Non-Abelian Generalization of Off-Diagonal Geometric Phases

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If a quantum system evolves in a noncyclic fashion the corresponding geometric phase or holonomy may not be fully defined. Off-diagonal geometric phases have been developed to deal with such cases. Here, we generalize these phases to the non-Abelian case, by introducing off-diagonal holonomies that involve evolution of more than one subspace of the underlying Hilbert space. Physical realizations of the off-diagonal holonomies in adiabatic evolution and interferometry are put forward.

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A quantal system that fails to return to its initial state after some prescribed elapse of time may acquire a well-defined geometric phase. An interesting feature of this noncyclic geometric phase is that it becomes undefined when the initial and final states are orthogonal. This gives rise to a nodal point structure that can be monitored experimentally in a history-dependent manner.

In the hope to recover some of the lost interference information at the nodal points of the noncyclic geometric phase, Manini and Pistolesi introduced off-diagonal geometric phases for adiabatic evolutions of pure states. These quantities may be defined in cases where the standard geometric phase is not. The adiabatic requirement on the evolution in Ref. was lifted by Mukunda et al., and Hasegawa et al. provided an experimental verification of the second order off-diagonal geometric phase for neutron spin. Theories for off-diagonal phases and holonomies for mixed quantal states have been developed.

Wilczek and Zee showed that the geometric phase factor generalizes to a unitary state change, often referred to as a non-Abelian quantum holonomy, when considering cyclic adiabatic evolution governed by a degenerate Hamiltonian. The relevance of non-Abelian holonomies for universal fault tolerant quantum computation has been demonstrated in Refs. The non-Abelian quantum holonomies have been generalized to nonadiabatic, discrete, and noncyclic evolutions. As for the geometric phase, the holonomy may be undefined when the evolution is noncyclic. In the non-Abelian case we also have the additional possibility that the holonomy is partially defined.

In this Letter, we extend Ref. and introduce non-Abelian off-diagonal holonomies. We demonstrate that the off-diagonal holonomies retain holonomy information when the standard noncyclic ones are undefined.

We also provide physical realizations of the off-diagonal holonomies in adiabatic evolution and interferometry. Consider a smoothly parameterized partitioning

$$H = H_1(s) + \cdots + H_\eta(s), \ s \in [0,1],$$

of an N-dimensional Hilbert space $H$ into $\eta$ mutually orthogonal subspaces. Assume that $\dim[H_\ell(s)] = n_\ell, \ \forall s \in [0,1], \ l = 1, \ldots, \eta$. Thus, each family $H_\ell(s)$ of subspaces defines a curve $C_\ell$ in the Grassmann manifold $G(N; n_\ell)$, i.e., the set of $n_\ell$-dimensional subspaces in the N-dimensional Hilbert space. For each such curve, we introduce the quantities

$$\Gamma_\ell = \lim_{\delta s \to 0} P_\ell(1)P_\ell(1 - \delta s) \cdots P_\ell(\delta s)P_\ell(0),$$

where $P_\ell(s)$ is the projection operator onto the subspace $H_\ell(s)$, and

$$\sigma_{kl} = P_k(0)\Gamma_l.$$  

Let $\{|k^{(s)}\rangle\}_{s=1}^{n_k}$ and $\{|l^{(s)}\rangle\}_{s=1}^{n_l}$ be orthonormal bases for subspaces $H_k(s)$ and $H_l(s)$, respectively, in terms of which

$$\sigma_{kl} = \sum_{ij} (\mathcal{F}_0^k|\mathcal{F}_1^l)^\dagger A_i(s)_{ij} |k^{(0)}\rangle \langle l^{(0)}|$$

$$= \sum_{ij} |A_{ij}^{kl}(s)|^2 |k^{(0)}\rangle \langle l^{(0)}|.$$  

Here, $(\mathcal{F}_0^k|\mathcal{F}_1^l)$ is a $n_k \times n_l$ matrix with components $(\mathcal{F}_0^k|\mathcal{F}_1^l)_{ij} = \langle k^{(0)}|l^{(1)}\rangle$ and $[A_i(s)]_{ij} = \langle \partial_s l^{(s)}|l^{(s)}\rangle$ is the Wilczek-Zee connection along $C_\ell$ in $G(N; n_\ell)$.

