Non-Abelian quantum holonomy of hydrogen-like atoms

Vahid Azimi Mousolou* and Carlo M. Canali†

School of Computer Science, Physics and Mathematics, Linnaeus University, Kalmar, Sweden

Erik Sjöqvist‡

Department of Quantum Chemistry, Uppsala University, Box 518, S-751 20 Uppsala, Sweden and Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, 117543 Singapore, Singapore

We study the Uhlmann holonomy [Rep. Math. Phys. 24, 229 (1986)] of quantum states for hydrogen-like atoms where the intrinsic spin and orbital angular momentum are coupled by the spin-orbit interaction and subject to a slowly varying magnetic field. We show that the holonomy for the orbital angular momentum and spin subsystems is non-Abelian, while the holonomy of the whole system is Abelian. Quantum entanglement in the states of the whole system is crucially related to the non-Abelian gauge structure of the subsystems. We analyze the phase of the Wilson loop variable associated with the Uhlmann holonomy, and find a relation between the phase of the whole system with corresponding marginal phases. Based on the result for the model system we provide evidence that the phase of the Wilson loop variable and the mixed-state geometric phase [E. Sjöqvist et al. Phys. Rev. Lett. 85, 2845 (2000)] are in general inequivalent.

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I. INTRODUCTION

The pioneering work by Berry [1] and Wilczek and Zee [2], have triggered considerable interest in effective gauge structures in the adiabatic evolution of non-relativistic quantum systems. Non-Abelian quantum holonomies have been examined in the context of nuclear rotations of diatoms [3], nuclear quadrupole resonance [4], semiconductor heterostructures [5], trapped atoms [6], quantum optics [7], and superconducting systems [8]. It has been pointed out [9] that non-Abelian holonomy may be used in the construction of universal sets of quantum gates for the purpose to achieve fault tolerant quantum computation.

In Refs. [2, 9], non-Abelian holonomies are related to the existence of degenerate energy eigenstates that can be controlled by a set of slowly changing parameters. In contrast, Uhlmann [10] has shown that non-Abelian gauge structures may appear along sequences of density operators representing mixtures of quantum states, irrespective of the degeneracy structure of the underlying Hamiltonian. Such non-Abelian structures may arise for subsystems of composite systems undergoing adiabatic evolution, since the marginal states are mixed if the instantaneous energy eigenstates of the whole system are entangled.

The purpose of the present paper is to follow the Uhlmann approach to examine non-Abelian gauge structure in the case of spin-orbit (LS) coupled hydrogen-like atoms subject to a slowly varying magnetic field. We show that the adiabatic Uhlmann holonomies for the spin (S) and orbital (L) parts become non-Abelian although the one of the whole LS state is Abelian. Studies of the same model were carried out previously [11] (see also [12]) by using the mixed-state geometric phase approach developed in Ref. [13]. In particular, in Ref. [11] it was shown that the mixed-state geometric phases of the L and S subsystems always sum up to the standard pure state geometric phase of the whole system. In contrast, we show here that the phases of Wilson loop variables associated with the Uhlmann holonomies satisfy this sum rule only for specific paths, while for other paths there is a deviation of π from the sum rule. This deviation from the sum rule demonstrates a striking non-trivial difference between the Uhlmann holonomy [10] and the mixed-state geometric phase [13].

The outline of the paper is as follows. In Sec. II the Uhlmann holonomy is briefly reviewed. The corresponding parallel transport equations for adiabatic rotation of angular momentum states are derived in Sec. III. In Sec. IV we compute the Uhlmann holonomies for the L and S subsystems as well as that of the total angular momentum. We examine in particular the non-Abelian nature of the subsystem holonomies as well as the additivity of the phases of the Wilson loop variables associated with the Uhlmann holonomies. The paper ends with the conclusions.

II. UHLMANN HOLOMONY

In this Section we summarize the main definitions and properties of the Uhlmann holonomy [10]. Let $C: [0, 1] \ni t \to \rho_t$ be a smooth path of density operators acting on
some Hilbert space $\mathcal{H}$. An operator $W_t$ such that $\rho_t = W_t W_t^\dagger$ is called an amplitude of $\rho_t$. $W_t$ can be written as $W_t = \sqrt{\rho_t} V_t$, where the “phase factor” $V_t$ is a partial isometry \cite{14} on $\mathcal{H}$. For any choice of $W_0 \equiv \tilde{W}_0$, there is a differentiable path $[0, 1] \ni t \to \tilde{W}_t$ of amplitudes over $C$ that satisfy the parallel transport condition

$$\tilde{W}^\dagger d \tilde{W} = d \tilde{W}^\dagger \tilde{W},$$

where $d \tilde{W} = d \tilde{W}_t$. Inserting $\tilde{W} = \sqrt{\rho_t}$ into Eq. (1) yields

$$d \tilde{W} \tilde{V}^\dagger \rho + p d \sqrt{\rho} \tilde{V}^\dagger = d \sqrt{\rho} \sqrt{\rho} - \sqrt{\rho} d \sqrt{\rho}.$$

By solving for $\tilde{V}$, we define the Uhlmann holonomy associated with the path $C$ to be

$$U_{\text{uhl}}(C) = \tilde{V}_1 \tilde{V}_0^\dagger. \quad (3)$$

The operator $U_{\text{uhl}}(C)$ is a unique partial isometry (unique unitary if all $\rho_t$ are full rank), gauge invariant (i.e., independent of the choice of $\tilde{W}_0$), and reparametrization invariant (i.e., independent of the speed of the evolution along $C$); thus, $U_{\text{uhl}}(C)$ is a property of the path $C$.

