I. INTRODUCTION

A particular instance of Berry’s discovery [1] of geometric phase factors accompanying adiabatic changes is the occurrence of sign reversal of eigenfunctions of real Hamiltonians when transported around certain types of degeneracies. Although already implied in a work by Darboux [2] in the late 19th century, the significance of such sign changes to physics was not realized until Longuet-Higgins and coworkers pointed out their existence in molecular theory [3, 4]. This latter insight led Mead and Truhlar to the notion of the molecular Aharonov-Bohm effect [5, 6], which has attracted experimental [7] and theoretical [8, 9] interest recently.

Sign reversal has been noted [10] in characteristic functions of vibrating membranes whose boundary is changed around closed paths. Such sign change patterns in the vicinity of degeneracies have been studied by experiments on microwave resonators [11, 12] and smectic films [13]. The microwave resonator experiments have been interpreted in terms of both the standard [14] and the off-diagonal [15] geometric phases, and they have motivated further theoretical studies concerning both the geometric phases and structure of the wave functions for real Hamiltonians [14, 15, 16, 17].

It was proved by Longuet-Higgins [16] that sign reversal of real electronic eigenfunctions when continuously transported around a loop in nuclear configuration space signals the existence of degeneracy points inside the loop. This topological result has been used to detect conical intersections in LiNaK [19] and ozone [20, 21]. On the other hand, there are cases where the Longuet-Higgins test fails, such as, e.g., when the loop encircles an even number of conical intersections [22]. This apparent limitation of the Longuet-Higgins theorem was resolved by the present authors [23], who put forward a topological test for degeneracies of real matrix Hamiltonians based upon consideration of their eigenvectors on loops in parameter space. This generalized test was further proved [24] to be optimal in the sense that it exhausts all topological information contained in the eigenvectors, related to the presence of degeneracies.

Continuous change of the eigenvectors of a real parameter dependent $n \times n$ matrix Hamiltonian around a closed path in parameter space may, if all geometric phase factors are unity, be viewed as a loop in the $n$ dimensional rotation group $SO(n)$. Based upon this observation, it was proved [23] that if the eigenvectors correspond to a nontrivial loop in $SO(n)$, then the loop must encircle at least one point of degeneracy. Thus, in order to apply the test we need to find a procedure to determine whether the change of the eigenvectors corresponds to a trivial loop in $SO(n)$ or not. In Ref. [23], methods particularly adapted to the special cases $n = 2, 3, 4$ were presented. The main focus of the present paper is to provide a method that makes the test applicable to any $n$.

Another important issue for the applicability of the test in Ref. [23] arises when noting that $n$ may be very large in many realistic scenarios. For example, the computed electronic eigenvectors in quantum chemical applications typically live in very large Hilbert spaces. This could make the test difficult to use in this important class of problems where degeneracy points play a vital dynamical role. To overcome this potential complication, we put forward a condition for when the test can be applied to subspaces of the full Hilbert space.

Stone [24] demonstrated a topological test that extended Longuet-Higgins’ original test [16] to the complex Hamiltonian case. In brief, this former test entails that if the standard geometric phase changes continuously by a nonzero integer multiple of $2\pi$ for a continuous set of loops in parameter space, starting and ending with infinitesimally small loops, then this set of loops must enclose a degeneracy point. As for Longuet-Higgins’ test,
Theorem 1. of Ref. [23] can be summarized in the following theorem. (F of the eigenvectors are unity, we may define the function loop and if all the concomitant geometric phase factors along Γ. If there are no points of degeneracy on the Q Γ otherwise around F a nontrivial loop was only treated in the Q previously. The outline of the paper is as follows. In the next II. TOPOLOGICAL TEST FOR DEGENERACITIES