The unitary part $\Phi[\sigma^{kl}]$ is associated with the (open) path $C_\ell$. It seems natural to ask whether we can interpret the matrices $\sigma^{kl}, \ k \neq l$, in a similar fashion. To answer this, we need to see how these matrices behave under a gauge transformation, i.e., a change of frames $|l^{(s)}\rangle \to |\tilde{l}^{(s)}\rangle = \sum_i U_i(s)_{ij} |l^{(s)}\rangle$, where $\{|U_i(s)\rangle\}_{i=1}^{n_\ell}$ are unitary matrices. Under such a transformation the matrices $Pe^{|A_i(s)\rangle \langle l^{(s)}|}$ and $(\mathcal{F}_0^k|\mathcal{F}_1^l)$ undergo the following

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changes
\[ P_C e^{i\int_0^1 A_i(s)ds} \rightarrow U_1^1(1) P_C e^{i\int_0^1 A_i(s)ds} U_1(0), \]
\[ \langle F^0_0|F^1_1 \rangle \rightarrow U^1_k(0) \langle F^0_0|F^1_1 \rangle U_1(1). \] (5)
Consequently, \( \sigma^{kl} \) transforms as
\[ \sigma^{kl} \rightarrow U^1_k(0) \sigma^{kl} U_1(0), \] (6)
i.e., noncovariantly unless \( k = l \). Thus, the matrix \( \sigma^{kl} \), \( k \neq l \), fail to reflect the geometry of the path \( C_l \). However, the specific behavior of \( \sigma^{kl} \) under gauge transformations suggests that we consider the operator
\[ \gamma_{l_1 \ldots l_\nu} = \sigma_{l_1 \nu} \sigma_{l_\nu l_{\nu-1}} \cdots \sigma_{l_2 l_1}, \]
\[ = \sum_{i,j} \langle \gamma^{l_1 \ldots l_\nu} \rangle_{ij} \langle l_i^1(0) \rangle \langle l_i^1(0) \rangle, \] (7)
where \( \gamma^{l_1 \ldots l_\nu} \) is the matrix
\[ \gamma^{l_1 \ldots l_\nu} = \sigma^{l_1 l_\nu} \sigma^{l_\nu l_{\nu-1}} \cdots \sigma^{l_2 l_1}. \] (8)
We can use these operators and matrices of this kind to define gauge covariant quantities, since \( \Phi_1^{\gamma^{l_1 \ldots l_\nu}} \rightarrow U_1^1(0) \Phi_1^{\gamma^{l_1 \ldots l_\nu}} U_1(0) \) from Eq. (6). Thus, we propose to take
\[ U^{(\nu)}_g[C_1, \ldots, C_\nu] = \Phi_1^{\gamma^{l_1 \ldots l_\nu}} \] (9)
as the gauge covariant non-Abelian holonomies of order \( \nu \), and thus generalizing the approach of Ref. [2] to the non-Abelian case. We extend the range of \( \nu \) by defining \( U^{(1)}_g[C_l] = \Phi_1^{\sigma^{ll}} \).

Note that the definition in Eq. (9) allows any sequence \((l_1, \ldots, l_\nu)\). This includes cases like, e.g., \( \gamma^{111} \), which is difficult to regard as an “off-diagonal” object. Hence, Eq. (9) can be regarded as a general definition of holonomies of degree \( \nu \), both diagonal and off-diagonal. To define genuinely off-diagonal holonomies we obtain a reasonable subclass if we require that \((l_1, \ldots, l_\nu)\) contains each number at most once. We let \( \nu^O \) denote all vectors \((l_1, \ldots, l_\nu)\) with \( l_j \in \{1, \ldots, \eta\} \), such that none of the numbers occurs twice, e.g., \((2, 5, 3) \in \nu^O \) but \((6, 4, 6, 2) \notin \nu^O \). We refer to the set of holonomies \( U^{(\nu)}_g[C_1, \ldots, C_\nu] \) with \((l_1, \ldots, l_\nu) \in \nu^O \) for \( 2 \leq \nu \leq \eta \), as “strictly off-diagonal holonomies”.