In Uhlmann’s approach, a system in a mixed state is thought to be a subsystem embedded in a larger quantum system which is in a pure state. The pure state is referred to as a purification of the mixed state. This is accomplished by introducing an auxiliary system with which the original system is entangled. The purification is equivalent to the amplitude $W_t$ of $\rho_t$. If $\tilde{W}_t$ satisfies the condition in Eq. (1) along the path $C$, then, inspired by the pure state geometric phase \cite{16}, one may assign the phase

$$\varphi_{\text{uhl}} = \arg \left[ \text{Tr} (\tilde{W}_0^\dagger \tilde{W}_1) \right], \quad (4)$$

to the Uhlmann holonomy $U_{\text{uhl}}(C)$. The definition $\varphi_{\text{uhl}}$ for Uhlmann phase has been used to investigate theoretically \cite{17, 19} and experimentally \cite{20} a possible relationship between the Uhlmann holonomy \cite{10} and the mixed-state geometric phase $\beta$ \cite{13}. The latter differs considerably from $\varphi_{\text{uhl}}$ in that it is, for cyclic unitary evolution, the sum of geometric phase factors of the eigenstates of the density operator weighted by the corresponding eigenvalues. Thus, contrary to $\varphi_{\text{uhl}}$, $\beta$ is essentially a decomposition dependent and Abelian geometric phase concept.

On the other hand, as for the case of the non-Abelian Wilczek-Zee phase factor \cite{2}, the Uhlmann holonomy in Eq. (3) for cyclic evolutions takes the form of a Wilson loop $P e^{-i \int_C A}$ for a vector potential $A$, where $P$ stands for path ordering. On the basis of this fact and on the fact that the Wilczek-Zee phase factor is a natural extension of the Berry phase \cite{1} to systems with degenerate spectra, one can argue that the phase of the Wilson loop variable $\text{Tr} \left( P e^{-i \int_C A} \right)$ is more natural quantity than $\varphi_{\text{uhl}}$, and define the Uhlmann phase as

$$\gamma = \arg \left[ \text{Tr} (U_{\text{uhl}}(C)) \right]. \quad (5)$$

Note that the two phase quantities $\varphi_{\text{uhl}}$ and $\gamma$ need not be equal. The focus of this paper is to turn our attention to the Uhlmann phase defined in Eq. (5). In particular, we demonstrate that $\gamma$ behaves very differently from the mixed-state geometric phase \cite{13}.

### III. UHLMANN HOLONOMY OF ANGULAR MOMENTA

As an introduction to the model studied in Sec. IV, we consider the case of adiabatic transport of a quantum angular momentum $S$. This angular momentum is assumed to be coupled to another quantum angular momentum $S^{(r)}$. The coupling is assumed to be spherically symmetric. Both $S$ and $S^{(r)}$ are exposed to an external classical magnetic field $B$. The Hamiltonian of the system takes the form $H = U^\text{tot}(\theta, \phi) H_z U^\text{tot} \dagger(\theta, \phi)$, where $U^\text{tot}(\theta, \phi) = e^{-i \phi S^z} e^{-i \theta S^z\text{tot}} e^{i \theta S^z}$ and $S^\text{tot} = S + S^{(r)} = (S^x, S^y, S^z)$ ($\hbar = 1$ from now on), $\theta, \phi$ are spherical polar angles parametrizing the direction $n = B/|B|$ of the external magnetic field.

$H_z$ is independent of the polar angles $(\theta, \phi)$ of the two-dimensional parameter sphere $S^2$ of all possible magnetic field directions. We assume that $S_z^\text{tot}, H_z = 0$ to make sure that $H$ is well defined on $S^2$. The energy eigenstates can be represented by the smooth vector-valued functions $|\psi(n)(\theta, \phi)\rangle = U^\text{tot}(\theta, \phi)|\psi(z)(n)\rangle$, well defined on the open patch $S^2 - \{\theta = \pi\}$, and $|\psi(n)(\theta, \phi)\rangle' = U^\text{tot}(\theta, \phi)|\psi(n')\rangle = U^\text{tot}(\theta, \phi)e^{-2i \phi S^z\text{tot}}|\psi(z')(n)\rangle$, well defined on the open patch $S^2 - \{\theta = 0\}$. Here, $H_z|\psi(z)(n)\rangle = E(n)|\psi(z)(n)\rangle$. The vectors $|\psi(n)(\theta, \phi)\rangle$ and $|\psi(n)(\theta, \phi)\rangle'$ define two monopole sections \cite{21} over the parameter sphere. These sections are related by a single-valued gauge transformation so that

$$|\psi(n)(\theta, \phi)\rangle (\theta, \phi) = |\psi(n)(\theta, \phi)\rangle' (\theta, \phi)$$

in any overlapping region on the parameter sphere.

The reduced density operator $\rho(n)(\theta, \phi)$ representing the marginal state of $S$, corresponding to the $n$th energy eigenstate of $H$, is obtained by partial trace $\text{Tr}_r$ over the degrees of freedom associated with $S^{(r)}$, i.e.,

$$\rho(n)(\theta, \phi) = U(\theta, \phi)|\psi(n)(\theta, \phi)\rangle \langle \psi(n)(\theta, \phi)| = U(\theta, \phi) \rho_z(n) U^\dagger(\theta, \phi). \quad (7)$$

