle \neq 0 \). Thus, the \( \pi \) shift in the qubit case is independent of the fulfillment of the parallel transport condition Eq. (11), a result that has been experimentally verified for neutron spin \( 25, 26 \).

Similarly, for the higher order off-diagonal geometric phases \( 27, 28 \), we obtain

\[
\gamma_{j_1...j_l}^{(l)} = \prod_{a=1}^{l} \Phi \left[ \langle \psi_j_a | U^\parallel(t) | \psi_{j_{a+1}} \rangle \right]
\times e^{-\int_{0}^{t} \langle \psi_j_a | U^\parallel(t') \tilde{U}(t') | \psi_j_a \rangle dt'}, \quad l \leq N
\]

(9)

upon substitution of Eq. (6) into Eq. (8). Once again, one may verify that \( \gamma_{j_1...j_l}^{(l)} \tilde{U}(t) = \gamma_{j_1...j_l}^{(l)} |\psi_j \rangle \langle \psi_j | \).

We now put forward a kinematic approach to the off-diagonal geometric phases of nondenerate mixed states proposed in Refs. 27, 28. Let

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

(10)

where for all nonzero eigenvalues we have \( \lambda_k \neq \lambda_{l \neq k} \). Furthermore, introduce the unitarity

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

(11)

in terms of which any pair of members \( \rho_{j_1}, \rho_{j_2}, j_1 \neq j_2 \), of the set

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

(12)

are unitarily connected and do not interfere since \( \text{Tr}(W^{j_2-j_1} \rho_{j_1}) \) vanishes. In analogy with the pure state case, the density operators \( \rho_n \) constitute a set of states in terms of which we may define the off-diagonal mixed state geometric phase factors as \( 27, 28 \)

\[
\gamma_{\rho_{j_1}...\rho_{j_l}}^{(l)} = \Phi \left[ \text{Tr} \left( \prod_{a=1}^{l} U^\parallel(t) \sqrt{\rho_{j_a}} \right) \right]
\]

(13)

as long as the trace in the argument of \( \Phi \) does not vanish. Here, \( U^\parallel(t) \) satisfies the parallel transport conditions in Eq. (11) and \( l \leq N \). Apparently \( \gamma^{(l)} \) are the standard mixed state geometric phase factors associated with the unitary paths \( \mathcal{M}_n : t \in [0, \tau] \rightarrow \rho_n(t) \) in state space. Furthermore, it has been demonstrated \( 27, 28 \) a physical scenario for the \( l = 2 \) case in terms of two-particle interferometry.

As the nonzero eigenvalues of all mixed states under consideration are nondegenerate, the parallel transport conditions are still given by Eq. (11) and \( U^\parallel(t) \) by Eq. (6). Substituting Eq. (6) into Eq. (13), we obtain the kinematic expression for the off-diagonal geometric phase factors for mixed states under evolution \( U(t) \) as
\[
\gamma^{(l)}_{i_1 \cdots i_l} = \Phi \left[ \sum_{i_1, \ldots, i_l=1}^{N} \sqrt{\lambda_{i_1-j_1+1} \cdots \lambda_{i_N-j_N+1}} \langle \psi_{i_1} | U(\tau) | \psi_{i_2} \rangle \langle \psi_{i_2} | U(\tau) | \psi_{i_3} \rangle \cdots \langle \psi_{i_N} | U(\tau) | \psi_{i_1} \rangle \right] \\
\times \exp \left( - \int_0^\tau \frac{1}{a} \sum_{a=1}^{l} \langle \psi_{i_a} | U^\dagger(t) \dot{U}(t) | \psi_{i_a} \rangle \, dt \right),
\]

where \( \lambda_{-p} = \lambda_{N-p}, \ p = 0, \ldots, N-1 \). One may verify that the phase factors \( \gamma^{(l)}_{i_1 \cdots i_l} \) are gauge invariant in that they are independent of the choice of \( U(t) \in \mathcal{S} \).