For a cyclic evolution, characterized by \( \mathcal{H}_l(1) = \mathcal{H}_l(0), \ l = 1, \ldots, \eta \), the standard holonomies \( U^{(1)}_g[C_l] \) are fully defined. On the other hand, in this case we have \( \gamma^{l_1 \ldots l_\nu} = 0 \), \((1, \ldots, l_\nu) \in \nu^O, \nu \geq 2 \), which implies that all strictly off-diagonal holonomies are undefined for cyclic evolution. Thus, just as in the Abelian case [3], the standard holonomies contain all nontrivial information about \( C_1, \ldots, C_\eta \) when these are loops.

In the case where \( n_l = 1, \ l = 1, \ldots, \eta \), the matrices \( \langle F^0_0|F^1_1 \rangle \) and \( P_C e^{i\int_0^1 A_i(s)ds} \) reduce to the complex numbers \( \langle k(0)\rangle l(1) \rangle \) and \( e^{-\int_0^1 \langle l(0)\rangle \delta l(s) \rangle ds} \), respectively. This leads to the off-diagonal geometric phase factors
\[ U^{(\nu)}_g[C_1, \ldots, C_\nu] = \Phi_1^{\langle l(0)\rangle l(1) \rangle \times e^{-\int_0^1 \langle l(0)\rangle \delta l(s) \rangle ds} \times \ldots \times e^{-\int_0^1 \langle l(2)\rangle l(1) \rangle \times \ldots \times e^{-\int_0^1 \langle l(\nu)\rangle l(1) \rangle}, \] (10)
which coincide with \( \Phi_1^{\gamma^{l_1 \ldots l_\nu}} \) in Ref. [3].

Manini and Pistolesi [3] suggest an interpretation of their off-diagonal geometric phases in terms of Berry phases for single closed paths. In the second order case, these paths consist of the segments \( C_k \), \( C_l \), and the geodesics \( G_{kl} \), and \( G_{lk} \), where \( G_{kl} \) connects the final point of \( C_k \) with the starting point of \( C_l \), and vice versa for \( G_{lk} \) (see Fig. 1 of Ref. [3]). In the general non-Abelian case, however, this interpretation is difficult to maintain. Apart from the special case when \( n_1 = n_2 = \ldots = n_\nu \), it is not possible to join the curves \( C_1, \ldots, C_\nu \), due to the mismatch of dimensions, and thus the closure using geodesics is not applicable.

Another consequence of the fact that we can have different \( n_l \) is that the rank of \( \gamma^{l_1 \ldots l_\nu} \) cannot be larger than the smallest \( n_l \) (see 2.17.8 of Ref. [17]), and thus may be less than \( n_l \). The non-Abelian character of the off-diagonal holonomies \( U^{(\nu)}_g[C_1, \ldots, C_\nu] \) implies that they are not invariant under cyclic permutations of the indexes \((l_1, \ldots, l_\nu)\). It may even be the case that two off-diagonal holonomies that differ only by a cyclic permutation have different rank, since the smallest \( n_l \) only provides an upper bound for the rank of \( \gamma^{l_1 \ldots l_\nu} \). Furthermore, as is exemplified below it is also possible that \( \sigma^{l_1 \ldots l_\nu} \) may have path dependent nodal points if \( \kappa \geq 2 \).