Let H(Q) be an n × n parameter dependent matrix Hamiltonian, written in the fixed basis {∣i⟩}i=1n of the n dimensional Hilbert space H. We suppose that H(Q) is real, symmetric, and continuous for each Q = (Q1, . . . , Qd) in parameter space Q, which we assume to be a simply connected subset of Rd. Consider a loop Γ in Q. Let {ψi(Q)}i=1n be a positively oriented set of orthonormalized real eigenvectors of H(Q) for each Q along Γ. If there are no points of degeneracy on the loop and if all the concomitant geometric phase factors of the eigenvectors are unity, we may define the function F : Γ → SO(n) as

\[
F(Q) = \begin{pmatrix}
⟨1|ψ_1(Q)⟩ & ⟨1|ψ_2(Q)⟩ & \cdots & ⟨1|ψ_n(Q)⟩ \\
⟨2|ψ_1(Q)⟩ & ⟨2|ψ_2(Q)⟩ & \cdots & ⟨2|ψ_n(Q)⟩ \\
\vdots & \vdots & \ddots & \vdots \\
⟨n|ψ_1(Q)⟩ & ⟨n|ψ_2(Q)⟩ & \cdots & ⟨n|ψ_n(Q)⟩
\end{pmatrix},
\]

such that F(Γ) is a loop in SO(n). Then, the main result of Ref. [23] can be summarized in the following theorem.

Theorem 1. If the n eigenvectors of H(Q) represent a nontrivial loop F(Γ) in SO(n) when taken continuously around Γ, then there must be at least one degeneracy point of H(Q) on every simply connected surface S bounded by Γ.

The predictive power of Theorem 1 stems from the existence of nontrivial loops in SO(n) ≥ 2. However, to determine to which homotopy class a given loop belongs was only treated in the n = 2, 3, 4 cases in Ref. [23], while the problem to find such a method for general n was left open. Here, we resolve this deficiency and put forward an explicit method that treats the general n case. Let F : [0, 1] → SO(n) be a loop in SO(n). Without loss of generality we assume that F(0) = F(1) equals the identity I on SO(n). This can always be achieved by multiplying the whole loop by F(0)−1 = F(0)T, an operation that does not change the homotopy class of F.

The space SO(n) of real orthogonal matrices with unit determinant forms a Lie group whose corresponding Lie algebra so(n) is the space of real antisymmetric matrices (see, e.g., Ref. [23], p. 172). Furthermore, the exponential map

\[
\exp : \mathfrak{so}(n) \to SO(n)
\]

\[
A \to I + \sum_{k=1}^{\infty} \frac{A^k}{k!}
\]

is continuous, onto, and exp(A) is well-defined for all A ∈ so(n). The function log : SO(n) → so(n) is defined as the inverse of the exponential map. It is multi-valued, i.e., there exist A ≠ B such that exp(A) = exp(B).

By continuity of the exponential map, any curve F : [0, 1] → so(n) satisfying exp(F(0)) = exp(F(1)) corresponds to a loop F in SO(n) via

\[
F(t) = \exp(F(t)).
\]

For brevity we say that continuous curves in so(n) for which exp(F(0)) = exp(F(1)) are l-curves. Our objective is to find a correspondence between classes of l-curves and the two homotopy classes of loops in SO(n) (n ≥ 3). This will make it possible to deduce whether a loop F in SO(n) is trivial by studying its corresponding l-curve F. We first make a classification of the l-curves.

Definition 1. Let F0 and F1 be l-curves in so(n). If there is a continuous function L : [0, 1] × [0, 1] → so(n) such that L(t, 0) = F0(t), L(t, 1) = F1(t), and exp(L(0, s)) = exp(L(1, s)) holds for all s ∈ [0, 1], then F0 and F1 are called l-homotopic. The function L is called an l-homotopy between F0 and F1.

Two l-curves are thus l-homotopic if they can be deformed into each other through a continuous family consisting solely of l-curves. The following connection between l-homotopy in so(n) and homotopy in SO(n) holds.

Proposition 1. If F0 and F1 are l-homotopic curves in so(n), then their corresponding loops F0 and F1 in SO(n) are homotopic.