Here, $U(\theta, \phi) = e^{-i \phi S^z} e^{-i \theta S^z} e^{i \theta S^z}$ is the rotation operator, $\tilde{U}(\theta, \phi) = U(\theta, \phi)e^{-2i \phi S^z}$, and $\rho_z(n) = \text{Tr}_r |\psi(z)(n)\rangle \langle \psi(z)(n)|$ is a “reference” state. $\rho(n)(\theta, \phi)$ defines the mixed state of our subsystem, for the $n$th energy eigenstate.
In the adiabatic regime, the path $\Gamma : [0, 1] \ni t \rightarrow (\theta_t, \phi_t)$ on the parameter sphere $S^2$ of magnetic field directions maps to the path $C^{(n)} : [0, 1] \ni t \rightarrow \rho^{(n)}(\theta_t, \phi_t)$ in state space of the considered angular momentum. Let $V^{(n)} = U(\theta, \phi)V^{(n)}$ be a partial isometry that satisfies parallel transport along $\Gamma$. With $d = d\theta d\phi$, we have
\begin{align}
&dV^{(n)}V^{(n)\dagger}\rho^{(n)}_z + \rho^{(n)}_z dV^{(n)}V^{(n)\dagger} = -2i\sqrt{\rho^{(n)}_z} \left( d\phi (1 - \cos \theta) S_z + d\phi \sin \theta (S_x \cos \phi + S_y \sin \phi) - d\theta (S_x \sin \phi + S_y \cos \phi) \right) \sqrt{\rho^{(n)}_z},
\end{align}
along $\Gamma$. Repeating the calculation for the other monopole section, by using the decomposition $\tilde{V}^{(n)} = \tilde{U}(\theta, \phi)\tilde{V}^{(n)}$, leads to the equation
\begin{align}
&d\tilde{V}^{(n)}\tilde{V}^{(n)\dagger}\rho^{(n)}_z + \rho^{(n)}_z d\tilde{V}^{(n)}\tilde{V}^{(n)\dagger} = 2i\sqrt{\rho^{(n)}_z} \left( d\phi (1 + \cos \theta) S_z - d\phi \sin \theta (S_x \cos \phi - S_y \sin \phi) + d\theta (S_x \sin \phi + S_y \cos \phi) \right) \sqrt{\rho^{(n)}_z},
\end{align}
along $\Gamma$. Since $[\rho^{(n)}_z, S_z] = 0$, $\tilde{V}^{(n)} = e^{2i\phi S_z}V^{(n)}$ for the choice $V^{(n)} = e^{2i\phi S_z}V^{(n)}$ satisfies Eq. [11]. Thus, the difference between $\tilde{V}^{(n)}$ and $V^{(n)}$ precisely compensates the difference between the rotation operators $\tilde{U}(\theta, \phi)$ and $U(\theta, \phi)$ so that the Uhlmann holonomy remains the same in the two representations. In other words, $U_{\text{ahl}}(C^{(n)})$ is independent of which monopole section we use. This implies that either of the above pair of monopole sections can be used to calculate the Uhlmann holonomy for any path on the parameter sphere.

IV. UHLMANN HOLOMONY OF HYDROGEN-LIKE ATOMS

In Ref. [11], the adiabatic geometric phases of the $LS$-coupled hydrogen atom in a slowly rotating magnetic field $B = Bn = B(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ were analyzed. The adiabatic geometric phases of the whole system and of the orbital ($L$) and spin ($S$) angular momentum subsystems were computed. In particular, it was demonstrated that the subsystem phases add up to the phase of the whole system. The purpose here is to compute the corresponding Uhlmann holonomies and to examine their relation.

A. Model system

We consider the spin-orbit ($LS$) part
\begin{align}
H_n = gn \cdot (L + 2S) + 2L \cdot S = U_f(\theta, \phi)H_zU^+_f(\theta, \phi),
\end{align}
of hydrogen-like atoms exposed to an external magnetic field pointing in a direction defined by the unit vector $\mathbf{n}$. The first and second terms are the Zeeman and $LS$-coupling contributions, respectively, $g$ is the Zeeman-$LS$ strength ratio (assumed to be time-independent), and $\mathbf{n}$ defines the adiabatic parameter sphere $S^2$ under slow changes in the direction of the external magnetic field. We may choose
\begin{align}
U_X(\theta, \phi) = e^{-i\phi X_s} e^{-i\theta X_z} e^{i\phi X_s}, \quad X = L, S, J,
\end{align}
where $\mathbf{J} = \mathbf{L} + \mathbf{S}$ is the total angular momentum and $H_z$ is the Hamiltonian at the north pole $\mathbf{n} = (0, 0, 1)$ of the parameter sphere.

The Hamiltonian $H_z$ is block-diagonalizable in one- and two-dimensional blocks with respect to the product basis with elements $|l, m, \pm \frac{1}{2}\rangle = |l, m|\pm\rangle$ being the common eigenvectors of $L^2, L_z, S^2, S_z$. Each block may be labeled by the eigenvalue $\mu = \pm \frac{1}{1}, -l+\frac{1}{1}, \ldots, l+\frac{1}{1}$ of $J_z$. The two extremal subspaces characterized by $|\mu| = l\pm\frac{1}{2} \equiv \mu_e$ are one-dimensional corresponding to the two product vectors $|\psi_{(l,\mu)}^{(l,\pm)}\rangle = |l, \pm\rangle|\pm\rangle$. The remaining blocks are two-dimensional, each of which spanned by the vectors $|l, m = \mu \pm \frac{1}{2}\rangle|\pm\rangle$, $|l, m = \mu \mp \frac{1}{2}\rangle|\pm\rangle$, $|\mu| < l\pm\frac{1}{2}$.

For each $\mu$, the corresponding energy eigenvectors $|\psi_{(l,\mu)}^{(l,\pm)}\rangle$ become $LS$ entangled. The amount of $LS$ entanglement may be measured in terms of concurrence [22]
\begin{align}
C^{(l,\mu)} = C(|\psi_{(l,\mu)}^{(l,\pm)}\rangle) = |\sin \alpha^{(l,\mu)}|,
\end{align}
where
\begin{align}
\cos \alpha^{(l,\mu)} = \frac{2\mu + g}{\sqrt{g^2 + 4g\mu + (2l + 1)^2}}.
\end{align}
Note that $C^{(l,\mu)}$ is independent of the $\pm$ label and varies between 0 for product states ($\alpha^{(l,\mu)} = 0, \pi$) and 1 for maximally entangled states ($\alpha^{(l,\mu)} = \pi/2$).

