Optimal Topological Test for Degeneracies of Real Hamiltonians

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We consider adiabatic transport of eigenstates of real Hamiltonians around loops in parameter space. It is demonstrated that loops that map to nontrivial loops in the space of eigenbases must encircle degeneracies. Examples from Jahn-Teller theory are presented to illustrate the test. We show furthermore that the proposed test is optimal.

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Sign reversal of real electronic eigenfunctions when continuously transported around a degeneracy was discovered by Herzberg and Longuet-Higgins [1] and was later used to construct a topological test for conical intersections [2]. Such intersections are abundant in molecular systems [3] and are important because they signal a breakdown of the Born-Oppenheimer approximation. The topological test in [2] has been used to detect conical intersections in LiNaK and ozone [4]. The sign change of the electronic eigenfunctions gives rise to the molecular Aharonov-Bohm effect [5], which has recently been experimentally tested [6] and theoretically investigated [7]. The structure of adiabatic wave functions and the sign change pattern in the vicinity of degeneracies have also been analyzed in the context of quantum billiards.

The behavior of the real wave functions for such systems, studied by analog experiments on microwave resonators [8], has been interpreted in terms of both the standard [9] and the off-diagonal [10] geometric phases. The microwave resonator experiments have motivated general theoretical treatments concerning both the concomitant geometric phases and structure of the wave functions [9, 10, 11].

In this Letter we study the eigenvectors of a real matrix Hamiltonian on a loop in parameter space. We show that the behavior of the eigenvectors may imply the presence of a degeneracy even if none of the eigenvectors changes sign around the loop. This result is a generalization of Longuet-Higgins’ topological test for intersections [2]. It is also proven that the generalized test exhausts all topological information associated with the behavior of the eigenvectors, concerning the presence of degeneracies.

We begin by the following topological fact. Let X and Y be topological spaces. If Γ is a trivial loop in X, and if $F : X \to Y$ is continuous, then $F(\Gamma)$ is a trivial loop in Y.

To prove this, note that if G is a homotopy between Γ and a point $x_0 \in X$, then $F \circ G$ is a homotopy between $F(\Gamma)$ and $F(x_0) \in Y$.

Now let $H(Q)$ be an $n \times n$ matrix Hamiltonian, written in the basis $\{|i\rangle\}$ of the n dimensional Hilbert space $\mathcal{H}$. We suppose that $H(Q)$ is real, symmetric, and continuous for each $Q = (Q_1, \ldots, Q_d)$ in parameter space $\mathcal{Q}$, which we assume to be a simply connected subset of $\mathbb{R}^d$. The eigenvectors of $H(Q)$ can always be chosen real. We call the space of real vectors $\mathcal{H}_{\text{real}}$, which through the expansion coefficients in the basis $\{|i\rangle\}$ can be identified with $\mathbb{R}^n$. The set $\mathcal{N}_{\text{real}}$ of normalized real vectors is the sphere $S^{n-1}$ in $\mathbb{R}^n$.

Consider a simply connected surface $S$ in $\mathcal{Q}$, bounded by the loop Γ. Longuet-Higgins’ theorem asserts that if a certain eigenvector $|\psi_i(Q)\rangle$ of $H(Q)$ changes sign when continuously transported around Γ, then there is a point on $S$ where $|\psi_i(Q)\rangle$ becomes degenerate with another state. We note that the theorem implies that if $H(Q)$ is nondegenerate on $S$, then $\pm|\psi_i(Q)\rangle$ represent two continuous functions from $S$ to $S^{n-1}$.