Proof. A homotopy K : [0, 1] × [0, 1] → SO(n) between F0 and F1 is given by

\[
K(t, s) = \exp(L(t, s)),
\]

where L is as in Definition 1. K defined in this way is continuous since it is the composition of two continuous functions. Furthermore t ↦ K(t, s) is a loop for each s since t ↦ L(t, s) is an l-curve for each s.
Let \( \exp(\overline{F}(0)) = \exp(\overline{F}(1)) = I \), we may choose \( \overline{F}(0) \) to be the zero matrix. \( \overline{F}(1) \) is denoted \( K \). We show that an \( l \)-curve \( \overline{F} \) between the zero matrix and \( K \) is \( l \)-homotopic, either to a point, or to an \( l \)-curve connecting the zero matrix to a matrix having only one nonzero \( 2 \times 2 \) block given by \( 2\pi i \sigma_y \). In the first case the corresponding loop \( F = \exp(\overline{F}) \) in \( SO(n) \) is trivial, and in the second case it is not. We also formulate a simple criterion that can be used to determine to which “\( l \)-homotopy class” \( F \) belongs.

On our way we need the following three lemmas, the first of which is a standard lemma from matrix theory \[20\].

**Lemma 1.** Let \( A \) be an antisymmetric matrix. Then there is an orthogonal matrix \( R \) and a block diagonal matrix \( D^A \) such that

\[
A = RD^AR^T,
\]

where the blocks of \( D^A \) are \( 2 \times 2 \) matrices of the form

\[
D^A_i = \begin{pmatrix} 0 & \alpha_i \\ -\alpha_i & 0 \end{pmatrix} \equiv i\alpha_i\sigma_y,
\]

with \( \alpha_i \geq 0 \). If the dimension \( n \) is odd, there is also a zero \( 1 \times 1 \) block.

For notational convenience, we assume from now on that \( n \) is even. The analysis for odd \( n \) is identical.

**Lemma 2.** Suppose that \( \lambda \) is a degenerate eigenvalue of \( \exp(A) \), and that the corresponding eigenspace is \( V \). Then \( \exp(RAR^T) = \exp(A) \) for any orthogonal matrix \( R \) acting nontrivially only on \( V \).

**Proof.**

\[
\exp(RAR^T) = R\exp(A)R^T = \exp(A),
\]

where the last equality follows since \( \exp(A) \) is \( \lambda I \) on \( V \).

**Lemma 3.** Let \( A \) and \( B \) be antisymmetric matrices such that \( \exp(A) = \exp(B) \), and let \( \overline{F} \) be an \( l \)-curve between them. Then the following statements hold.

(a) \( \overline{F} \) is \( l \)-homotopic to any other \( l \)-curve connecting \( A \) to \( B \). Specifically it is \( l \)-homotopic to the straight line \( t \mapsto (1 - t)A + tB \).

(b) If \( X \) is an antisymmetric matrix commuting with both \( A \) and \( B \), then \( L(t, s) = \overline{F}(t) - sX \) is an \( l \)-homotopy. The \( l \)-curve \( L(t, 1) \) connects \( A \) to \( B \).

(c) Let \( \lambda \) be a degenerate eigenvalue of \( \exp(A) \), and \( V \) be the corresponding eigenspace. If \( R \) is an orthogonal transformation with unit determinant acting nontrivially only on \( V \), then \( \overline{F} \) is \( l \)-homotopic to an \( l \)-curve connecting \( RAR^T \) to \( B \).

**Proof.** (a) Follows since \( so(n) \) is a vector space, and thus simply connected. To prove (b) we note that \( L \) is continuous and that

\[
\exp(L(0, s)) = \exp(A - sX) = \exp(A)\exp(-sX) = \exp(B)\exp(-sX) = \exp(B - sX) = \exp(L(1, s)). \tag{8}
\]

For (c), note that since \( R \) acts nontrivially only on \( V \), it is possible to write \( R = \exp(\overline{C}) \), where \( C \) is an antisymmetric matrix whose null space contains the orthogonal complement of \( V \). This means that \( \exp(\overline{C}) \) acts nontrivially only on \( V \) for any real number \( r \). Lemma \[2\] is thus applicable, and \( \exp(\overline{\exp(-rC)}\overline{A}\exp(\overline{rC})) = \exp(A) \) for any \( r \). We may thus define the \( l \)-homotopy

\[
L(t, s) = \exp((1 - t)sC)\overline{F}(t)\exp((t - 1)sC). \tag{9}
\]

We see that \( L(t, 0) = \overline{F}(t) \), \( L(0, 1) = RAR^T \), and \( L(1, 1) = B \) as required.