### III. OFF-DIAGONAL GEOMETRIC PHASES FOR DEGENERATE DENSITY OPERATORS

We now generalize the concept of off-diagonal geometric phases of nondegenerate mixed states to degenerate mixed states. Let

\[
\rho_1 = \lambda_1 P^{(m_1)}_{1:1} + \cdots + \lambda_K P^{(m_K)}_{1:K},
\]

where the nonzero eigenvalue \( \lambda_k, k = 1, \ldots, K \leq N \), is \( m_k \) fold degenerate and \( P^{(m_k)}_{1:k} \) the corresponding projector of rank \( m_k \). The choice \( |\psi_1\rangle, \ldots, |\psi_N\rangle \) of orthonormal Hilbert space basis and concomitant permutation unitarity \( W = |\psi_1\rangle \langle \psi_N| + |\psi_N\rangle \langle \psi_1| + \cdots + |\psi_2\rangle \langle \psi_1| \), defines a set of noninterfering density operators

\[
\rho_n = \lambda_1 P^{(m_1)}_{n:1} + \cdots + \lambda_K P^{(m_K)}_{n:K}, \quad n = 1, \ldots, N,
\]

where \( P^{(m_k)}_{n:k} = W^{-1} P^{(m_k)}_{1:k} (W^\dagger)^{n-1} \), \( n = 1, \ldots, N \). Note that \( P^{(m_k)}_{n:k} \neq P^{(m_k)}_{n':k} \) for \( n \neq n' \).

The parallel transport conditions for a unitary path \( t \to \rho_n(t) \) with \( \rho_n(0) = \rho_n \), could be taken as

\[
F^{(m_k)}_{n:k} U^\dagger_n(t) \dot{U}_n(t) F^{(m_k)}_{n:k} = 0, \quad k = 1, \ldots, K.
\]

In terms of the orthonormal Hilbert space basis \( |\psi_1\rangle, \ldots, |\psi_N\rangle \), Eq. (17) is equivalent to the more familiar parallel transport conditions

\[
\langle \psi_t | U^\dagger_n(t) \dot{U}_n(t) | \psi_t \rangle = 0, \quad \forall \ n \in \mathcal{P}_{n:k},
\]

which reduces to those of Ref. 11 in the nondegenerate case where \( K = N \).

Now, suppose there is a one-parameter family of unitaries \( \{ U(t) | t \in [0, \tau], U(0) = I \} \) defining the paths \( \mathcal{M}_n : t \in [0, \tau] \to \rho_n(t) = U(t) \rho_n U^\dagger(t), n = 1, \ldots, N \). Then, for each \( \rho_n \), there is an equivalence set \( \mathcal{S}_n \) of unitaries \( \tilde{U}_n(t) \) that all realize \( \mathcal{M}_n \), namely those of the form

\[
\tilde{U}_n(t) = U(t) V_n(t)
\]

with

\[
V_n(t) = \alpha_{n:1}(t) + \cdots + \alpha_{n:K}(t),
\]

where \( \alpha_{n:k}(t) \) is unitary on the \( k \)th degenerate subspace, i.e., \( \alpha_{n:k}(t) \alpha_{n:k}^\dagger(t) = \alpha_{n:k}(t) \alpha_{n:k}^\dagger(t) = P^{(m_k)}_{n:k} \), and \( \alpha_{n:k}(0) = P^{(m_k)}_{n:k} \). We can identify \( \tilde{U}_n(t) \in \mathcal{S}_n \) by substituting \( \tilde{U}_n(t) = \tilde{U}_n(t) \) into Eq. (17), and obtain

\[
\alpha^\dagger_{n:k}(t) = P^{(m_k)}_{n:k} T \exp \left( - \int_0^t P^{(m_k)}_{n:k} U^\dagger(t') \dot{U}(t') P^{(m_k)}_{n:k} \, dt' \right) P^{(m_k)}_{n:k},
\]

where \( T \) denotes time ordering. The parallel transporting unitary operators for \( \rho_n \) may be expressed as \( U^\dagger_n(t) = U(t) V_n^\dagger(t) \) with supplementary operators \( V_n(t) = \alpha^\dagger_{n:1}(t) + \cdots + \alpha^\dagger_{n:K}(t) \).

In the presence of degenerate subspaces, some of the parallel transporting unitaries \( U^\dagger_n(t) \) must be different from each other. Thus, unlike the nondegenerate case, where a common parallel transporting \( U^\dagger(t) \) can always be found, such a common operator parallel transporting all the states \( \rho_n \) does not exist in the degenerate case; we need to take \( U^\dagger(t) \), \( U^\dagger(t) \), \( U^\dagger(t) \) to parallel transport \( \rho_1, \ldots, \rho_N \), respectively. Substituting \( \tilde{U}^\dagger_n(t) = U(t) V_n^\dagger(t) \), \( a = 1, \ldots, l \), into Eq. (17) for the \( a \)th \( U(t) \), we obtain the off-diagonal geometric phase factors of the degenerate mixed states as

\[
\gamma^{(l)}_{i_1 \cdots i_l} = \Phi \left[ \text{Tr} \left( \prod_{a=1}^{l} U(\tau) V_{j_a}^\dagger(\tau) \sqrt{\rho_{j_a}} \right) \right]
\]

for nonvanishing trace in the argument of \( \Phi \). The phase value calculated in Eq. (21) is manifestly gauge invariant under choice of the set \( \{ \tilde{U}_n(t) \} \), which shows that it is
IV. EXAMPLE: PSEUDOPURE STATES