The instantaneous energy eigenvectors of $H_n$ are related to the eigenvectors of $H_z$ according to
\begin{align}
|\psi_{(l,\mu)}^{(l,\pm)}; \theta, \phi\rangle = U_f(\theta, \phi)|\psi_{(l,\mu)}^{(l,\pm)}\rangle
= U_L(\theta, \phi)U_S(\theta, \phi)|\psi_{(l,\mu)}^{(l,\pm)}\rangle.
\end{align}
Let $\Gamma : [0, 1] \ni t \rightarrow (\theta_t, \phi_t)$ be a parametrized path on the parameter sphere. Assume that the external magnetic field slowly traverses $\Gamma$ so that the adiabatic approximation is valid. With this assumption $\Gamma$ maps to the paths
\begin{align}
C_{X,\pm}^{(l,\mu)} : [0, 1] \ni t \rightarrow \rho_{X,\pm}^{(l,\mu)}(\theta_t, \phi_t)
&= U_X(\theta_t, \phi_t)\rho_{X,\pm}^{(l,\mu)}U^+_X(\theta_t, \phi_t), \quad X = L, S, J.
\end{align}
in the spaces of density operators, where
\[
\rho_{J,\pm}^{(l,\mu)} = |\psi_{\pm}^{(l,\mu)}(\psi_{\pm}^{(l,\mu)}|^, \\
\rho_{L,\pm}^{(l,\mu)} = \text{Tr}_S|\psi_{\pm}^{(l,\mu)}|^\langle \psi_{\pm}^{(l,\mu)}|, \\
\rho_{S,\pm}^{(l,\mu)} = \text{Tr}_L|\psi_{\pm}^{(l,\mu)}|^\langle \psi_{\pm}^{(l,\mu)}|.
\]
(16)

In the following subsections we compute the Uhlmann holonomies of the total angular momentum \(J\) of the atom and its subsystems \(L\) and \(S\) under the assumption \(g \neq 0\).

**B. Holonomy of total angular momentum**

Let \(V_{J,\pm}^{(l,\mu)}\) denote the solution of Eq. (5) with reference state \(|\psi_{\pm}^{(l,\mu)}\rangle\langle \psi_{\pm}^{(l,\mu)}|\). We obtain the partial isometry
\[
V_{J,\pm;1}^{(l,\mu)} = e^{-i\mu f_{1}(1-\cos \theta)d\phi}|\psi_{\pm}^{(l,\mu)}\rangle\langle \psi_{\pm}^{(l,\mu)}|V_{J,\pm;0}^{(l,\mu)},
\]
(17)

which yields the Uhlmann holonomy
\[
U_{\text{uhl}}(C_{J,\pm}^{(l,\mu)}) = e^{-i\mu f_{1}(1-\cos \theta)d\phi} \\
\times U_{J}(\theta_{1}, \phi_{1})|\psi_{\pm}^{(l,\mu)}\rangle\langle \psi_{\pm}^{(l,\mu)}|U_{J}^\dagger(\theta_{0}, \phi_{0}).
\]
(18)

To compare with the corresponding geometric phase factor \(e^{i\mathcal{B}(C_{J,\pm}^{(l,\mu)})}\), we note that while this geometric phase factor is a unit modulus complex number, \(U_{\text{uhl}}(C_{J,\pm}^{(l,\mu)})\) in Eq. (15) is a partial isometry with \(U_{\text{uhl}}(C_{J,\pm}^{(l,\mu)})(U_{\text{uhl}}(C_{J,\pm}^{(l,\mu)})^\dagger)\) being projection operators onto the initial and final states, respectively. In particular, this shows that while the geometric phase \(\mathcal{B}(C_{J,\pm}^{(l,\mu)})\) is undefined if the two end points of \(C_{J,\pm}^{(l,\mu)}\) correspond to orthogonal states, \(U_{\text{uhl}}(C_{J,\pm}^{(l,\mu)})\) is a well-defined partial isometry. On the other hand, a direct calculation yields
\[
\text{Tr}[U_{\text{uhl}}(C_{J,\pm}^{(l,\mu)})] = |\text{Tr}[U_{\text{uhl}}(C_{J,\pm}^{(l,\mu)})]|e^{i\mathcal{B}(C_{J,\pm}^{(l,\mu)})}
\]
(19)

that demonstrates an explicit relation between the Wilson loop variable associated with the Uhlmann holonomy and the geometric phase factor, unless \(\text{Tr}[U_{\text{uhl}}(C_{J,\pm}^{(l,\mu)})]\) vanishes, which happens precisely when the initial and final states are orthogonal. These results establish a one-to-one relation between the standard pure state geometric phase \(\mathcal{B}\) and the corresponding Uhlmann holonomy of the whole system.

**C. Holonomy of the \(L\) and \(S\) subsystems**

Now we compute the Uhlmann holonomies of the \(L\) and \(S\) subsystems. Let us start with the extremal states \(\mu = \pm \mu_{c}\). We note that the eigenvectors
\[
|\psi_{\pm}^{(l,\pm \mu_{c})}\rangle = U_{L}(\theta, \phi)|l, \pm l\rangle U_{S}(\theta, \phi)|\pm\rangle
\]
(20)
of \(H_{n}\) are tensor products of states of the two subsystems \(L\) and \(S\). We thus find the Uhlmann holonomies for the \(L\) and \(S\) subsystems as
\[
U_{\text{uhl}}(C_{L,\pm}^{(l,\pm \mu_{c})}) = e^{-i\mu f_{1}(1-\cos \theta)d\phi} \\
\times U_{L}(\theta_{1}, \phi_{1})|l, \pm l\rangle U_{L}^\dagger(\theta_{0}, \phi_{0}),
\]
\[
U_{\text{uhl}}(C_{S,\pm}^{(l,\pm \mu_{c})}) = e^{-i\mu f_{1}(1-\cos \theta)d\phi} \\
\times U_{S}(\theta_{1}, \phi_{1})|\pm\rangle U_{S}^\dagger(\theta_{0}, \phi_{0}).
\]
(21)

Note that the associated holonomies are \(g\)-independent and satisfy the product relation
\[
U_{\text{uhl}}(C_{J,\pm}^{(l,\pm \mu_{c})}) = U_{\text{uhl}}(C_{L,\pm}^{(l,\pm \mu_{c})}) \otimes U_{\text{uhl}}(C_{S,\pm}^{(l,\pm \mu_{c})}).
\]
(22)