Let us now analyze what happens if the rank of some of the overlap matrices \( \langle F^0_0|F^1_1 \rangle \) is less than their subspace dimension \( n_l \). This is a situation where the corresponding holonomies become partial [12]. To aid us in this analysis we introduce the unitary \( N \times N \) matrix
\[ S_{tot} = \begin{pmatrix} \sigma^{l_1} & \cdots & \sigma^{l_\eta} \\ \vdots & \ddots & \vdots \\ \sigma^{l_1} & \cdots & \sigma^{l_\eta} \end{pmatrix}. \] (11)
It follows from unitarity that \( R(S_{tot}) = N \), where \( R(X) \) denotes the rank of matrix \( X \). Furthermore, for every \( l = 1, \ldots, \eta \), it holds that \( \sum_k \langle l|\sigma^{lk} \rangle \langle \sigma^{lk}|l \rangle = \sum_k \langle l|\sigma^{lk} \rangle \sigma^{lk} = 1_{n_l \times n_l} \), where \( 1_{n_l \times n_l} \) denotes the \( n_l \times n_l \) identity matrix. This entails that (see 2.17.2 and 2.17.5 of Ref. [17])
\[ \sum_k R(\sigma^{lk}) \geq n_l \text{ and } \sum_k R(\sigma^{lk}) \geq n_l. \] So, if \( R(\sigma^{lk}) = n_l - n \), then \( \sum_k R(\sigma^{lk}) \geq n \) and \( \sum_k R(\sigma^{lk}) \geq n \). In other words, when the overlap matrix \( \langle F^0_0|F^1_1 \rangle \) decreases by \( n_l \) in rank, the lower bound for the sum of the ranks of the matrices \( \sigma^{kl} \) increases by the same amount. Thus, the “holonomy information” that is lost when the holonomy of the curve \( C_l \) becomes partial is transferred to the matrices \( \sigma^{kl} \).
A perhaps more significant question is whether the rank of the matrices $\gamma_{l_1\ldots l_\kappa}$ depends on the rank of the overlap matrix $(F_0^i|F_i^j)$ in a manner similar to what was discussed above for the matrices $\sigma^{kl}$. One can demonstrate with a simple counterexample that no such relation exists. Assume $\eta = 3$ and $n_1 = n_2 = n_3 = 2$. Furthermore, assume that $\sigma^{13}, \sigma^{21},$ and $\sigma^{32}$ are the $2 \times 2$ zero matrix, and

$$\sigma^{11} = \sigma^{22} = \sigma^{33} = \sigma^{12} = \sigma^{23} = \sigma^{31} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$ 

One may verify that the corresponding matrix $S_{\text{tot}}$ is unitary. In this example $\gamma_{l_1l} = 0$, $\forall (k, l) \in \mathbb{I}_2^n$, and $\gamma_{l_1\ldots l_\kappa} = 0$, $\forall (k, l, m) \in \mathbb{I}_2^n$. Hence, although none of the overlap matrices $(F_0^i|F_i^j)$ are of full rank, all strictly off-diagonal holonomies are undefined.

Now, we ask what happens if the matrices $\sigma^{kl}$ are zero for all $l = 1, \ldots, \eta$. We prove by reductio ad absurdum that at least one of the strictly off-diagonal $\gamma$'s must have nonzero rank. Assume $\sigma^{kl} = 0$, for $l = 1, \ldots, \eta$, and $\gamma_{l_1\ldots l_\kappa} = 0$, for $(l_1, \ldots, l_\kappa) \in \mathbb{I}_2^n$, $\kappa \geq 2$. Consider an arbitrary string $(l_1, \ldots, l_\nu)$ consisting of the integers 1 to $\eta$, and with $\nu \geq 2$. If $(l_1, \ldots, l_\nu) \in \mathbb{I}_2^n$ ($\nu \leq \eta$), then by assumption $\gamma_{l_1\ldots l_\nu} = 0$. If $(l_1, l_\nu) \notin \mathbb{I}_2^n$, then take one of the smallest subsequences $(l_{a}, l_{a+1}, \ldots, l_{b-1}, l_{b})$ that begins and ends with the same number (i.e., $l_b = l_a$). This subsequence there is no other repetitions (otherwise there exists a smaller subsequence). It follows that $\gamma_{l_1\ldots l_\nu} = \gamma_{l_{a+1}l_a\ldots l_{b-1}l_b} = \cdots = \gamma_{l_1\ldots l_b} = 0$ by assumption. We proceed by noting that

$$\text{Tr}(S_{\text{tot}}^\nu) = \sum_{(l_1, \ldots, l_\nu)} \text{Tr}(\gamma_{l_1\ldots l_\nu}) = 0,$$

for all $\nu = 1, 2, \ldots, \eta$, as a consequence of our assumptions. However, this cannot be the case since $S_{\text{tot}}$ is a unitary matrix. Therefore, our assumptions must be wrong, and at least one of the strictly off-diagonal $\gamma$'s must have nonzero rank.

