Noncyclic geometric changes of quantum states

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(Received 6 December 2005; revised manuscript received 5 June 2006; published 25 August 2006)

Non-Abelian quantum holonomies, i.e., unitary state changes solely induced by geometric properties of a quantum system, have been much under focus in the physics community as generalizations of the Abelian Berry phase. Apart from being a general phenomenon displayed in various subfields of quantum physics, the use of holonomies has lately been suggested as a robust technique to obtain quantum gates; the building blocks of quantum computers. Non-Abelian holonomies are usually associated with cyclic changes of quantum systems, but here we consider a generalization to noncyclic evolutions. We argue that this open-path holonomy can be used to construct quantum gates. We also show that a structure of partially defined holonomies emerges from the open-path holonomy. This structure has no counterpart in the Abelian setting. We illustrate the general ideas using an example that may be accessible to tests in various physical systems.

DOI: 10.1103/PhysRevA.74.022106 PACS number(s): 03.65.Vf, 03.67.Lx

I. INTRODUCTION

Berry's discovery [1] of geometric phase factors associated with slowly changing external parameters initiated intense studies of geometric phase effects in quantum mechanics. Wilczek and Zee [2] extended Berry's work by pointing out the existence of geometric effects as a generic feature of quantum adiabatic evolution. They showed that the Abelian geometric phase factors generalize to unitary state changes, often referred to as non-Abelian quantum holonomies, in the case of Hamiltonians with degeneracies. Such effects have been shown to occur in a variety of systems, ranging from molecules [3,4] and extended systems [5] to atomic nuclei [6,7] and fields [8]. Lately, the interest in holonomies has been refueled due to the insight that they can be used to implement fault tolerant quantum gates [9,10]. This has led to work on holonomy effects for implementations of quantum computation [11–15] and quantum information [16–19].

In the aforementioned work, holonomy is associated only to loops, i.e., to closed paths of slowly changing parameters. But what happens if the path is not closed? In this work, we address this question and propose an approach to noncyclic non-Abelian holonomies.

Above we have used the language of parameter dependent Hamiltonians in order to describe the emergence of holonomies, where the motion of the eigenspaces of the Hamiltonian gives rise to the holonomy. However, the Hamiltonian is not a necessary component. We may instead consider just a subspace moving in the total Hilbert space of the system. As above, this moving subspace can be realized as an eigenspace of a Hamiltonian, but could alternatively be achieved through a sequence of projective measurements of observables with the subspace as an eigenspace. We use this more general "subspace approach" in our definition of open-path holonomy, and extend Ref. [20] to the non-Abelian case. However, in order to connect with more familiar settings, we also present the open-path holonomy in terms of parallel transport, as well as resulting from adiabatic evolution of parameter dependent Hamiltonians.

Our generalized holonomy contains previous notions, such as that of Ref. [2] in the case of cyclically evolving Hamiltonians, and that of Ref. [21] for particular paths associated with the dynamical invariants of a Hamiltonian. We further demonstrate a concept of open-path holonomic quantum gates that may be of use in the context of quantum information processing. Finally we demonstrate that for some relative orientations of the initial and final subspaces of the open path, the holonomy is only partially defined. This we call partial holonomy; a phenomenon that has no counterpart in the Abelian case.

II. OPEN PATH HOLONOMY

Consider a smooth curve $\mathcal{C}$ in the Grassmann manifold $\mathcal{G}(N;K)$ [22], i.e., the set of K-dimensional subspaces in an N-dimensional Hilbert space. The holonomy for subspaces should only depend on the properties of this curve. There is a natural bijection between the Grassmann manifold and the collection of projectors of rank K. Thus, corresponding to our curve $\mathcal{C}$ in the Grassmann manifold, we may define a curve $P(s)$ being a family of projectors parametrized by $s \in [0,1]$. Let us now construct the intrinsically geometric quantity

$$\Gamma = P(1)P(1-\delta s)\cdots P(\delta s)P(0), \tag{1}$$

where δs is the step size in a discretization of the curve. We are interested in the operator Γ in the limit of small δs. In order to find an expression for Γ in this limit we let $\{|a_k(s)\rangle\}_{k=1}^{K}$ be an orthonormal basis of the subspace $\mathcal{C}(s)$, for each s, and we assume that this family of bases is chosen in a smooth way. Note that