Next, we compute the Uhlmann holonomy in adiabatic evolution of non-extremal energy eigenstates characterized by \(|\mu| < l + \frac{1}{2}\). The marginal states are rank-two density operators obtained by adiabatically evolving the states \(\rho_{L,\pm}^{(l,\mu)}\) and \(\rho_{S,\pm}^{(l,\mu)}\) under unitaries \(U_{L}\) and \(U_{S}\), respectively. One may solve Eq. (5) with reference states \(\rho_{L,\pm}^{(l,\mu)}\) for a path \(\Gamma\) on the parameter sphere to obtain the Uhlmann holonomy of the \(L\) subsystem,
\[
U_{\text{uhl}}(C_{L,\pm}^{(l,\mu)}) = U_{L}(\theta_{1}, \phi_{1})P_{\text{e}}^{-i\mu f_{1}(A_{L,\theta}^{(l,\mu)} + A_{L,\phi}^{(l,\mu)})} \\
\times U_{L}^\dagger(\theta_{0}, \phi_{0}).
\]
(23)

Here, we have introduced the vector potential components
\[
A_{L,\theta}^{(l,\mu)} = \frac{1}{2}\mu c_{l,\mu}^{(l,\mu)} \left( \begin{array}{cc}
0 & -ie^{-i\phi} \\
-e^{-i\phi} & 0
\end{array} \right) d\theta,
\]
(24)

\[
A_{L,\phi}^{(l,\mu)} = \mu(1-\cos \theta) \left( \begin{array}{cc}
1 & 0 \\
0 & 1
\end{array} \right) d\phi \quad + \frac{1}{2} \left( \begin{array}{cc}
-1+\cos \theta & \mu c_{l,\mu}^{(l,\mu)} \sin \theta e^{i\phi} \\
\mu c_{l,\mu}^{(l,\mu)} \sin \theta e^{-i\phi} & 1-\cos \theta
\end{array} \right) d\phi.
\]

The vector potential \(A_{L,\mu}^{(l,\mu)} = A_{L,\theta}^{(l,\mu)} + A_{L,\phi}^{(l,\mu)}\) is expressed in the basis \(\{|\mu-\frac{1}{2}\rangle, |\mu+\frac{1}{2}\rangle\}\) and \(w = \sqrt{(l+\frac{1}{2})^{2} - \mu^{2}} > 0\).

It is worth noting that the vector potential \(A_{L,\mu}^{(l,\mu)}\) exhibits a \(U(1)\) part being proportional to the identity. In the case where \(\Gamma\) is a loop, this part gives rise to the global geometric phase factor \(e^{-i\mu f_{1}(1-\cos \theta)d\phi} = e^{-i\mu \Omega}\), \(\Omega\) being the solid angle enclosed by \(\Gamma\) on the parameter sphere \(S^{2}\).

Similarly, for the \(S\) subsystem we have
\[
U_{\text{uhl}}(C_{S,\pm}^{(l,\mu)}) = U_{S}(\theta_{1}, \phi_{1})P_{\text{e}}^{-i\mu f_{1}(A_{S,\theta}^{(l,\mu)} + A_{S,\phi}^{(l,\mu)})} \\
\times U_{S}^\dagger(\theta_{0}, \phi_{0})
\]
(25)

with vector potential components
\[
A_{S,\theta}^{(l,\mu)} = \frac{1}{2} c_{l,\mu}^{(l,\mu)} \left( \begin{array}{cc}
0 & ie^{-i\phi} \\
-i e^{-i\phi} & 0
\end{array} \right) d\theta,
\]
(26)

\[
A_{S,\phi}^{(l,\mu)} = \frac{1}{2} \left( \begin{array}{cc}
1-\cos \theta & c_{l,\mu}^{(l,\mu)} \sin \theta e^{-i\phi} \\
\mu c_{l,\mu}^{(l,\mu)} \sin \theta e^{i\phi} & -1+\cos \theta
\end{array} \right) d\phi.
\]
in the \{\{+\rangle,\{-\}\rangle\} basis. Note that \(A_S^{(l,\mu)}\) does not have a \(U(1)\) part.

Unlike the extremal case, the marginal Uhlmann holonomies are \(g\)-dependent via the concurrence \(C^{(l,\mu)}\). Furthermore, there is a dimensional mismatch between the rank-one holonomy of the \(J\) system and the rank-two holonomies of the \(L\) and \(S\) subsystems; in general this mismatch implies that there is no path for which a product rule similar to that in Eq. (22) holds.

It is noticed that when \(\alpha^{(l,\mu)} \neq 0, \pi, i.e., when the concurrence \(C^{(l,\mu)}\) is non-zero, the vector potentials contain non-Abelian components. In other words, the non-Abelian nature of the subsystem holonomies is due to entanglement. This is analogous to the Lévy geometric phase defined for two-qubit systems [23], which is a path-dependent unit quaternion that may find realization in two-particle interferometry [24]. The holonomy group associated with this geometric phase becomes, just as the Uhlmann holonomy of the subsystems, Abelian in the product state case.

In the “classical” limit characterized by \(l \rightarrow \infty\) and \(|\mu| = O(l)\), \(C^{(l,\mu)}\) vanishes as \(q^{(l,\mu)}\) tends to zero. Thus, the \(L\) and \(S\) holonomies turn Abelian in this limit. We further see that for cyclic evolution in the \(l/|\mu|, l/|g| \rightarrow \infty\) limit, \(C^{(l,\mu)}\) tends to its maximum value 1, i.e., the energy eigenvector becomes maximally entangled, and the holonomies turn into the transpose of the Wilczek-Zee holonomy for nuclear quadrupole resonance setup discussed in Ref. [25] and experimentally studied in Refs. [4, 26].

D. Figure-8 Curve

In order to investigate the consequences of the non-Abelian structure of the Uhlmann holonomies of the \(L\) and \(S\) subsystems, we consider here the class of “figure-8” loops on the parameter sphere of magnetic field directions shown in Fig. 1 for which the holonomies can be calculated explicitly. These loops are chosen to enclose no net area. Since any Abelian geometric phase of a angular momentum system is proportional to the area enclosed on the parameter sphere [1], any such phase must vanish for the figure-8 loops; a fact that has been used to demonstrate the Abelian nature of the Berry phase experimentally by using nuclear magnetic resonance techniques [27]. Similarly, the mixed-state geometric phases [13] and the Berry phases in the \(LS\) system are all zero due to their Abelian nature. In contrast, we show that the Uhlmann phases of the subsystems along this class of loops are in general non-zero, which is a clear signature of the non-Abelian structure of the underlying Uhlmann holonomy.