As a first step towards a generalization of Longuet-Higgins’ theorem we consider two-level systems. The set of normalized vectors $\mathcal{N}_{\text{real}}$ is then the circle $S^1$. We prove that if an eigenvector of a real two-level system represents a nontrivial loop in $S^1$ when continuously transported along a loop Γ, then Γ must encircle a degeneracy. The proof is by reductio ad absurdum. Suppose that $H(Q)$ is nondegenerate on the surface $S$ bounded by Γ. A real eigenvector $|\pm(Q)\rangle$ then represents a continuous function $F$ from $S$ to $\mathcal{N}_{\text{real}} = S^1$. Since Γ is trivial ($S$ being simply connected), so is the loop traced out by $|\pm(Q)\rangle$.

As an illustration, let us consider the coupling matrix Hamiltonian of the $E \otimes \epsilon$ Jahn-Teller system [12]

$$H(\rho, \theta) = \begin{pmatrix}
k \rho \cos \theta + \frac{1}{2} g \rho^2 \cos 2\theta & k \rho \sin \theta - \frac{1}{2} g \rho^2 \sin 2\theta \\
k \rho \sin \theta - \frac{1}{2} g \rho^2 \sin 2\theta & -k \rho \cos \theta - \frac{1}{2} g \rho^2 \cos 2\theta \end{pmatrix},$$

(1)

where $\rho$ and $\theta$ are polar coordinates of parameter space $Q = \mathbb{R}^2$, and $k$ and $g$ are the linear and quadratic coupling strengths, respectively. In this system there are four degeneracies: one at the origin $\rho = 0$ and three at $\rho = 2k/g$ and $\theta = \pi/3$, $\pi$, and $5\pi/3$. Continuous transport of an eigenvector around any single degeneracy produces a sign change [12]. Longuet-Higgins’

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test applied to such a loop would thus imply a degeneracy. Consider instead a circular loop \( \Gamma \) given by \( \rho \gg 2k/q \) and \( \theta \in [0, 2\pi] \), encircling all four degeneracies. The eigenvectors \( | - (\theta) \rangle \approx \sin \theta | 1 \rangle + \cos \theta | 2 \rangle \) and \( | + (\theta) \rangle \approx -\cos \theta | 1 \rangle + \sin \theta | 2 \rangle \) do not change sign as the loop is traversed. However, viewed as elements of the circle \( S^1 \), \( | \pm (\theta) \rangle \) both make a complete clock-wise turn. This means that each eigenvector traces out a nontrivial loop in \( \mathcal{N}_{\text{real}} = S^1 \). In this way the presence of degeneracies encircled by \( \Gamma \) can be detected.

For the two-level case we have thus obtained a generalization of Longuet-Higgins' test: also loops along which the eigenvectors trace out nontrivial loops in \( S^1 \) encircle degeneracies on every surface bounded by them. However, for \( n \geq 3 \), the space of real normalized vectors \( \mathcal{N}_{\text{real}} = S^{n-1} \) is simply connected, i.e., it contains only trivial loops. Thus, following a single eigenvector along the loop is insufficient. To generalize the test in this case, we consider instead a complete set \( \{|\psi_i(Q)\rangle\}_{i=1}^n \) of normalized eigenvectors of \( H(Q) \).

If \( H(Q) \) is nondegenerate on \( S \), then \( \pm |\psi_i(Q)\rangle \) are, for each \( i \), two continuous and globally defined functions from \( S \) to \( S^{n-1} \). Without loss of generality we may assume that \( \{|\psi_i(Q)\rangle\}_{i=1}^n \) represents a positively oriented orthonormal basis of \( \mathcal{H}_{\text{real}} = \mathbb{R}^n \). Every such basis can be thought of as an element of the \( n \) dimensional rotation group \( \text{SO}(n) \). We may thus define a continuous function \( F : S \rightarrow \text{SO}(n) \) as

\[
F(Q) = \begin{pmatrix}
|\psi_1(Q)\rangle & \cdots & |\psi_n(Q)\rangle \\
\vdots & \ddots & \vdots \\
|n\psi_1(Q)\rangle & \cdots & |n\psi_n(Q)\rangle
\end{pmatrix}.
\]