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$$P(s+\delta s)P(s) = \sum_{kl} [\boldsymbol{B}(s)]_{kl} |a_k(s+\delta s)\rangle\langle a_l(s)|, \tag{2}$$

where $[\boldsymbol{B}(s)]_{kl} = \delta_{kl} + \delta s \langle \dot{a}_k(s) | a_l(s)\rangle$. This allows us to rewrite Γ as

$$\Gamma = \sum_{kl} [\boldsymbol{B}(1-\delta s)\boldsymbol{B}(1-2\delta s)\cdots\boldsymbol{B}(0)]_{kl} |a_k(1)\rangle\langle a_l(0)|. \tag{3}$$

We observe that to the first order in δs, $\boldsymbol{B}(s) = \mathbf{1} + \delta s \boldsymbol{A}(s) = \exp(\delta s \boldsymbol{A}(s))$, where $\mathbf{1}$ is the $K \times K$ unit matrix and

$$[\boldsymbol{A}(s)]_{kl} = \langle \dot{a}_k(s) | a_l(s)\rangle. \tag{4}$$

Hence, in the limit $\delta s \to 0$, we obtain

$$\Gamma = \sum_{kl} [\boldsymbol{P} e^{\int_0^1 \boldsymbol{A}(s)ds}]_{kl} |a_k(1)\rangle\langle a_l(0)|, \tag{5}$$

where $\boldsymbol{P}$ denotes path ordering.

A gauge transformation is a change of frames

$$|a_k(s)\rangle \to |a_k'(s)\rangle = \sum_l [\boldsymbol{U}(s)]_{lk} |a_l(s)\rangle, \tag{6}$$

$\boldsymbol{U}(s)$ being a unitary matrix. The set of K-frames, i.e., ordered orthonormal K-tuples in an N-dimensional Hilbert space, forms the Stiefel manifold [22]. The Stiefel manifold can be regarded as a fiber bundle with the Grassmannian as base manifold and with the set of $K \times K$ unitary matrices as fibers. The gauge transformation given by Eq. (6) can be seen as a motion along the fiber over a point $\mathcal{C}(s)$ in the Grassmannian.

The quantity Γ is manifestly gauge invariant. On the other hand, the matrix $\boldsymbol{P} e^{\int_0^1 \boldsymbol{A}(s)ds}$ transforms as

$$\boldsymbol{P} e^{\int_0^1 \boldsymbol{A}(s)ds} \to \boldsymbol{U}^\dagger(1) \boldsymbol{P} e^{\int_0^1 \boldsymbol{A}(s)ds} \boldsymbol{U}(0). \tag{7}$$

Hence, the eigenvalues of $\boldsymbol{P} e^{\int_0^1 \boldsymbol{A}(s)ds}$ are not gauge invariant [2,23] since we may have $\boldsymbol{U}(1) \neq \boldsymbol{U}(0)$. In order to deal with this we must somehow find a way to relate the initial and final frames. This can be achieved by introducing the concept of parallel frames [24–27].