One can parametrize the loop \(\Gamma = \Gamma'' \circ \Gamma'\) in Fig. 1 as

\[
\Gamma'((\theta_t, \phi_t)) = \begin{cases} 
\Gamma_0' : (\theta_0'(t) \in [0, \pi], \phi_0) \\
\Gamma_1' : (\pi, \phi_0'(t) \in [\phi_0, \phi_1]) \\
\Gamma_2' : (\theta_1'(t) \in (\pi, 0), \phi_1) \\
\Gamma_3' : (0, \phi_1'(t) \in [\phi_1, \phi_1 + \pi])
\end{cases}
\]

and

\[
\Gamma''(\theta_t, \phi_t) = \begin{cases} 
\Gamma_{0''} : (\theta_0''(t) \in [0, \pi], \phi_1 + \pi) \\
\Gamma_1'' : (\pi, \phi_0''(t) \in [\phi_1 + \pi, \phi_0 + \pi]) \\
\Gamma_2'' : (\theta_1''(t) \in (\pi, 0), \phi_0 + \pi) \\
\Gamma_3'' : (0, \phi_1''(t) \in [\phi_0 + \pi, \phi_0])
\end{cases}
\]

with \(\{\theta_0''(t), \ldots, \phi_1''(t)\}\) being a time ordered set of smooth functions.

For the extremal subspaces \(\mu = \pm \mu_e\), the holonomies of the \(L, S, J\) systems are trivial in the sense that \(U_{uhl}(C_{X,\pm}^{(l,\mu)}), X = L, S, J\), become projection operators. This follows from the Abelian nature of the extremal states and from the fact that the net area vanishes for \(\Gamma\).

On the other hand, in the case where \(|\mu| < l + \frac{1}{2}\), the holonomies turn non-Abelian and the corresponding Uhlmann phases might be non-zero. We demonstrate this in detail for the \(L\) subsystem.

By using that \(U_L(0, \phi) = \mathbb{1}\), integration along \(\Gamma'\) and \(\Gamma''\) yields

\[
U_{uhl}(C_{L,\pm}^{(l,\mu)}) = e^{-i2\mu(\phi_1-\phi_0)} \begin{pmatrix} a_L & b_L \\ -b_L^* & a_L^* \end{pmatrix},
\]

\[
U_{uhl}(C_{L,\pm}^{(l,\mu)}) = e^{i2\mu(\phi_1-\phi_0)} \begin{pmatrix} a_L^* & b_L \\ -b_L^* & a_L \end{pmatrix}.
\]

Here,

\[
a_L = e^{i(\phi_1-\phi_0)} \cos^2 \left(\frac{\chi_L}{2}\right) + \sin^2 \left(\frac{\chi_L}{2}\right),
\]

\[
b_L = \cos \left(\frac{\chi_L}{2}\right) \sin \left(\frac{\chi_L}{2}\right) \left( -e^{i\phi_1} + e^{i\phi_0} \right),
\]

where \(\chi_L = wC^{(l,\mu)}\pi\). Consequently

\[
U_{uhl}(C_{L,\pm}^{(l,\mu)}) = \begin{pmatrix} |a_L|^2 - |b_L|^2 & 2a_L^*b_L \\ -2a_Lb_L^* & |a_L|^2 - |b_L|^2 \end{pmatrix}.
\]
where $C^{(l,\mu)} = C^{\mu}_{l,\mu} \circ C^{(l,\mu)}$.

We may interpret the Uhlmann holonomy in Eq. (31) as a rotation in an abstract space defined by the two states $|l, \mu \pm \frac{1}{2}\rangle$. Explicitly, if we let $\frac{2\pi}{b^L} = \tan \frac{\pi}{2} e^{-i\phi}$, and introduce the effective Pauli operators $\sigma^{L,\mu}_{l} = |l, \mu + \frac{1}{2}\rangle \langle l, \mu - \frac{1}{2}| + h.c$, $\sigma^{L}_\mu = -i|l, \mu + \frac{1}{2}\rangle \langle l, \mu - \frac{1}{2}| + h.c$, and $\sigma^{L}_\mu = |l, \mu + \frac{1}{2}\rangle \langle l, \mu + \frac{1}{2}| - |l, \mu - \frac{1}{2}\rangle \langle l, \mu - \frac{1}{2}|$, defining an internal $xyz$ coordinate system, the Uhlmann holonomy in Eq. (31) can be viewed as a rotation by an angle $\kappa$ around an axis in the internal space.

By applying the definition in Eq. (5) to the Uhlmann holonomy given by Eq. (31), we obtain the Uhlmann phase as

$$\gamma^{(l,\mu)}_{L,\pm} = \arg \left[ \text{Tr} \left( U_{\text{uhl}}(C^{(l,\mu)}_{L,\pm}) \right) \right] = \arg \xi, \quad (32)$$

where

$$\xi = 2\cos (\phi_1 - \phi_0) \sin^2 (\chi_L) + \cos^2 (\chi_L). \quad (33)$$

Hence,

$$\gamma^{(l,\mu)}_{L,\pm} = \begin{cases} 0, & \xi > 0 \\ \pi, & \xi < 0 \\ \text{undefined}, & \xi = 0 \end{cases} \quad (34)$$

The points in the space $(\phi_1 - \phi_0, \chi_L \propto C^{(l,\mu)})$ where $\xi$ vanishes form a nodal line along which the Uhlmann phase $\gamma^{(l,\mu)}_{L,\pm}$ is undefined. The points along this line are analogous to the nodal points found in Ref. 11 in the case of the mixed-state geometric phase for this system.

![FIG. 2](Color online) $\xi$ defined in Eq. (33) as a function of $\phi_1 - \phi_0$, for $l = 3$, $\mu = \frac{1}{2}$, and the coupling strengths $g = 3, 13, 37, 50$. The corresponding phase $\gamma^{(l,\mu)}_{L,\pm}$ of the Wilson loop variable associated with the Uhlmann holonomy of the $L$ subsystem is given arg $\xi$.