We illustrate the off-diagonal holonomies by an example in the adiabatic context. We let the system evolve under the action of a slowly varying Hamiltonian. Let us consider the triad system modeled by the parameter dependent four-state Hamiltonian

$$H(s) = \omega |e)(\sin \theta |e| + \sin \phi |\varphi(s)| + \cos \theta |s\rangle \langle a| + \text{h.c.},$$

exhibiting two nondegenerate 'bright' states $|F_+\rangle = \{|B^\pm(s)\rangle\}$ with energy $\pm \omega$ and a doubly degenerate 'dark' zero energy subspace $|F_0\rangle = \{|D^1(s)\rangle, |D^2(s)\rangle\}$. Explicitly, we may choose

$$|B^\pm\rangle = \frac{1}{\sqrt{2}} \left( |e\rangle + \sin \theta |e\rangle + \sin \phi |s\rangle + \cos \phi |\varphi(s)\rangle \pm \cos \theta |s\rangle \right),$$

$$|D^1\rangle = \cos \theta |e\rangle + \cos \phi |\varphi(s)\rangle - \sin \theta |s\rangle,$$

$$|D^2\rangle = -\sin \phi |s\rangle + \cos |e\rangle.$$ 

Consider paths $0,0 \rightarrow (\theta_1, \phi_1)$ in parameter space $(\theta, \phi)$. For each such path the energy eigenstates define paths $C_\pm$ in $G(4;1)$ and $C_0$ in $G(4;2)$. We obtain

the geometric phase factors $U^{(1)}[C_\pm] = 1$ for $\theta_1 \neq \pi$ and $U^{(2)}[C_\pm, C_\mp] = 1$ for $\theta_1 \neq 0$. $U^{(1)}[C_\pm]$ are undefined at $\theta_1 = \pi$ and similarly $U^{(2)}[C_\pm, C_\mp]$ at $\theta_1 = 0$. In Ref. [12] it was shown that $U^{(1)}[C_\pm]$ is fully defined, except when the path ends at $\theta_1 = \pi/2$, where the holonomy becomes partial. The strictly off-diagonal holonomies involving the dark subspace are undefined when $\sin \theta_1 = 0$. For $\sin \theta_1 \neq 0$, let $Z = \int_0^\phi \sin \theta \rho(s)ds$ and we obtain

$$U^{(2)}[C_\mp, C_d] = -U^{(3)}[C_\pm, C_\mp, C_d] = -\frac{\cos \varphi - Z}{\cos(\varphi - Z)},$$

$$U^{(3)}[C_d, C_{\mp}, C_{\mp}] = -\frac{\cos Z \cos \varphi + \sin Z \cos \varphi}{\cos Z \sin \varphi}.$$

While $U^{(2)}[C_d, C_{\mp}]$ and $U^{(3)}[C_d, C_\pm, C_{\mp}]$ are nonzero partial isometries, there are path dependent nodal points of $U^{(2)}[C_d, C_d]$, $U^{(3)}[C_\pm, C_\mp, C_d]$, and $U^{(3)}[C_\pm, C_d, C_{\mp}]$, namely where $\cos(\varphi - Z) = 0$.