Given a fixed K-frame $\mathcal{A} = \{|a_k\rangle\}_{k=1}^K$ in the subspace $\mathcal{L}_a$ we wish to find a K-frame $\mathcal{B} = \{|b_k\rangle\}_{k=1}^K$ in the subspace $\mathcal{L}_b$ that in some sense is as parallel as possible to $\mathcal{A}$. A reasonable approach would be to minimize the following function over all possible choices of $\mathcal{B}$

$$D(\mathcal{A},\mathcal{B}) = \sum_{k=1}^K \| |a_k\rangle - |b_k\rangle \|^2 = 2K - 2\mathrm{Re\ Tr}\, \boldsymbol{M}(\mathcal{A},\mathcal{B}), \tag{8}$$

where

$$[\boldsymbol{M}(\mathcal{A},\mathcal{B})]_{kl} = \langle a_k | b_l\rangle. \tag{9}$$

Thus, in order to minimize $D(\mathcal{A},\mathcal{B})$ we have to maximize $\mathrm{Re\ Tr}\, \boldsymbol{M}(\mathcal{A},\mathcal{B})$, where it is assumed that $\mathcal{B}$ spans over all possible K-frames of $\mathcal{L}_b$. We refer to the matrix $\boldsymbol{M}(\mathcal{A},\mathcal{B})$ as the overlap matrix.

Let $\tilde{\mathcal{B}} = \{|\tilde{b}_k\rangle\}_{k=1}^K$ be some arbitrary but fixed K-frame of $\mathcal{L}_b$. Every other K-frame $\mathcal{B}$ of $\mathcal{L}_b$ we may write as a unitary transformation of the elements of $\tilde{\mathcal{B}}$. All possible overlap matrices can thus be written as $\boldsymbol{M}(\mathcal{A},\mathcal{B}) = \boldsymbol{M}(\mathcal{A},\tilde{\mathcal{B}})\boldsymbol{V}$, where $\boldsymbol{V}$ spans over the set of unitary $K \times K$ matrices. Let $\boldsymbol{M}(\mathcal{A},\tilde{\mathcal{B}}) = \boldsymbol{R}\boldsymbol{U}_M$, with $\boldsymbol{R}$ positive semidefinite ($\boldsymbol{R} \geq 0$)and $\boldsymbol{U}_M$ unitary, be a polar decomposition [28]. If $\boldsymbol{R}$ is positive definite ($\boldsymbol{R} > 0$), then its inverse $\boldsymbol{R}^{-1}$ exists and $\boldsymbol{U}_M$ is unique and can be constructed as $\boldsymbol{U}_M = \boldsymbol{R}^{-1}\boldsymbol{M}(\mathcal{A},\tilde{\mathcal{B}})$.

Note that the positive definiteness of $\boldsymbol{R}$ is a property of the pair of subspaces $\mathcal{L}_a$ and $\mathcal{L}_b$, and not a property of the specific choice of frames. In the following we say that two subspaces $\mathcal{L}_a$ and $\mathcal{L}_b$ are overlapping if, for any choice of frames, the positive part $\boldsymbol{R}$ of the overlap matrix is positive definite. One may note that this equivalently could be stated as the overlap matrix having K nonzero singular values [28]. In the case when the number of nonzero eigenvalues of $\boldsymbol{R}$ is greater than zero but less then K, we say the two subspaces are partially overlapping. If all the eigenvalues of $\boldsymbol{R}$ are zero, the two subspaces are orthogonal.

In the case when the two subspaces are overlapping one can show that the maximum of $\mathrm{Re\ Tr}\,(\boldsymbol{M}(\mathcal{A},\tilde{\mathcal{B}})\boldsymbol{V})$ is obtained if we choose $\boldsymbol{V} = \boldsymbol{U}_M^\dagger$. Thus, the optimal choice of K-frame $\bar{\mathcal{B}}$ is uniquely determined as

$$|\bar{b}_k\rangle = \sum_l [\boldsymbol{U}_M]_{kl}^* |\tilde{b}_l\rangle. \tag{10}$$

It follows that

$$\inf_{\mathcal{B}} D(\mathcal{A},\mathcal{B}) = 2K - 2\,\mathrm{Tr}\sqrt{\boldsymbol{M}(\mathcal{A},\bar{\mathcal{B}})\boldsymbol{M}^\dagger(\mathcal{A},\bar{\mathcal{B}})} \tag{11}$$

with $\boldsymbol{M}(\mathcal{A},\bar{\mathcal{B}}) = \boldsymbol{R}$. An alternative route to find the parallel frame in Eq. (10) is to note that the overlap matrix $\boldsymbol{M}(\mathcal{A},\mathcal{B}) > 0$ if and only if $\mathcal{B}$ is the parallel frame $\bar{\mathcal{B}}$.