Let us illustrate the above for pseudopure states, which take the form

\[ \rho_n = \frac{1 - \epsilon}{N} I + \epsilon |n⟩⟨n|, \quad n = 1, \ldots, N \geq 2 \]  

with \( 0 < \epsilon \leq 1 \), and \( |n⟩ \) any \( p \)-qubit state. Such states have a single nondegenerate eigenvector \( |n⟩ \) with eigenvalue \((1 + (N - 1)\epsilon)/N\) and an \( N - 1 \) fold degenerate eigenvalue \((1 - \epsilon)/N\) with eigenprojector \( I - |n⟩⟨n| \). Pseudopure states appear generically as input states to standard liquid-state NMR quantum computers, in case of which \( N = 2^p \), \( p \) being the number of nuclear spin qubits.

\[ U_n = U_{\|} = I - P_{nm} + U_{nm}(t) \]

where \( P_{nm} \) is the projection operator onto the subspace spanned by \{\( |n⟩, |m⟩ \}\) and \( U_{nm}(t)U_{nm}^\dagger(t) = U_{nm}(t)U_{nm}^\dagger(t) = P_{nm} \). In the case of liquid-state NMR quantum protocols, one may for example take

\[ |n⟩ = |0⟩_1 \otimes \ldots \otimes |0⟩_q \otimes \ldots \otimes |0⟩_p, \]

\[ |m⟩ = |0⟩_1 \otimes \ldots \otimes |1⟩_q \otimes \ldots \otimes |0⟩_p, \]

where \( 1 \leq q \leq p \) so that \( U(t) \) represents single-qubit operations on the \( q \)th nuclear spin. Using Eq. \( 19 \), we obtain the parallel transporting unitarities

\[ U_{nm} = \left( \frac{(N - 2)}{2} \right) \left( (N - 2)(1 - \epsilon) + \eta(1 + (N - 1)\epsilon)e^{-i\Omega/2} + \eta(1 - \epsilon)e^{i\Omega/2} \right) \]

The above form of the specific family of states, there is a single unitarity parallel transporting both \( \rho_n \) and \( \rho_m \). This property may be advantageous in experimental tests of the \( l = 1 \) and \( l = 2 \) geometric phases for \( \rho_n \) and \( \rho_m \). Note that a separate treatment of the random mixture (\( \epsilon = 0 \)) yields \( U_n = C_n^\dagger = I \).

Let us first analyze the \( l = 1 \) geometric phase factors for \( \rho_n \) and \( \rho_m \) in the \( \epsilon \geq 0 \) case. Inserting Eqs. \( 22 \) and \( 24 \) into Eq. \( 21 \) yields

\[ \gamma^{(1)}_{\rho_n} = \gamma^{(1)}_{\rho_m} = \Phi \left[ \frac{\eta N \epsilon \sin \frac{\Omega}{2}}{(N - 2)(1 - \epsilon) + \eta(2 + (N - 2)\epsilon) \cos \frac{\Omega}{2}} \right] \]

whenever the phase factor is defined. Here, \( \Omega \) is the geodesically closed solid angle on the Bloch sphere defined by projection of the two-dimensional subspace spanned by the pure state components \( |n⟩ \) and \( |m⟩ \) and \( \eta = |⟨n|U_{nm}|n⟩| = |⟨m|U_{nm}|m⟩| \) is the pure state visibility. In the absence of noise (\( \epsilon = 1 \)) the \( l = 1 \) geometric phases become undefined if \( \eta = 0 \), corresponding to the case where \( |n⟩ \) and \( |m⟩ \) are interchanged. When \( \eta \neq 0 \), we obtain the standard pure state geometric phases \( \gamma^{(1)}_{\rho_n} = \gamma^{(1)}_{\rho_m} = e^{-i\pi/2} \). In the general case (\( 0 < \epsilon < 1 \)), the nodal points, defined as those points in parameter space \((\eta, \epsilon, \Omega)\) where \( \gamma^{(1)}_{\rho_n} \) and \( \gamma^{(1)}_{\rho_m} \) are undefined, are obtained as solutions of

\[ \left( (N - 2)(1 - \epsilon) + \eta(2 + (N - 2)\epsilon) \cos \frac{\Omega}{2} \right)^2 + \eta^2 N^2 \epsilon^2 \sin^2 \frac{\Omega}{2} = 0. \]