Thus, if \( H(Q) \) is nondegenerate on \( S \), then its eigenvectors represent a continuous function from \( S \) to \( \text{SO}(n) \). Analogous to the two-level case it follows that the loop in \( \text{SO}(n) \) traced out by \( F(Q) \) as \( Q \) varies along \( \Gamma \), is a trivial loop. By reductio ad absurdum we consequently arrive at the following result. If the \( n \) eigenvectors of \( H(Q) \) represent a nontrivial loop in \( \text{SO}(n) \) when taken continuously around \( \Gamma \), then there must be at least one degeneracy of \( H(Q) \) on every simply connected surface \( S \) bounded by \( \Gamma \).

This result makes it possible to detect the presence of a degeneracy by considering eigenvectors on a loop in \( Q \) even if they do not change sign around the loop. It constitutes the promised generalization of Longuet-Higgins' test.

We note that \( \text{SO}(2) \) is homeomorphic to \( S^1 \) and is thus infinitely connected: it contains one class of nontrivial loops for each nonzero integer. The fundamental group of \( \text{SO}(2) \) is the additive group of integers \( \mathbb{Z} \). Determining whether a loop is trivial amounts to counting the number of times the eigenvector encircles the origin. For each \( n \geq 3 \), however, \( \text{SO}(n) \) contains only one class of nontrivial loops, that all become trivial when traversed twice. The fundamental group of \( \text{SO}(n \geq 3) \) is the two-element group \( \mathbb{Z}_2 \). In order to apply the test in this latter situation, we need to know how to determine whether a loop in \( \text{SO}(n) \) with \( n \geq 3 \) is trivial or not. In principle, this can be done by lifting the loop to the universal covering space \( \text{Spin}(n) \) of \( \text{SO}(n) \). In practice, though, it seems difficult to find a method, that works for all \( n \) and is easily implemented. Below we show explicitly how to use the test in the cases \( n = 3 \) and \( n = 4 \). We use examples from Jahn-Teller theory as physical illustrations.

First, let us consider the \( n = 3 \) case. \( \text{SO}(3) \) is homeomorphic to the closed ball of radius \( \pi \) with antipodal points on its surface identified. A vector \( \phi \hat{\nu} \) in the ball represents a rotation around the unit vector \( \hat{\nu} \) by the angle \( \phi \in [0, \pi] \). Antipodal points on the surface must be identified since a rotation by the angle \( \pi \) is the same transformation regardless of whether the rotation axis is plus or minus \( \hat{\nu} \). A loop in \( \text{SO}(3) \) can thus be viewed as a curve that may exit the closed ball at the boundary, and enter again at the antipodal point. The loop is trivial if and only if the number of piercings of the boundary is divisible by two. Such a piercing is characterized by \( \phi = \pi \) and that \( \hat{\nu} \) abruptly changes sign.

We apply the method to the linear \( T \otimes \tau_2 \) Jahn-Teller system, described by the coupling matrix (2)

\[
H(R) = \begin{pmatrix}
0 & -Z & -Y \\
Z & 0 & -X \\
Y & X & 0
\end{pmatrix},
\]

where \( R = (X, Y, Z) \) parametrizes \( Q = \mathbb{R}^3 \). The Hamiltonian is doubly degenerate on eight rays in \( \mathbb{R}^3 \) that go out from the origin and into the middle of each octant. At the origin there is a three-fold degeneracy. We consider a loop \( \Gamma \) lying completely in the \( X-Y \) plane. In planar polar coordinates \( \rho \) and \( \theta \), the eigenvectors arranged according to increasing energy read \( |\psi_1(\theta)\rangle = \frac{1}{\sqrt{2}} (\sin \theta |1\rangle + \cos \theta |2\rangle + |3\rangle) \), \( |\psi_2(\theta)\rangle = \cos \theta |1\rangle - \sin \theta |2\rangle \), and \( |\psi_3(\theta)\rangle = \frac{1}{\sqrt{2}} (\sin \theta |1\rangle + \cos \theta |2\rangle - |3\rangle) \). Note that the eigenvectors are independent of \( \rho \) and that none of them changes sign around any loop that does not pass through the origin. The function \( F \) along the loop is