If we assume that the initial subspace $\mathcal{C}(0)$ and final subspace $\mathcal{C}(1)$ are overlapping, we can rewrite Eq. (5) using a final frame $\{|\bar{a}_k(1)\rangle\}_{k=1}^K$ that is parallel to the initial frame $\{|a_k(0)\rangle\}_{k=1}^K$. This results in

$$\Gamma = \sum_{kl} [\boldsymbol{U}_g]_{kl} |\bar{a}_k(1)\rangle\langle a_l(0)|, \tag{12}$$

where

$$\boldsymbol{U}_g = \boldsymbol{U}_M \boldsymbol{P} e^{\int_0^1 \boldsymbol{A}(s)ds}. \tag{13}$$

Here, $\boldsymbol{U}_M$ is the unitary part of the polar decomposition of the overlap matrix of the initial frame and the original final frame. Under a gauge transformation of the form given by Eq. (6), one can show that the overlap matrix transforms as

$$\boldsymbol{M} \to \boldsymbol{M}' = \boldsymbol{U}^\dagger(0)\boldsymbol{M}\boldsymbol{U}(1). \tag{14}$$

This entails that the unitary part of $\boldsymbol{M}$ must transform as $\boldsymbol{U}_M \to \boldsymbol{U}_M' = \boldsymbol{U}^\dagger(0)\boldsymbol{U}_M\boldsymbol{U}(1)$. This fact and Eq. (7) entail that the matrix $\boldsymbol{U}_g$ transforms as

$$\boldsymbol{U}_g \to \boldsymbol{U}_g' = \boldsymbol{U}^\dagger(0)\boldsymbol{U}_g\boldsymbol{U}(0). \tag{15}$$

Hence, the eigenvalues of $\boldsymbol{U}_g$ are gauge invariant and we define $\boldsymbol{U}_g$ to be the holonomy for subspaces.

Let us consider some special cases of this holonomy. If $\mathcal{A}(0)=\{|a_k(0)\rangle\}_{k=1}^K$ and $\bar{\mathcal{A}}(1)=\{|\bar{a}_k(1)\rangle\}_{k=1}^K$ are two parallel frames such that $|\bar{a}_k(1)\rangle=|a_k(0)\rangle$, for all k, then we obtain $\boldsymbol{M}(\mathcal{A}(0),\bar{\mathcal{A}}(1))=\mathbf{1}$. Hence, $\boldsymbol{U}_M=\mathbf{1}$ and $\boldsymbol{U}_g=\boldsymbol{P}e^{\int_0^1\boldsymbol{A}(s)ds}$. This corresponds to the Wilczek-Zee holonomy [2] in the case of adiabatic evolution. Furthermore, when the subspaces are one-dimensional the matrices reduce to complex numbers. In this case we may use Eq. (13) to obtain

$$\boldsymbol{U}_g = e^{i\arg(\langle a(0)|a(1)\rangle)+\int_0^1\langle\dot{a}(s)|a(s)\rangle ds}, \tag{16}$$

which fully agrees with the geometric phase factor in Ref. [20].