For \( N = 2 \) (nondegenerate case), the nodal points are those where \( \eta = 0 \), which is consistent with Refs. \( 27, 28 \), and when \( \eta \neq 0 \) we have

\[ \gamma^{(1)}_{\rho_n} = \gamma^{(1)}_{\rho_m} = \exp \left( -i \arctan \left( \epsilon \tan \frac{\Omega}{2} \right) \right) \]
which is consistent with Refs. [11, 16] by identifying \( \epsilon \) as the length of the Bloch vector. For \( N \geq 3 \) a necessary condition for a nodal point is \( \Omega/2 = (2k+1)\pi \), \( k \) integer, and \( \eta \neq 0 \). For these solid angles, Eq. (24) reduces to

\[
\eta = \frac{(N - 2)(1 - \epsilon)}{2 + (N - 2)\epsilon}.
\]

(29)

Physical solutions (i.e., fulfilling \( \eta \leq 1 \)) of this equation exist provided

\[
\epsilon \geq \frac{N - 4}{2(N - 2)}.
\]

(30)

Thus, for \( N \geq 5 \), there is a lower bound on the amount of noise for the existence of nodal points, i.e., in too noisy input states the \( l = 1 \) geometric phases are always well-defined for this \( U \).

Let us now turn to the \( l = 2 \) geometric phase for \( \rho_n \) and \( \rho_m \). First notice that \( \gamma_{\rho_n, \rho_m}^{(2)} = \gamma_{\rho_m, \rho_n}^{(2)} \), which is due to the symmetry of trace under cyclic permutations. Explicit calculation yields

\[
\gamma_{\rho_n, \rho_m}^{(2)} = \Phi \left[ (N - 2)(1 - \epsilon) + (2 + (N - 2)\epsilon)(-1 + \eta^2) + 2\eta^2 \sqrt{(1 - \epsilon)(1 + (N - 1)\epsilon) \cos \Omega} \right].
\]

(31)

Thus, \( \gamma_{\rho_n, \rho_m}^{(2)} = \pm 1 \), changing sign across a nodal surface in the parameter space \((\epsilon, \eta, \Omega)\). This nodal surface is defined by vanishing argument of \( \Phi \) in Eq. (31), i.e., the solution of

\[
\eta^2 = \frac{2(N - 2)\epsilon - N + 4}{2 + (N - 2)\epsilon + 2\sqrt{(1 - \epsilon)(1 + (N - 1)\epsilon) \cos \Omega}}.
\]

(32)

If \( \cos \Omega \geq 0 \), solutions fulfilling \( \eta \leq 1 \) always exist for all \( N \) as long as Eq. (32) is satisfied. In the case where \( \cos \Omega < 0 \), however, \( 0 \leq \eta^2 \leq 1 \) yields

\[
\frac{N - 4}{2(N - 2)} \leq \epsilon \leq \frac{(N - 2)^2 - 4 \cos^2 \Omega}{4(N - 1) \cos^2 \Omega + (N - 2)^2}.
\]

(33)

Thus, there are nodal points only for the amount of noise satisfying the above equation. In the limiting case \( N = 2 \), the upper bound on \( \epsilon \) is negative and thus no nodal points exist, which is consistent with Refs. [24, 25].

Now we wish to check \( \gamma_{\rho_n, \rho_m}^{(2)} \) at the nodal points of \( \gamma_{\rho_n, \rho_m}^{(1)} = (\gamma_{\rho_n, \rho_m}^{(1)})^* \). For \( N = 2 \) we obtain that the nodal points for \( l = 1 \) and \( l = 2 \) never coincide. For \( N \geq 3 \), insert \( \Omega/2 = (2k+1)\pi \), \( k \) integer, into Eq. (32) and eliminate \( \epsilon \) by using Eq. (20), yielding

\[
\eta^2 + \eta - 1 + \frac{2 \eta^2}{N - 2} \sqrt{\eta(N - 2 - \eta)} = f(\eta, N) = 0
\]

(34)

the solutions of which are the common nodal points of \( \gamma_{\rho_n, \rho_m}^{(2)} \) and \( \gamma_{\rho_n, \rho_m}^{(1)} \). In Fig. 1 we have depicted \( f(\eta, N) \) for \( N = 3, 4, 5, 6 \) and we conclude that there are coinciding nodal points for \( N > 2 \). For these rare parameter values one has to resort to \( l \geq 3 \) geometric phases to retain some information about the geometry of the path in state space.