Before we proceed it is convenient to introduce some notation to describe block diagonal matrices. First, \( A_1 \oplus \ldots \oplus A_m \) will denote a block diagonal matrix with blocks \( A_1, \ldots, A_m \). Secondly, for any numbers \( \lambda_1, \ldots, \lambda_n/2 \) we define \( [\lambda_1, \ldots, \lambda_n/2] \equiv (i\lambda_1\sigma_y) \oplus \ldots \oplus (i\lambda_n/2\sigma_y) \). Note that any two matrices of this form commute. Thirdly, \( I_m \) and \( 0_m \) denote the \( m \)-dimensional unit and zero matrix, respectively.

Now, we return to our \( l \)-curve \( \overline{F} \) connecting \( 0_n = \overline{F}(0) \) to \( K \equiv \overline{F}(1) \). Let \( R \) be as in Lemma \[1\] so that \( K = RD^KR^T \), with \( D^K = [a_1, \ldots, a_n/2] \). Note that since \( \exp(K) = I \), we must have \( \alpha_i = 2\pi k_i \) for some integers \( k_i \). At the possible cost of having some \( k_i < 0 \) we may assume \( R \) to have unit determinant. This implies that \( \overline{F} \) is \( l \)-homotopic to any \( l \)-curve connecting \( 0_n \) and \( D^K \). To see this, let \( R = \exp(\overline{C}) \) and define

\[
L(t, s) = \exp(-sC)\overline{F}(t)\exp(sC). \tag{10}
\]

Clearly \( L(t, 0) = \overline{F}(t) \) and \( L(t, 1) \) goes from \( 0_n \) to \( D^K \). Furthermore, \( L \) is continuous, and

\[
\exp(L(0, s)) = I = \exp(L(1, s)). \tag{11}
\]

Thus, \( L \) is an \( l \)-homotopy, and by Lemma \[3\](a), \( \overline{F} \) is \( l \)-homotopic to the \( l \)-curve

\[
\overline{F}_{\text{block}}(t) = tD^K. \tag{12}
\]

Our goal is to make as many as possible of the \( k_i \) disappear through \( l \)-homotopies. We begin by reducing each of them to zero or one. Assume that \( k_i \geq 2 \). The case \( k_i \leq -1 \) can be treated similarly. Define \( Y_i = [0, \ldots, 0, 2\pi, 0, \ldots, 0] \), where the \( 2\pi \) appears at the \( i \)-th place. \( Y_i \) commutes with \( 0_n \) and \( D^K \), i.e.,

\[
L(t, s) = \overline{F}_{\text{block}}(t) - sY_i. \tag{13}
\]
is an $l$-homotopy transforming $\tilde{F}_{\text{block}}$ into $\tilde{F}_i = (t - 1)Y_i + t(D^K - Y_i)$. This $l$-curve starts at $-Y_i$ and terminates in the matrix $D^K - Y_i = 2\pi[k_1, \ldots, k_{i-1}, k_i, -1, k_{i+1}, \ldots, k_n]$. Furthermore $\exp(-Y_i) = I$. This makes Lemma 3(c) applicable, $V$ being the whole space. For $i \geq 2$ (the case $i = 1$ is similar), we choose the orthogonal transformation $R$ as

$$R = I_{2i-3} \oplus (-I_1) \oplus \sigma_x \oplus I_{n-2i},$$

(14)

where $\sigma_x$ is the $x$ component of the standard Pauli matrices. $R$ thus defined has unit determinant, and

$$R(-Y_i)R^T = 0_{2i-2} \oplus (-i2\pi\sigma_x\sigma_y\sigma_x) \oplus 0_{n-2i} = 0_{2i-2} \oplus (i2\pi\sigma_y) \oplus 0_{n-2i} = Y_i.$$

Consequently, by Lemma 3(c) $\tilde{F}_i$ is $l$-homotopic to an $l$-curve between $Y_i$ and $D^K - Y_i$, and thus to the $l$-curve

$$\tilde{F}_{\text{block},i-}(t) = t(D^K - 2Y_i).$$

(16)

If we compare this to Eq. (12), and note that $D^K - 2Y_i = 2\pi[k_1, \ldots, k_{i-1}, k_i - 2, k_{i+1}, \ldots, k_n]$, we see that we have reduced $k_i$ by two.