Next, we view the holonomy in terms of parallel transport along the curve $\mathcal{C}$. Intuitively, parallel transport is based on the notion of transporting a subspace without locally rotating it. Assume that we have a family of K-frames $\mathcal{A}(s)=\{|a_k(s)\rangle\}_{k=1}^K$ parametrized by $s\in[0,1]$. Parallel transport is achieved if and only if $\mathcal{A}(s+\delta s)$ is parallel to $\mathcal{A}(s)$, $\forall s\in[0,1)$. As mentioned above, two frames are parallel if and only if their overlap matrix, as defined by Eq. (9), is positive definite. The overlap matrix of the frames $\mathcal{A}(s)$ and $\mathcal{A}(s+\delta s)$ can, to first order in δs, be expressed as

$$[\boldsymbol{M}(\mathcal{A}(s),\mathcal{A}(s+\delta s))]_{kl}=\delta_{kl}-\delta s[\boldsymbol{A}(s)]_{kl}, \tag{17}$$

with $\boldsymbol{A}(s)$ as in Eq. (4). Since $\boldsymbol{A}(s)$ is anti-Hermitian, the overlap matrix is positive definite only if $\boldsymbol{A}(s)=0$ for all $s\in[0,1]$. Hence, under parallel transport the holonomy takes the form $\boldsymbol{U}_g=\boldsymbol{U}_M$, where $\boldsymbol{U}_M$ is the unitary part of the polar decomposition of the overlap matrix between the initial frame and the parallel transported final frame.

Let us now consider adiabatic evolution. Assume $H(s)$ is a one-parameter family of Hamiltonians all having a degenerate energy eigenspace of dimension K corresponding to the energy $E(s)$. Furthermore, assume that $\{|a_k(s)\rangle\}_{k=1}^K$ is a basis for the eigenspace. Consider an adiabatic change from $s=0$ to $s=1$ during an elapse of time T. The evolution imposed on a state, initially in the degenerate subspace, can be written as

$$U(1,0)P(0)=e^{-iT\int_0^1E(s)ds}\sum_{kl}[\boldsymbol{P}e^{\int_0^1\boldsymbol{A}(s)ds}]_{kl}|a_k(1)\rangle\langle a_l(0)|, \tag{18}$$

where $U(1,0)$ is the evolution operator taking the system from $s=0$ to $s=1$ and $P(0)$ is the projector onto the initial eigenspace. If we assume that the final eigenspace is overlapping with the initial eigenspace, we may as before consider a final frame that is parallel to the initial frame. Using this we may rewrite Eq. (18) as $U(1,0)P(0)=e^{-iT\int_0^1E(s)ds}\Gamma$, with Γ as in Eq. (12). The first factor of the right-hand side of this equation we recognize as the dynamical phase factor, while the second contains the open-path holonomy.

The total action of Γ in Eq. (12) can be decomposed into two parts. One part is given by the partial isometry $T=\sum_{k=1}^K|\bar{a}_k(1)\rangle\langle a_k(0)|$, which maps the initial frame to its parallel frame. The second part is $R=\sum_{k,l=1}^K[\boldsymbol{U}_g]_{kl}|\bar{a}_k(1)\rangle\langle\bar{a}_l(1)|$, which is a unitary transformation on the final subspace given by the holonomy. This decomposition of Γ provides an understanding of how the holonomy should behave under a gauge transformation. In order for the unitary transformation on the final subspace to be independent of gauge, the holonomy must transform unitarily, as displayed in Eq. (15).

In the language of quantum computation, one may say that we choose to let the parallel frame $\{|\bar{a}_k(1)\rangle\}_{k=1}^K$ in the final space correspond to the computational basis $\{|a_k(0)\rangle\}_{k=1}^K$ in the initial space. The holonomy then appears as the resulting operation with respect to these choices of computational bases. An aspect of this is that the computational basis becomes path dependent. One might, as an example, consider a sequence of open-path holonomic implementations of operations. If this sequence happens to join into a cyclic path, it might be the case that the initial computational basis does not coincide with the final computational basis, although they span the same subspace.