\[
F(\theta) = \begin{pmatrix}
\frac{1}{\sqrt{2}} \sin \theta & \cos \theta & \frac{1}{\sqrt{2}} \sin \theta \\
\frac{1}{\sqrt{2}} \cos \theta & -\sin \theta & \frac{1}{\sqrt{2}} \cos \theta \\
\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}}
\end{pmatrix}.
\]

We aim to determine which loops in the \( X-Y \) plane that map to nontrivial loops in \( \text{SO}(3) \) under \( F \). The rotation angle \( \phi \) and rotation vector \( \hat{\nu} \) of \( F(\theta) \) are given by

\[
\phi(\theta) = \arccos \left( -1 + \frac{1}{2} \left( 1 - \frac{1}{\sqrt{2}} \right) (1 - \sin \theta) \right),
\]

\[
\hat{\nu}(\theta) = \frac{1}{N} (-\cos \theta, \sin \theta - 1, (1 - \sqrt{2}) \cos \theta),
\]

respectively, where \( N \) is a normalization constant. Eq. (4) shows that \( \phi(\theta) = \pi \) only for \( \theta = \pi/2 \). It is also
clear that \( \hat{\mathbf{v}} \) is continuous everywhere except on the ray \( \theta = \pi/2 \), where it abruptly changes sign. A plot of \( \phi \) and \( \hat{\mathbf{v}} \) as functions of \( \theta \) appears in Fig. 1. Thus, exactly the loops in the X-Y plane that cross the ray \( \theta = \pi/2 \) an odd number of times are mapped to nontrivial loops in SO(3). This is a concrete manifestation of the validity of the test, since any loop that passes \( \theta = \pi/2 \) an odd number of times must encircle the degenerate subset of \( \mathcal{Q} \).

Consider now the case \( n = 4 \). Let \( F(t) = (F_{ij}(t)) \) be a loop in SO(4) parametrized by \( t \in \mathbb{R} \). The first column \( f(t) \equiv (F_{11}(t), F_{21}(t), F_{31}(t), F_{41}(t)) \) of \( F(t) \) then represents an element of \( S^3 \) tracing out a loop. Define the matrix

\[
T(f(t)) = \begin{pmatrix}
F_{11}(t) & F_{21}(t) & F_{31}(t) & F_{41}(t) \\
-F_{21}(t) & F_{11}(t) & -F_{41}(t) & F_{31}(t) \\
-F_{31}(t) & F_{41}(t) & F_{11}(t) & -F_{21}(t) \\
-F_{41}(t) & -F_{31}(t) & F_{21}(t) & F_{11}(t)
\end{pmatrix},
\]

being orthogonal and continuous as a function of \( f \in S^3 \). It follows that \( T(t) \equiv T(f(t)) \in \text{SO}(4) \) since it can be continuously connected to the identity matrix, corresponding to \( f = (1,0,0,0) = \hat{\mathbf{e}}_1 \in S^3 \). Furthermore, since \( f(t) \) is a loop in \( S^3 \), \( T(t) \) is a trivial loop. We consider the loop in SO(4) given by \( T(t)F(t) \). This loop is nontrivial exactly when \( F(t) \) is, since \( T(t) \) is trivial. However, the loop \( T(t)F(t) \) is simpler than \( F(t) \). Carrying out the matrix multiplication, yields

\[
T(t)F(t) = \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & A_{11}(t) & A_{12}(t) & A_{13}(t) \\
0 & A_{21}(t) & A_{22}(t) & A_{23}(t) \\
0 & A_{31}(t) & A_{32}(t) & A_{33}(t)
\end{pmatrix},
\]

Thus, the loop \( T(t)F(t) \) is trivial if and only if the loop \( A(t) = (A_{ij}(t)) \) in \( \text{SO}(3) \) is trivial.