Proceeding in this way we may show that $\tilde{F}_{\text{block}}$ is $l$-homotopic to $\tilde{F}_{\text{red}}(t) = tP$, where $P = 2\pi[\delta_1, \ldots, \delta_n]$, and $\delta_i$ is defined by

$$\delta_i = \begin{cases} 1 & \text{if } k_i \text{ is odd} \\ 0 & \text{if } k_i \text{ is even.} \end{cases}$$

(17)

Our next task is to reduce the number of nonzero $\delta_i$ to one or zero. We will show that any pair $\delta_i = \delta_j = 1$ can be eliminated through $l$-homotopies. The procedure for doing this is similar to the reduction of the $k_i$.

Suppose that $i < j$. First deform $\tilde{F}_{\text{red}}$ by

$$L(t, s) = \tilde{F}_{\text{red}}(t) - \frac{s}{2}(Y_i + Y_j),$$

(18)

yielding $\tilde{F}_{i,j}(t)$ starting at $-Y \equiv -\frac{1}{2}(Y_i + Y_j)$. Note that $\exp(-Y)$ is four-fold degenerate with eigenvalue $-1$. The eigenspace is $\text{supp}(Y)$. We apply Lemma 3(c) with $R$ defined by

$$R = I_{2(i-1)} \oplus \sigma_x \oplus I_{2(j-i-1)} \oplus \sigma_x \oplus I_{n-2j},$$

(19)

This matrix is orthogonal and has unit determinant. Also, we may verify that

$$R(-Y)R^T = Y.$$ 

(20)

Consequently, as we went from $\tilde{F}_{\text{block}}(t) = tD^K$ to $\tilde{F}_{\text{block},i-}(t) = t(D^K - 2Y_i)$, we can go from $\tilde{F}_{\text{red}}(t) = tP$ to $\tilde{F}_{\text{red},i-}(t) = t(P - 2Y_i) = t(P - Y_i - Y_j)$. The matrix $P - Y_i - Y_j$ has the same structure as $P$, but has $\delta_i = \delta_j = 0$. Continuing in this fashion we can reduce the number of nonzero $\delta_i$ to one (zero) if this number was odd (even) to begin with. Note that this number is odd (even) exactly when $\sum_{i=1}^{n/2} k_i$ is odd (even). At long last we arrive at the following main result.

**Theorem 2.** Suppose that $F$ is a loop in $SO(n)$ starting at $I$ and that $\tilde{F}$ is an $l$-curve that maps to $F$ under the exponential map Eq. (3). Then there is an orthogonal transformation $R$ so that

$$\tilde{F}(1) = R2\pi(ik_1\sigma_y) \oplus \ldots \oplus (ik_{n/2}\sigma_y)R^T,$$

(21)

for some integers $k_1, \ldots, k_{n/2}$. Furthermore $F$ is trivial if and only if $h = \sum_{i=2}^{n/2} k_i$ is even.

Note that in case of odd $n$, the matrix $R^T\tilde{F}(1)R$ has one zero $1 \times 1$ block that can be ignored.

**Proof.** The theorem follows from the above discussion, and from Proposition 4. If $h$ is even, then $\tilde{F}$ is $l$-homotopic to a point. Otherwise it is $l$-homotopic to $\tilde{F}_Y(t) = tY_i$ for some $i$, which makes $\exp(\tilde{F}_Y(t))$ nontrivial.

**Theorem 2** reduces the task of determining the homotopy class of a loop in $SO(n)$ that starts at the identity to computing the logarithm $\tilde{F}$ and block diagonalizing its ending point.