III. PHYSICAL EXAMPLE

In order to illustrate the concept of open-path holonomy, as well as to provide an explicit example of an open-path holonomic implementation of a single qubit gate, we now consider a specific model system. This model was first examined in connection to non-Abelian holonomies in Ref. [29] and would be accessible to tests in various physical systems, such as ion traps [12,29], atoms [13], superconducting nanocircuits [14], and semiconductor nanostructures [15]. The Hamiltonian of the system reads

$$H(s)=\omega_0(s)|e\rangle\langle 0|+\omega_1(s)|e\rangle\langle 1|+\omega_a(s)|e\rangle\langle a|+\text{H.c.}, \tag{19}$$

where $|0\rangle,|1\rangle,|a\rangle$, and $|e\rangle$ are orthonormal and $\omega_0(s)$, $\omega_1(s)$, and $\omega_a(s)$ are tunable coupling parameters. We assume that the parameters combine to a real vector $(\omega_0(s),\omega_1(s),\omega_a(s))$ of unit length. Thus the parameter space forms a unit 2-sphere, which we may parametrize using the polar angle θ and the azimuthal angle φ. The Hamiltonian $H(s)$ has a doubly degenerate zero-energy eigenspace, which is spanned by the eigenstates

$$\begin{aligned}|D_1(s)\rangle &= \cos\theta(s)\cos\varphi(s)|0\rangle+\cos\theta(s)\sin\varphi(s)|1\rangle\\ &\quad-\sin\theta(s)|a\rangle,\\ |D_2(s)\rangle &= -\sin\varphi(s)|0\rangle+\cos\varphi(s)|1\rangle,\end{aligned} \tag{20}$$

where $\theta(s)\in[0,\pi]$ and $\varphi(s)\in[0,2\pi)$. In this context, the states $|D_1(s)\rangle$ and $|D_2(s)\rangle$ are often referred to as "dark states."

Let us now assume that the parameter s is changed slowly enough for the evolution to be adiabatic. Further, let $(\theta(0),\varphi(0))=(0,0)$ and $(\theta(1),\varphi(1))=(\theta_1,\varphi_1)$. The overlap matrix between the initial frame $\mathcal{A}(0)=\{|0\rangle,|1\rangle\}$ and the final frame $\mathcal{A}(1)=\{|D_1(1)\rangle,|D_2(1)\rangle\}$ is

$$\boldsymbol{M}(\mathcal{A}(0),\mathcal{A}(1))=\begin{pmatrix}\cos\theta_1\cos\varphi_1 & -\sin\varphi_1\\ \cos\theta_1\sin\varphi_1 & \cos\varphi_1\end{pmatrix}. \tag{21}$$

The unitary part of the overlap matrix is

$$\boldsymbol{U}_M = \begin{pmatrix} \dfrac{\cos\theta_1\cos\varphi_1}{|\cos\theta_1|} & -\sin\varphi_1 \\ \dfrac{\cos\theta_1\sin\varphi_1}{|\cos\theta_1|} & \cos\varphi_1 \end{pmatrix}, \tag{22}$$

which holds under the assumption that $\theta_1 \neq \pi/2$. If we furthermore assume that $0 \leq \theta_1 < \pi/2$, we may write $\boldsymbol{U}_M = e^{-i\varphi_1\boldsymbol{\sigma}_y}$, where $\boldsymbol{\sigma}_y$ is the y component of the standard Pauli matrices. For the frame in Eq. (20), we obtain $\boldsymbol{A}(s) = i\cos\theta(s)\dot{\varphi}(s)\boldsymbol{\sigma}_y$, yielding

$$\boldsymbol{U}_g = e^{-i\boldsymbol{\sigma}_y[\varphi_1 - \int_0^1 \cos\theta(s)\dot{\varphi}(s)ds]} = e^{-i\boldsymbol{\sigma}_y(\varphi_1 - \int_C \cos\theta d\varphi)} = e^{-i\boldsymbol{\sigma}_y\gamma}, \tag{23}$$

where the quantity γ equals the solid angle swept by the geodesic closure of the curve C on the parameter sphere.