To measure \( \gamma_{\rho_1, \rho_2}^{(2)} \) we add an ancillary system \( a \) and consider pure states \( |\Psi_n\rangle \in \mathcal{H}_a \otimes \mathcal{H}_a \), \( \dim \mathcal{H}_a = N \), such that the partial trace \( \text{Tr}_a|\Psi_n\rangle\langle\Psi_n| = \rho_n \). For pseudopure states, the purifications take the form

\[
|\Psi_n\rangle = \sqrt{\frac{1 - \epsilon}{N}} \sum_{k \neq n} |k\rangle \otimes |\varphi_k\rangle + \sqrt{\epsilon + \frac{1 - \epsilon}{N}} |n\rangle \otimes |\varphi_n\rangle,
\]

(35)

where \( |\varphi_1\rangle, \ldots, |\varphi_N\rangle \) is an orthonormal basis of \( \mathcal{H}_a \). \( \gamma_{\rho_1, \rho_2}^{(2)} \) may be measured interferometrically as a shift in the interference pattern

\[
\mathcal{I} \propto |U_s \otimes U_a|\langle\Psi_n| + V_s \otimes V_a|\Psi_n\rangle|^2
\]

by choosing \( U_s = e^{i\chi W^{m-n}} \), \( V_s = U_s^\dagger \), \( U_a = W^{m-n} \), and \( V_a = (U_a^\dagger)^T \), \( T \) being transpose with respect to the ancilla basis \( |\varphi_1\rangle, \ldots, |\varphi_N\rangle \) and \( \chi \) a variable \( U(1) \) phase shift.

In liquid-state NMR, such a test could in principle be implemented as follows. By adding an ‘auxiliary’ nuclear spin qubit pair in the state \( |0\rangle \otimes |0\rangle \), prepare the total input

\[
|\Gamma\rangle = |0\rangle \otimes |0\rangle \otimes |\Psi_n\rangle. \quad (37)
\]

Apply \( H \otimes H \otimes I_s \otimes I_s \), \( H \) being Hadamard on each auxiliary qubit, followed by the conditional transformation

\[
U_c = |0\rangle\langle 0| \otimes |0\rangle\langle 0| \otimes U_s \otimes U_a + |1\rangle\langle 1| \otimes |1\rangle\langle 1| \otimes V_s \otimes V_a. \quad (38)
\]
with $U_s, U_a, V_s,$ and $V_a$ chosen as above. Finally, apply another Hadamard transform on the auxiliary qubits and measure the output in the 00 channel. The resulting intensity should confirm Eq. 38.

V. CONCLUSIONS

We have put forward a kinematic approach to the off-diagonal geometric phases of pure states 23 and nondegenerate mixed states 27, 28. The kinematic approach to off-diagonal geometric phases presented in this paper emphasizes the path in state space as the primary concept for the geometric phase and provides a tool to efficiently calculate off-diagonal geometric phases for arbitrary unitary operators and arbitrary density matrices. We have extended the concept of off-diagonal geometric phases of nondegenerate mixed states to degenerate mixed states. This kind of extension is essential since the geometric phase of degenerate mixed states 12 is undetermined in the case where the interference visibility between the initial and final states vanishes leading to an interesting nodal point structure in the experimental parameter space that could be monitored in a history-dependent manner. On the other hand, the notion of off-diagonal geometric phase put forward for nondegenerate mixed state in Refs. 27, 28 breaks down in the case of degenerate mixed states, while the latter case does really include the most general quantum states and therefore this extension is physically important. Our extension makes it possible to obtain information of the geometry along the path in state space when the standard notion of geometric phase for degenerate density operators is undetermined. We have argued that liquid-state NMR protocols constitute a possible physical scenario for test of off-diagonal geometric phases for degenerate mixed quantal states.

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[31] By saying that the unitarily connected mixed states $\rho_1, \ldots, \rho_i$ have the same degeneracy structure, we mean that an eigenvector $|\psi\rangle$ of $\rho_i$ corresponding to an $m_i$-fold degenerate eigenvalue $\lambda_i$ is also an eigenvector of $\rho_{i'} \neq \rho_i$ corresponding to an $m_{i'}$-fold degenerate eigenvalue $\lambda_{i'}$. Note that $\lambda_i \neq \lambda_{i'}$, in general.