We illustrate the procedure by determining the homotopy class of a loop in $SO(3)$. Let

$$F(\theta) = \left( \begin{array}{ccc} \frac{1}{2}(\cos \theta + 1) & -\frac{1}{\sqrt{2}} \sin \theta & \frac{1}{2}(\cos \theta - 1) \\ \frac{1}{\sqrt{2}} \sin \theta & \cos \theta & \frac{1}{\sqrt{2}} \sin \theta \\ \frac{1}{2}(\cos \theta - 1) & -\frac{1}{\sqrt{2}} \sin \theta & \frac{1}{2}(\cos \theta + 1) \end{array} \right),$$

(22)

where $\theta \in [0, 2\pi]$ parametrizes the loop. This loop appears in the analysis of the $T \otimes \gamma_2$ Jahn-Teller system. In fact, Eq. (22) represents the loop in Eq. (4) of Ref. [23] multiplied by its inverse at Jahn-Teller system.

Note that $\tilde{F}$ is undefined at $\theta = 0$ and $2\pi$, since $F(0) = F(2\pi) = I$. It is straightforward to check that $\exp(\tilde{F}(\theta)) = F(\theta)$ if we define

$$\tilde{F}(\theta) = \phi(\theta) \begin{pmatrix} 0 & \hat{v}_3(\theta) & \hat{v}_2(\theta) \\ \hat{v}_3(\theta) & 0 & \hat{v}_1(\theta) \\ \hat{v}_2(\theta) & \hat{v}_1(\theta) & 0 \end{pmatrix} \begin{pmatrix} \theta \\ 0 \\ 0 \end{pmatrix} = \frac{\theta}{\sqrt{2}} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}.$$ 

(24)

This curve is continuous everywhere, starts at the zero matrix and ends, by continuity, at

$$K = \pi \sqrt{2} \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}.$$ 

(25)
The orthogonal transformation
\[ R = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 0 & 1 \\ 0 & \sqrt{2} & 0 \\ 1 & 0 & 1 \end{pmatrix} \] (26)
block diagonalizes $K$. Explicitly, we have
\[ D^K = R^T K R = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 2\pi \\ 0 & -2\pi & 0 \end{pmatrix} \] (27)
Thus, $h = k_1 = 1$ and the loop is nontrivial.

III. APPLICATION TO SUBSPACES

Here, we demonstrate how to apply the test to a subspace of Hilbert space. Specifically, we show that if $p < \dim \mathcal{H}$ eigenvectors of a parameter dependent Hamiltonian can be well approximated by their projections in some fixed $p$ dimensional subspace of Hilbert space, then the $p$ dimensional version of the test in Ref. [23] is applicable. This result may be of use in quantum chemical applications, where the detection of degeneracy points for electronic Hamiltonian matrices of large dimension becomes pertinent.

Suppose that $\{|i\rangle\}_{i=1}^p$ is an orthonormal set of fixed real vectors. We consider $p$ eigenvectors $\{|\psi_i(Q)\rangle\}_{i=1}^p$ of $H(Q)$ and their projections in $\text{Span}\{|i\rangle\}$. Define
\[ P = \sum_{i=1}^p |i\rangle\langle i|, \]
\[ |\phi_i(Q)\rangle = P|\psi_i(Q)\rangle, \]
\[ |\phi_i^+(Q)\rangle = |\psi_i(Q)\rangle - |\phi_i(Q)\rangle \] (28)
The eigenvectors $|\psi_i(Q)\rangle$ are mutually orthogonal, but $|\phi_i(Q)\rangle$ need not be. In fact they may even be linearly dependent. This, however, can occur only if $\langle \phi_i(Q)|\phi_i(Q)\rangle$ is sufficiently small for some $i$. This is formalized in Proposition 2.

Lemma 4. Let $v_1, \ldots, v_p$ be linearly dependent unit vectors in a real vector space. Then for some pair $v_j, v_k$ with $j \neq k$ we have
\[ |v_j \cdot v_k| \geq \frac{1}{p - 1}. \] (29)
Proof. Let $\text{Span}\{v_1, \ldots, v_p\}$ have dimension $m$. It is enough to prove the statement for $m = p - 1$, since if it is false for some $m$, then it is false for all higher $m$.

Intuitively, to make all scalar products as small as possible, we need to “spread” the vectors as much as possible, i.e., the vectors should point to the vertices of a regular $(p - 1)$-simplex [29]. The scalar product between any two distinct vectors is then $\frac{1}{p - 1}$ [30]. This proves the statement. \hfill \square

Proposition 2. Suppose that
\[ \langle \phi_i|\phi_i \rangle > 1 - \frac{1}{p} \] (30)
holds for all $i$. Then $\{|\phi_i\rangle\}$ is a linearly independent set.