Let us now examine possible experimental realizations of $U^{(3)}_g[C_\pm, C_\pm]$. Consider the Mach-Zehnder interferometer in FIG. [1] with the two path states represented...
by $|0\rangle$ and $|1\rangle$. We let the internal state of the particle (e.g., spin) be represented by the Hilbert space $\mathcal{H}$. Let $U$ on $\mathcal{H}$ be the total unitary evolution caused by an adiabatic evolution of a time-dependent Hamiltonian. We can then write $U = \sum_i e^{i\phi_i} \Gamma_i$, where $\phi_i$ is the dynamical phase $\phi_i = \int_0^s E_i(s)\,ds$, and $E_i(s)$ the eigenvalue corresponding to eigenspace $\mathcal{H}_i(s)$ of the Hamiltonian. The total system is prepared in the state $|0\rangle\langle 0| \otimes P_1(0)/n_1$. We first apply a beam-splitter, followed by the unitary operations $|0\rangle\langle 0| \otimes U + |1\rangle\langle 1| \otimes V$, and $|0\rangle\langle 0| \otimes U + |1\rangle\langle 1| \otimes P$, where $V$ is a variable unitary operator assumed to be chosen such that $[V, P_{1}(0)] = 0$ for all $l$. Next, we perform a filtering corresponding to the projection operator $|0\rangle\langle 0| \otimes P_{l}(0) + |1\rangle\langle 1| \otimes \mathbb{1}$, i.e., the particle is “removed” if it is found in path 0 with its internal state outside subspace $\mathcal{H}_2$. Thereafter, we again apply the adiabatic evolution $|0\rangle\langle 0| \otimes U + |1\rangle\langle 1| \otimes \mathbb{1}$, and the filtering $|0\rangle\langle 0| \otimes P_{l}(0) + |1\rangle\langle 1| \otimes \mathbb{1}$. This procedure is repeated until we have applied the adiabatic evolution $n$ times. After this, we apply a final filtering $|0\rangle\langle 0| \otimes P_{l}(0) + |1\rangle\langle 1| \otimes \mathbb{1}$, and recombine the two paths with a beam splitter. We finally measure the probability $p$ to find the particle in path 0. This probability becomes

$$p = \frac{1}{4} + \frac{1}{4n_1} \text{Tr}(\gamma_{l_1} ... \gamma_{l_n}^T \gamma_{l_1} ... \gamma_{l_n})$$

$$+ \frac{1}{4n_1} \text{Re}[e^{i\sum_{k=1}^n \phi_k \text{Tr}(\gamma_{l_1} ... \gamma_{l_n} V_{ij})}],$$

(14)

where $V_{ij} = \langle l^i_1|0\rangle\langle 0| l^j_1\rangle$. Note that $V$ is a unitary matrix since $[V, P_{1}(0)] = 0$. By varying $V$ we find that the maximal detection probability is obtained when $V = e^{i\sum_{k=1}^n \phi_k U_g^{(s)}(C_{l_1}, ..., C_{l_n})}$. Hence, up to the dynamical phases we have found the holonomy.

One can consider an alternative approach based entirely on filtering, where we approximate the evolution in the spirit of Eq. (2). This procedure has the advantage that it does not generate any dynamical phase. We begin with the same initial state, beam-splitter, and variable unitary $V$, as in the previous case. Next we apply a sequence of filterings $|0\rangle\langle 0| \otimes P_{l}(s_j) + |1\rangle\langle 1| \otimes \mathbb{1}$, where $s_j$ forms a discretization of the interval $[0, 1]$. For the next step we apply the sequence of filterings $|0\rangle\langle 0| \otimes P_{l}(s_j) + |1\rangle\langle 1| \otimes \mathbb{1}$, and we continue up $l_k$. We finally apply $|0\rangle\langle 0| \otimes P_{l}(0) + |1\rangle\langle 1| \otimes \mathbb{1}$, followed by a beam splitter, and measure the probability to find the particle in path 0. One can show that the probability is as in Eq. (14) apart from that the dynamical phases do not appear.

In conclusion, noncyclic evolution of quantum systems may lead to well-defined off-diagonal holonomies that involve more than one subspace of Hilbert space. These holonomies reduce to the off-diagonal geometric phases in Ref. [2] for one-dimensional subspaces. The set of off-diagonal holonomies are undefined for cyclic evolution but must contain members of nonzero rank when all the standard holonomies are undefined. While the nodal point structure of the holonomy for an open continuous path can only depend on the end-points of the path, this structure can be path dependent in the off-diagonal case. Furthermore, we have put forward physical realizations of the off-diagonal holonomies in the context of adiabatic evolution and interferometry that may open up the possibility to test these quantities experimentally.

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[14] For a matrix $Z$, $\Phi[Z] \equiv (\sqrt{Z})^T \sqrt{Z}$, $\otimes$ being the Moore-Penrose pseudoinverse obtained by inverting all nonzero eigenvalues of $\sqrt{Z}$. If $\det \sqrt{Z} \neq 0$ then the MP pseudoinverse of $\sqrt{Z}$ coincides with the inverse.