We have applied the above procedure numerically to the \( G \otimes g \) Jahn-Teller system. The coupling matrix for this system reads

\[
H(g) = -q k^G_g \sqrt{2} \times \begin{pmatrix}
g_3 & g_4 & g_1 - g_3 & g_2 + g_4 \\
g_4 & -g_3 & -g_2 + g_4 & g_1 + g_3 \\
g_1 - g_3 & -g_2 + g_4 & -g_1 & g_2 \\
g_2 + g_4 & g_1 + g_3 & g_2 & g_1
\end{pmatrix},
\]

where \( g = (g_1, \ldots, g_4) \) are normal modes and \( k^G_g \) is the linear coupling constant. We consider a loop \( \Gamma \) described by \( qg_1 = qg_4 = \cos \theta \) and \( qg_2 = qg_3 = \sin \theta \), \( \theta \in [0,2\pi] \). This loop encircles a four-fold degeneracy at the origin of parameter space and it can be checked that none of the eigenvectors changes sign along \( \Gamma \). Fig. 2 shows the angle and vector of rotation of the matrix \( A(\theta) \) along \( \Gamma \). \( \phi \) equals \( \pi \) once, meaning that the loop in SO(4) traced out by the eigenvectors is nontrivial. The four-fold degeneracy at the origin is thus detected.

Let us now consider whether there can be a better topological test than the present one. It is easy to find loops encircling degeneracies that map to trivial loops in \( \text{SO}(n) \). This means that the test does not find every degeneracy, so there may be room for improvement. The rest of this Letter we devote to an argument showing that if we are only allowed to consider eigenvectors on a loop in

![FIG. 1: Rotation angle \( \phi \) in radians and components of the rotation vector \( \hat{\mathbf{v}} \), as functions of \( \theta \) also in radians. \( \phi \) and \( \hat{\mathbf{v}} \) are computed from the matrix \( F(\theta) \) of Eq. (1) representing eigenvectors in the \( T \otimes \tau_2 \) system. The first, second, and third component of \( \hat{\mathbf{v}} \) are represented by the solid, dotted, and dashed curves, respectively. Note that \( \phi \) equals \( \pi \) at \( \theta = \pi/2 \), and that \( \hat{\mathbf{v}} \) changes sign at that point.](image1)

![FIG. 2: The same plot as in Fig. 1 but \( \phi \) and the vector components are calculated from the matrix \( A(\theta) \) of the \( G \otimes g \) system along the loop \( \Gamma \). Since \( \phi \) equals \( \pi \) at one point, \( \Gamma \) must encircle a degeneracy.](image2)
parameter space $Q$, and if the only information we have about the Hamiltonian is that it is continuous, then there is no test that can do better in implying degeneracies. To prove this, assume that the eigenvectors $\{|\psi_i(Q(t))\rangle\}_{i=1}^n$ and corresponding eigenvalues $\{\lambda_i(Q(t))\}_{i=1}^n$ are known along the loop $\Gamma$ parametrized by $t \in \mathbb{R}$. Suppose that the eigenvectors are nondegenerate along $\Gamma$ so that $\lambda_1(Q(t)) < \lambda_2(Q(t)) < \ldots < \lambda_n(Q(t))$ holds for all $t$, and that the corresponding loop $F(Q(t))$ in $SO(n)$ is trivial. Under these conditions we show that there always exists a Hamiltonian $H(Q)$, continuous and nondegenerate on all $Q$, having exactly the eigenvectors $\{|\psi_i(Q(t))\rangle\}_{i=1}^n$ and eigenvalues $\{\lambda_i(Q(t))\}_{i=1}^n$ on $\Gamma$. Thus, if $F(Q(t))$ is trivial, the Hamiltonian can be nondegenerate everywhere, meaning that no test can imply a degeneracy.