Proof. Assume that Eq. (30) holds for each $i$, and that the vectors $|\phi_i\rangle$ are linearly dependent. We show that this leads to a contradiction. With $|\phi_i\rangle = |\phi_i^N\rangle \sqrt{\langle \phi_i|\phi_i \rangle}$, there are by Lemma 4 $j \neq k$ such that
\[ \langle \phi_j|\phi_k \rangle = \sqrt{\langle \phi_j|\phi_k \rangle \langle \phi_k^N|\phi_k^N \rangle} \]
\[ > \left(1 - \frac{1}{p}\right) \frac{1}{p - 1} = \frac{1}{p}. \] (31)
Note however that
\[ 0 = \langle \psi_j|\psi_k \rangle = \langle \phi_j|\phi_k \rangle + \langle \phi_j^+|\phi_k^+ \rangle \] (32)
and thus that
\[ |\langle \phi_j|\phi_k \rangle| = |\langle \phi_j^+|\phi_k^+ \rangle| \leq \left(\langle \phi_j^+|\phi_j^+ \rangle \langle \phi_k^+|\phi_k^+ \rangle\right)^{1/2} \]
\[ = \left(1 - \langle \phi_j|\phi_j \rangle\right)\left(1 - \langle \phi_k|\phi_k \rangle\right)^{1/2} \]
\[ < \frac{1}{p}. \] (33)
contradicting Eq. (31). \hfill \square

We are now in a position to give a condition for when the $p$ dimensional test is applicable to a subspace of Hilbert space. Let $S$ be a simply connected surface in $Q$, bounded by the loop $\Gamma$, and let the $p$ eigenvectors along $\Gamma$ be denoted $\{|\psi_i(Q)\rangle\}_{i=1}^p$. Assume that for $|\phi_i(Q)\rangle$ defined by Eq. (28), the inequality
\[ \langle \phi_i(Q)|\phi_i(Q)\rangle > 1 - \frac{1}{p}. \] (34)
holds for each $i$, and for each $Q \in S$. The set $\{|\phi_i(Q)\rangle\}_{i=1}^p$ is then linearly independent by Proposition 2. This means that the Gram-Schmidt orthonormalization procedure can be applied to $\{|\phi_i(Q)\rangle\}_{i=1}^p$, for any $Q \in S$. This procedure is continuous, and produces an orthonormal set $\{|\phi_i^{GS}(Q)\rangle\}_{i=1}^p$, which can be interpreted as an element $F(Q) \in SO(p)$. Thus, given that Eq. (34) holds and that $H(Q)$ is nondegenerate on $S$, we have a continuous function $F : S \to SO(p)$. By the same reasoning as in Ref. [23] we arrive at the following result.

Proposition 3. Suppose that the projections $|\phi_i(Q)\rangle$ of the $p$ eigenvectors of $H(Q)$ satisfy Eq. (27) for each $Q \in S$. Suppose furthermore that $F(Q)$ defined as above traces out a nontrivial loop in $SO(p)$ as $Q$ varies along $\Gamma$. Then $H(Q)$ becomes degenerate somewhere in $S$.

Note that the result in Proposition 4 concerns the exact Hamiltonian $H(Q)$, but is based upon the behavior of the approximate eigenvectors $|\phi_i(Q)\rangle$. 

IV. STONE’S TEST

The original test by Longuet-Higgins 18, as well as its generalization 22, suffers from the limitation of being applicable only to real Hamiltonians. When the test of Longuet-Higgins is applicable, the loop in parameter space maps to an open curve in $\mathbb{R}^n$ representing the Hilbert space. In this case the corresponding loop in the space of states $\mathbb{R}P^{n-1}$ is nontrivial. Similarly, the generalization makes use of the existence of nontrivial loops in $SO(n)$, the space of eigenbases. A pertinent question is whether there exist analogous results for the general complex case.