In Fig. 2 we have plotted $\xi$, as a function of $\phi_1 - \phi_0$ for $l = 3$, $\mu = \frac{1}{2}$, and $g = 3, 13, 37, 50$. The figure shows that $\xi$ can in fact satisfy each of the three possible conditions displayed in Eq. (34). In other words, there exist figure-8 loops for which the Uhlmann phase $\gamma^{(l,\mu)}_{L,\pm}$ is $\pi$, in contrast to the corresponding mixed-state geometric phases that always vanish for such loops. This result is due to the non-Abelian nature of the underlying Uhlmann holonomy for non-extremal states. The existence of non-zero $\gamma^{(l,\mu)}_{L,\pm}$ is furthermore related to entanglement in a non-trivial way: one can show that a non-zero $\gamma^{(l,\mu)}_{L,\pm}$ may occur only if $\frac{1}{4\sqrt{((l+\frac{1}{2})^2-\mu^2)^2}} < C^{(l,\mu)} < \frac{1}{4\sqrt{((l+\frac{1}{2})^2-\mu^2)^2}}$.

One may verify that the phase $\gamma^{(l,\mu)}_{L,\pm}$ of the Wilson loop variable associated with the Uhlmann holonomy of the $S$ subsystem may similarly be $\pi$ for certain figure-8 loops, while 0 or undefined for other loops. Note in particular that the necessary condition on concurrence for a non-zero $\gamma^{(l,\mu)}_{L,\pm}$ now reads $\frac{1}{4} < C^{(l,\mu)} < \frac{3}{4}$, which is different from the above condition for the $L$ subsystem. Thus, there may be energy eigenstates that allows for a non-zero $\gamma^{(l,\mu)}_{L,\pm}$ while $\gamma^{(l,\mu)}_{L,\pm}$ must be zero and vice versa. In fact, if $(l+\frac{1}{2})^2 - \mu^2 > 9$, then only one of the two Uhlmann phases can be $\pi$ for any given loop on the parameter sphere.

**E. Additivity**

In this section, we explore the relation between the Uhlmann phases of the whole system and the subsystems. We restrict to cyclic evolutions, for which the Uhlmann holonomy takes the Wilson loop form.

For $|\mu| < l + \frac{1}{2}$, we put $A^{(l,\mu)}_{L;SU(2)} = A^{(l,\mu)}_{L;U(1)} + A^{(l,\mu)}_{L;SU(2)}$, where $A^{(l,\mu)}_{L;U(1)} = \mu(1 - \cos \theta) d\phi$, and obtain

$$\gamma^{(l,\mu)}_{J,\pm} = \gamma^{(l,\mu)}_{L,\pm} + \gamma^{(l,\mu)}_{S,\pm} - \arg \left[ \text{Tr} \left( \text{Pe}^{-i f^L_{\text{uhl}} A^{(l,\mu)}_{L;SU(2)}} \right) \right] \quad (35)$$

Since the trace of an SU(2) matrix is real, the deviation $\Delta \gamma^{(l,\mu)}_{J,\pm}$ from the sum rule $\gamma^{(l,\mu)}_{J,\pm} = \gamma^{(l,\mu)}_{L,\pm} + \gamma^{(l,\mu)}_{S,\pm}$ can only be $\pi$ for a cyclic evolution in this model system. Similar to the nodal points found in Ref. 11 for the mixed-state geometric phases $\xi^{(l,\mu)}$ of the $L$ and $S$ subsystems, there exist loops for which either $\text{Tr} \left( \text{Pe}^{-i f^L_{\text{uhl}} A^{(l,\mu)}_{L;SU(2)}} \right)$ or $\text{Tr} \left( \text{Pe}^{-i f^S_{\text{uhl}} A^{(l,\mu)}_{S;SU(2)}} \right)$ vanish so that $\Delta \gamma^{(l,\mu)}_{J,\pm}$ becomes undefined. These loops are nodal points of $\gamma^{(l,\mu)}_{L,\pm}$ or $\gamma^{(l,\mu)}_{S,\pm}$, respectively.

We demonstrate that $\Delta \gamma^{(l,\mu)}_{J,\pm}$ can be zero, non-zero, or undefined for the “orange slice” loop defined in Eq. (27), which connects the two poles on the parameter sphere twice along geodesics at $\phi_0$ and $\phi_1$. 

The holonomy of the $L$ subsystem for the orange slice loop $\Gamma'$ can be found in Eq. (29). For the $S$ subsystem, we obtain

$$U_{\text{uhl}}(C_{S,\pm}^{(l,\mu)}) = \begin{pmatrix} a_S^* & -b_S^* \\ b_S & a_S \end{pmatrix},$$

where $a_S$ and $b_S$ are obtained from $a_L$ and $b_L$ in Eq. (30) by replacing $\chi_L$ with $\chi_S = C^{(l,\mu)}$. The corresponding Uhlmann phases read

$$\gamma_{J;\pm}^{(l,\mu)} = -\mu(\phi_1 - \phi_0),$$

$$\gamma_{L;\pm}^{(l,\mu)} = -\mu(\phi_1 - \phi_0) + \arg \left[ \cos^2 \left( \frac{\chi_L}{2} \right) \cos (\phi_1 - \phi_0) + \sin^2 \left( \frac{\chi_L}{2} \right) \right],$$

$$\gamma_{S;\pm}^{(l,\mu)} = \arg \left[ \cos^2 \left( \frac{\chi_S}{2} \right) \cos (\phi_1 - \phi_0) + \sin^2 \left( \frac{\chi_S}{2} \right) \right].$$

(37)

Thus, $\Delta \gamma^{(l,\mu)} = -\arg \zeta$, where

$$\zeta = \left[ \cos^2 \left( \frac{\chi_L}{2} \right) \cos (\phi_1 - \phi_0) + \sin^2 \left( \frac{\chi_L}{2} \right) \right] \times \left[ \cos^2 \left( \frac{\chi_S}{2} \right) \cos (\phi_1 - \phi_0) + \sin^2 \left( \frac{\chi_S}{2} \right) \right].$$

(38)

$\Delta \gamma^{(l,\mu)}$ is 0 if $\zeta > 0$, $\pi$ if $\zeta < 0$, and undefined if $\zeta = 0$. All these three cases are visible in Fig. (3), in which we have plotted $\zeta$ as a function of $\phi_1 - \phi_0$ for fixed $l$, $\mu$, and $g = 3, 20, 50$. Figure 3 confirms that there are some loops on the parameter sphere for which $\Delta \gamma^{(l,\mu)} \neq 0$, and therefore $\gamma_{J;\pm}^{(l,\mu)} \neq \gamma_{L;\pm}^{(l,\mu)} + \gamma_{S;\pm}^{(l,\mu)}$.