If we instead assume that $\pi/2 < \theta_1 \leq \pi$, we obtain

$$\boldsymbol{U}_M = \begin{pmatrix} -\cos\varphi_1 & -\sin\varphi_1 \\ -\sin\varphi_1 & \cos\varphi_1 \end{pmatrix}, \tag{24}$$

which can be written as $\boldsymbol{U}_M = e^{-i\varphi_1\boldsymbol{\sigma}_y}(-\boldsymbol{\sigma}_z)$, where $\boldsymbol{\sigma}_z$ is the z component of the standard Pauli matrices. In this case the holonomy takes the form

$$\boldsymbol{U}_g = e^{-i\varphi_1\boldsymbol{\sigma}_y}(-\boldsymbol{\sigma}_z)e^{-i\boldsymbol{\sigma}_y\int_C \cos\theta d\varphi}. \tag{25}$$

Due to the fact that the different components of the Pauli matrices do not commute, the holonomy is no longer determined by the solid angle swept by the geodesic closure of the curve C on the parameter sphere. In the first case the holonomy had an Abelian structure (in the sense of Ref. [23]) due to the fact that $[\boldsymbol{A}(s), \boldsymbol{A}(s')] = 0$ for any $s, s' \in [0,1]$ and $[\boldsymbol{U}_M, e^{\int_0^1 \boldsymbol{A}(s)ds}] = 0$. The latter is not fulfilled in the second case, where the holonomy is truly non-Abelian. Hence, for this physical example open paths seems to be a necessary prerequisite in order to achieve truly non-Abelian holonomies.

IV. PARTIAL HOLONOMY

So far we have assumed that the initial and final subspaces of the open path are overlapping. In the special case of a one-dimensional subspace there are two cases, either the subspaces are overlapping, or they are orthogonal. As a consequence the holonomy either exists uniquely, or is undefined. In the non-Abelian case, however, there is an additional case, namely, that the subspaces are partially overlapping. In this case the holonomy is only partially determined. When the two subspaces are partially overlapping the positive part $\boldsymbol{R}$ of the overlap matrix is not invertible, no matter the choice of frames. However, we may use the Moore-Penrose (MP) pseudoinverse [28]. Since $\boldsymbol{R}$ is a positive semidefinite matrix, its MP-inverse $\boldsymbol{R}^{\ominus}$ can be calculated by inverting the nonzero eigenvalues in its spectral decomposition. The matrix $\boldsymbol{U}_M$ can now be defined as the partial isometry $\boldsymbol{U}_M = \boldsymbol{R}^{\ominus}\boldsymbol{M}$. This results in a partial isometry $\boldsymbol{R}^{\ominus}\boldsymbol{M}\boldsymbol{P}e^{\int_0^1 \boldsymbol{A}(s)ds}$ that we shall call a partial holonomy.

Let us examine how the partial holonomy behaves under a gauge transformation. The overlap matrix between the initial and final subspaces transforms as in Eq. (14). It follows that

$$\boldsymbol{R}' = \sqrt{\boldsymbol{M}'\boldsymbol{M}'^{\dagger}} = \sqrt{\boldsymbol{U}^{\dagger}(0)\boldsymbol{M}\boldsymbol{U}(1)\boldsymbol{U}^{\dagger}(1)\boldsymbol{M}^{\dagger}\boldsymbol{U}(0)} = \boldsymbol{U}^{\dagger}(0)\boldsymbol{R}\boldsymbol{U}(0), \tag{26}$$

where $\boldsymbol{R} = \sqrt{\boldsymbol{M}\boldsymbol{M}^{\dagger}}$. We note the following property of the MP inverse. Suppose that $\boldsymbol{U}$ and $\boldsymbol{V}$ are unitary matrices. Then, for any matrix $\boldsymbol{X}$, we have (see p. 434 in Ref. [28])

$$(\boldsymbol{U}\boldsymbol{X}\boldsymbol{V})^{\ominus} = \boldsymbol{V}^{\dagger}\boldsymbol{X}^{\ominus}\boldsymbol{U}^{\dagger}. \tag{27}$$