For a generic Hamiltonian, the degenerate subsets of parameter space have co-dimension 3 24, 31, meaning that any such test must consider eigenvectors on a closed surface, rather than on a closed loop. An eigenstate taken around the surface represents a 2-loop in projective space, being the $n-1$ dimensional complex projective space $\mathbb{C}P^{n-1}$.

Stone 24 put forward a topological test relating the behavior of a single eigenvector on a closed surface $S$ in parameter space, to the presence of degeneracies inside the surface. Potentially, this test might be possible to generalize in the same manner as the one by Longuet-Higgins. However, as shown below, this is impossible.

Despite that it preceded Berry’s work 1 by eight years, Stone’s test is conveniently formulated in the language of geometric phases. The surface $S$ is swept out by a continuous set $\{L_i\}_{i=1}^N$ of loops, where $L_1$ and $L_N$ are infinitesimally small. The cyclic geometric phases $\{\gamma_i\}_{i=1}^N$ along these loops are modulo $2\pi$ quantities. However, if we require continuity in the index $i$ and choose $\gamma_1 = 0$, $\gamma_N$ becomes uniquely determined, and equal to $2\pi k$ for some integer $k$. Stone proved that if $k \neq 0$, then there must be a degeneracy point somewhere inside $S$.

The integer $k$ can be topologically interpreted as labeling the homotopy class to which the 2-loop represented by the states around $S$ belongs. Equivalently, $k$ characterizes the topological structure of the monopole bundle with fiber $U(1)$ representing state vectors and base space $S^2$ representing the surface $S$ (see, e.g., Ref. 25, p. 320).

It turns out that it is possible to define a global and continuous state vector around $S$ if and only if $k = 0$, i.e., if and only if Stone’s test does not signal a degeneracy. Let us try to construct a test that works even for some cases when $k = 0$ by considering a complete set of eigenvectors around $S$. We then have a continuous function from the surface $S$ to the space of eigenbases $U(n)$. This can contain topological information only if $U(n)$ contains nontrivial 2-loops. This, however, is not the case (see, e.g., Ref. 25, pp. 120-121). Consequently, Stone’s test exhausts all topological information contained in the eigenvectors around $S$.

We conclude this section by noting that, while Stone’s test is optimal for general Hamiltonians, topological tests similar to that of Ref. 23 may be constructed for Hamiltonians obeying additional symmetries.

V. CONCLUSIONS

The need to demonstrate whether or not there exist degeneracy points in the spectra of Hamiltonians is of relevance in many fields of physics. For example, such points are abundant in molecular systems 32 and are important because they signal a breakdown of the Born-Oppenheimer approximation. Another instance where the presence of degeneracy points become pertinent is in the recently proposed paradigm of adiabatic quantum computation 33, 54, whose efficiency relies crucially upon the presence of nonvanishing energy gaps along certain paths in parameter space.

Topological tests to detect degeneracies have been put forward in the past by Longuet-Higgins 18 and Stone 24. More recently, the present authors 23 extended Longuet-Higgins’ test by consideration of complete sets of eigenvectors of real parameter dependent Hamiltonian matrices as paths in $SO(n)$. This extended test can detect degeneracies even in cases where Longuet-Higgins’ original test fails.

In this paper, we have put forward a method that makes the topological test in Ref. 23 applicable to any dimension $n$ of the Hamiltonian matrix. This method is based upon the multi-valuedness of the function log : $SO(n) \mapsto so(n)$, that connects $SO(n)$ with its corresponding Lie algebra $so(n)$ of real antisymmetric matrices. We have further demonstrated under what conditions the topological test in Ref. 23 is applicable to subspaces of the full Hilbert space. These two major findings of the present paper open up the possibility to use the test in realistic scenarios, such as, e.g., for computed electronic eigenvectors in various molecular systems or for the eigenfunctions of quantum billiards. Our final result concerns Stone’s test for degeneracies of complex Hamiltonians. We have shown that Stone’s test is optimal in the sense that no other topological test can do better in detecting degeneracies in systems that need a description in terms of general complex Hamiltonians.

Acknowledgments

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[2] G. Darboux, Lecons sur la Théorie Générale des Sur-
[29] A regular $n$-simplex is the generalization to higher dimensions of an equilateral triangle (the 2-simplex) and a tetrahedron (the 3-simplex).