For the proof we need to assume that the loop $\Gamma$ is homeomorphic to $S^1$ and that there is a homeomorphism $D$ from $\mathbb{R}^d$ onto itself, such that $D(\Gamma)$ is the unit circle in the $X_1$-$X_2$ plane. $(X_1, \ldots, X_d) = X = D(Q)$ denotes the coordinates of the image of a point $Q \in \mathbb{R}^d$ under $D$. Such a $D$ exists for all physically interesting $\Gamma$.

We consider first the unit disc in the $X_1$-$X_2$ plane, parametrized by the usual polar coordinates $\rho \in [0, 1]$ and $\theta \in [0, 2\pi)$. By the homeomorphism $D$ we may view $F(Q(t))$ and $\{\lambda_i(Q(t))\}_{i=1}^n$ as functions of $\theta$, i.e., $F(\theta) \equiv F(D^{-1}(\cos \theta, \sin \theta, 0, \ldots, 0))$ and $\lambda_i(\theta) \equiv \lambda_i(D^{-1}(\cos \theta, \sin \theta, 0, \ldots, 0))$. The eigenvalues can be continuously extended to the unit disc preserving the nondegeneracy by defining $\tilde{\lambda}_i(\rho, \theta) = \rho \lambda_i(\theta) + (1 - \rho) A_i$, where $A_i$ are any real numbers satisfying $A_1 < A_2 < \ldots < A_n$. Let $\tilde{\Lambda}(\rho, \theta) = \text{diag}[\tilde{\lambda}_1(\rho, \theta), \ldots, \tilde{\lambda}_n(\rho, \theta)]$. Also the eigenvectors can be continuously extended to the disc. This is exactly because they represent a trivial loop in $SO(n)$. Let the function $G : [0, 1] \times [0, 1] \to SO(n)$ be a homotopy between the loop $F(\theta)$ and a constant element $R_0$ of $SO(n)$ such that $G(0, s) = R_0$ for all $s \in [0, 1]$ and $G(1, \theta/2\pi) = F(\theta)$. A continuous extension of $F$ to the whole disc is $\tilde{F}(\rho, \theta) = G(\rho, \theta/2\pi)$.

We are now in a position to construct a suitable Hamiltonian as a function of the coordinate $X$. Let $\rho$ take any value in $[0, +\infty)$. Define

$$\tilde{H}(X) = \begin{cases} \tilde{F}(\rho, \theta) \tilde{\Lambda}(\rho, \theta) \tilde{F}(\rho, \theta)^T, & \text{if } \rho \leq 1 \\ \tilde{F}(1, \theta) \tilde{\Lambda}(1, \theta) \tilde{F}(1, \theta)^T, & \text{if } \rho > 1, \end{cases} \tag{9}$$

where $T$ denotes matrix transposition. Note that $\tilde{H}(X)$ defined in this way is independent of the coordinates $X_3, \ldots, X_d$, that it is continuous and nondegenerate for all $X$, and that it has $\{|\psi_i(\theta)\rangle\}_{i=1}^n$ as eigenvectors and $\{\lambda_i(\theta)\}_{i=1}^n$ as eigenvalues on the unit circle in the $X_1$-$X_2$ plane. To obtain the desired Hamiltonian as a function of $Q$, simply define $H(Q) = \tilde{H}(D(Q))$.

In conclusion, we have described a test for degeneracies of real Hamiltonians based on the behavior of their eigenvectors on a loop in parameter space. If one considers a complete set of eigenstates, one may detect a degeneracy even if none of the corresponding vectors changes sign. The test works for all real quantum systems with finite dimensional Hilbert spaces, including quantum billiards and Jahn-Teller systems, and could find explicit use in quantum chemistry applied to computed eigenvectors. We show also that no other topological test can do better in detecting degeneracies.

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