Thus,

$$\begin{aligned} \boldsymbol{U}'_M &= (\boldsymbol{R}')^{\ominus}\boldsymbol{M}' = (\boldsymbol{U}^{\dagger}(0)\boldsymbol{R}\boldsymbol{U}(0))^{\ominus}\boldsymbol{U}^{\dagger}(0)\boldsymbol{M}\boldsymbol{U}(1) \\ &= \boldsymbol{U}^{\dagger}(0)\boldsymbol{R}^{\ominus}\boldsymbol{M}\boldsymbol{U}(1), \end{aligned} \tag{28}$$

which is precisely the way $\boldsymbol{R}^{-1}\boldsymbol{M}$ transforms if $\boldsymbol{R}$ is invertible. Hence, the transformation of $\boldsymbol{U}_M$ takes the same form independently of whether or not the matrix $\boldsymbol{R}$ is invertible. Moreover, the path ordered part of the holonomy, $\boldsymbol{P}e^{\int_0^1 \boldsymbol{A}(s)ds}$, always constitutes a unitary matrix that transforms according to Eq. (7). Thus the partial holonomy transforms unitarily just as the holonomy, as displayed in Eq. (15).

As an example of a partial holonomy, let us revisit the previous model system, now assuming that $\theta_1 = \pi/2$. The overlap matrix $\boldsymbol{M}(\mathcal{A}(0), \mathcal{A}(1))$ reduces to

$$\boldsymbol{M}(\mathcal{A}(0), \mathcal{A}(1)) = e^{-i\varphi_1\boldsymbol{\sigma}_y}\boldsymbol{Q}, \quad \boldsymbol{Q} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{29}$$

and $\boldsymbol{R} = e^{-i\varphi_1\boldsymbol{\sigma}_y}\boldsymbol{Q}e^{i\varphi_1\boldsymbol{\sigma}_y}$, which happens to be a one-dimensional projector, and thus equal to its own MP inverse. Consequently, $\boldsymbol{U}_M = \boldsymbol{M}(\mathcal{A}(0), \mathcal{A}(1))$ and the partial holonomy becomes

$$\boldsymbol{U}_g = e^{-i\varphi_1\boldsymbol{\sigma}_y}\boldsymbol{Q}e^{i\int_0^1 \cos\theta(s)\dot{\varphi}(s)ds\boldsymbol{\sigma}_y}. \tag{30}$$

One may note that the existence of a loop (in this case the equator $\theta_1 = \pi/2$ of the parameter sphere) along which the holonomy is not fully defined is a topologically enforced prerequisite for the discontinuous transition between the Abelian and non-Abelian character of the holonomy, that we have found in this example.

V. CONCLUSIONS

To summarize, we consider subspaces moving in the Hilbert space of a quantum system, and the concomitant unitary transformation associated with the geometry of the traversed path; the non-Abelian quantum holonomy. The standard non-Abelian quantum holonomy is defined for closed paths of such subspace motions, while we consider an open-path generalization. Due to the openness of the path, the initial and final subspaces do not coincide in general. In order to "extract" the unitary transformation on the final subspace, i.e., the holonomy, we use a concept of parallelity in order to decide which basis in the final subspace corresponds to the basis in the initial subspace. Under suitable conditions on the relative orientation between the initial and final subspaces, this procedure results in a uniquely defined non-Abelian quantum holonomy for open paths. This enables the con-

struction of quantum gates in the open-path setting, where the action of the gates is given by the proposed holonomy. The idea of open-path holonomic gates may be useful when analyzing noncyclic errors [30,31] of standard implementations of holonomic quantum computation. We finally point out the existence of partially defined holonomies, which has no counterpart in the Abelian case.

ACKNOWLEDGMENTS

We wish to thank Patrik Thunström for useful comments. J.Å. wishes to thank the Swedish Research Council for financial support and the Centre for Quantum Computation at DAMTP, Cambridge, for hospitality. E.S. acknowledges partial financial support from the Swedish Research Council.

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