To compare with the mixed state geometric phase proposed in Ref. [13], we first consider the spectral decomposition $\{p_k, |\psi_k\rangle\}$ of an arbitrary non-degenerate density operator $\rho$ that undergoes cyclic unitary evolution. The resulting mixed state geometric phase $\beta$ reads $\beta = \arg \left( \sum_k p_k e^{i\gamma_k} \right)$, where $\gamma_k$ is the cyclic pure state geometric phase of $|\psi_k\rangle$. Using this expression, the mixed-state geometric phases $\beta(C_{L;\pm}^{(l,\mu)})$ and $\beta(C_{S;\pm}^{(l,\mu)})$ of the $L$ and $S$ subsystems read

$$\beta(C_{L;\pm}^{(l,\mu)}) = -\mu \Omega \pm \arctan \left( \frac{\cos \alpha^{(l,\mu)}}{\tan \Omega} \right),$$

$$\beta(C_{S;\pm}^{(l,\mu)}) = \mp \arctan \left( \frac{\cos \alpha^{(l,\mu)}}{\tan \Omega} \right),$$

(39)

which implies the sum rule $\beta(C_{L;\pm}^{(l,\mu)}) + \beta(C_{S;\pm}^{(l,\mu)}) = -\mu \Omega = \beta(C_{J;\pm}^{(l,\mu)})$. Thus, the sum rule for $\beta$ is satisfied for any loop $\Gamma$ on the parameter sphere. This again demonstrates the difference between the phase of the Wilson loop variable associated with the Uhlmann holonomy and the mixed-state geometric phase defined in Ref. [13].

We note that, the alternative Uhlmann phase $\varphi_{\text{uhl}}$ defined in Eq. (11) is in general non-zero for the figure-8 path in Fig. 1 as a consequence of the non-Abelian nature of the underlying Uhlmann holonomy. On the other hand, the corresponding deviation $\Delta \varphi_{\text{uhl}}^{(l,\mu)}$ from the sum rule is no longer restricted to 0 or $\pi$, but can take any real value for cyclic evolutions. Thus, in general there is a difference between $\varphi_{\text{uhl}}$ and $\gamma$, and they both differ, in the sense of the sum rule, from the mixed-state geometric phase in Ref. [13].

V. CONCLUSIONS

Uhlmann’s quantum holonomy along density operators is a concept that allows for studies of geometric phases of general quantum states undergoing arbitrary quantum evolutions. Its relevance to various aspects of physics have been demonstrated in the past, such as for open system evolution [28], interferometry [29], many-body quantum systems [30], as well as for Yang-Mills theory [31] and Thomas precession in special relativity [32]. These works have been triggered in part by the need to test the conjectured resilience of holonomic quantum gates for quantum computation to various kinds of errors, such as noise and decoherence. Recently, a first experimental test of the related Uhlmann geometric phase, utilizing nuclear magnetic resonance techniques, has been carried out [20].

Here, we have analyzed Uhlmann’s quantum holonomy by considering a physical model system in which the Uhlmann holonomies for LS-coupled hydrogen-like atoms in a slowly rotating magnetic field have been computed. We have shown that the holonomy of the total angular momentum has Abelian structure. Furthermore, its corresponding phase is exactly the associated standard geometric phase for open or closed paths on the parameter sphere of magnetic field directions. For the holonomies of the $L$ and $S$ subsystems, we have shown that, in analogy with the Lévy geometric phase defined for two-qubit systems [23], depending
on whether the energy eigenstate of the whole system is a product state or an entangled state, the corresponding holonomies are Abelian or non-Abelian, respectively. In the case of entangled states, there is an explicit dependence of the gauge field vector potential on the concurrence [22], which interpolates the standard Abelian (Berry) and non-Abelian (Wilczek-Zee) cases. In other words, our analysis demonstrates that the rich geometrical nature of the Uhlmann holonomy incorporates as a limiting case the Wilczek-Zee holonomy, which is characterized by maximum quantum entanglement between the L and S subsystems.

In the analysis of the phase of the Wilson loop variable associated with the Uhlmann holonomy, we have pointed out that this phase, unlike the mixed-state geometric phase [13], possesses a non-Abelian structure and may therefore be non-zero even for loops on the parameter sphere that enclose no net area. We have also elucidated that the phases of the Wilson loop variables of the corresponding Uhlmann holonomies for the L and S subsystems add up to that of the whole system for specific paths; for other paths the sum may differ by $\pi$ from the Berry phase of the whole system.

Furthermore, we would like to point out that previous theoretical [17–19] and experimental [20] work analyzing the relation between the Uhlmann holonomy and the mixed-state geometric phase all employ a notion of the Hilbert-Schmidt overlap between the initial and parallel transported final Uhlmann amplitude. In Ref. [20] it was also pointed out that other definitions of mixed-state geometric phases, which differ both from the geometric phase considered in Ref. [13] and the (Hilbert-Schmidt) Uhlmann phase are in principle possible and experimentally relevant. It is important that these different definitions of mixed-state geometric phases be thoroughly investigated and compared with the phases associated to the Uhlmann holonomy in model systems, where exact or computationally feasible solutions exist. Our paper is a contribution in this direction.

The results for the phase of the Wilson loop variable suggest it would be of interest to test the relation between this phase and various mixed-state geometric phases experimentally. This would further improve our understanding of the relation between the Uhlmann holonomy [10] and the mixed-state geometric phase [13]. It would also help shed light on which of these phases is the most robust and, at the same time, the most accessible experimentally and the most amenable to external manipulation.

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