

Topological Phases near a Triple Degeneracy

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We study the pattern of three-state topological phases that appears in systems with real Hamiltonians and wave functions. We give a simple geometric construction for representing these phases. We then apply our results to understand previous work on three-state phases. We show that the “mirror symmetry” of wave functions noticed in microwave experiments can be simply understood in our framework.

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There has been considerable work on the geometric phase in recent years [1–3], and the phenomenon is now quite well understood in differential geometric terms as the twisting of a line bundle over the ray space of quantum mechanics. In a two-state system, this abstract picture can be made quite visualizable using the Poincaré sphere. The ray space is identified with the Poincaré sphere and the geometric phase is half the solid angle enclosed by the ray in its quantum evolution. Thus, for two-state systems, the abstract differential geometric picture can be made quite concrete and brought to bear on the interpretation of experiments. Indeed, this field has seen a fruitful interplay between theory and experiment. The geometric phase appears in a wide variety of wave phenomena. The theory has been tested in situations as diverse as optics [2], molecular spectroscopy [4], nuclear magnetic resonance [2], and microwave cavities [5].

For three-state systems the situation is not as satisfactory. While the abstract differential geometric picture is, of course, correct and complete, it does not lead to simple visualizable pictures or formulas that can directly be compared with experiment. There have been attempts in this direction [6], but it is fair to say that the general three-state geometric phase is considerably less accessible to the experimental community than the two-state geometric phase. In this paper we take up a special case of this general problem: our Hamiltonians (and wave functions) are restricted to be real. This restriction considerably simplifies the problem and renders it tractable. While complex Berry phases take values on the unit circle and are correctly described as geometric, real Berry phases can only take values ± 1 . These should be thought of as topological phases, since they are insensitive to continuous deformations of the system history. Even though these real Berry phases are topological, the pattern of three-state topological phases that emerges is surprisingly rich, as we will see. The aim of this Letter is to explore this rich structure and present it in a form suitable for direct comparison with experiments.

The motivation for this work comes from experiments with microwave cavities. Lauber *et al.* [5] have performed experiments in which they perturb a rectangular microwave cavity by deforming its shape adiabatically. The unperturbed cavity has a threefold degeneracy, which is lifted

by the perturbation. As the perturbation is varied cyclically, the system returns to its original state but sometimes picks up a topological phase of π . There has been some discussion of the interpretation of this experiment. Lauber *et al.* suggested that the phase changes they were seeing were not related to Berry’s phase but were a new and independent phenomenon related to “mirror symmetry.” Manolopoulos and Child [7] posed a specific theoretical problem and partially solved it, thereby gaining insight into the pattern of Berry phases that are expected from the general theory. Reference [7] also applied their theory to the experiment of Lauber *et al.* and were able to explain the experimentally observed closed path phases as Berry phases. This work has been criticized by Pistolesi and Manini [8] on the grounds that the formalism of Ref. [7] incorrectly predicts the open path [9] phases. They attribute this to the presence of additional “satellite” degeneracies near the main degeneracy which was not taken into account in Ref. [7].

In this paper we will completely solve the problem posed in Ref. [7]. We first motivate and pose the problem that we address. We then present our solution to this problem. Finally we use our solution to critically understand the previous theoretical and experimental work in this area.

A general perturbation of the system will remove the threefold degeneracy and can be represented in the adiabatic approximation by a 3×3 symmetric matrix, H . (The approximation consists of neglecting transition amplitudes between the three states of interest and other states.) We are interested in the eigenspaces of H . These are not affected by rescaling H or adding a multiple of the identity to it. One can thus arrange that H be traceless $\text{Tr}(H) = 0$. The space of traceless symmetric matrices is a five-dimensional vector space. This space has a natural inner product $\langle H_1, H_2 \rangle = \text{Tr}(H_1 H_2)$. Let us choose a basis Q_α ($\alpha = 0, 1, 2, 3, 4$) in this vector space which is orthonormal: $\langle Q_\alpha, Q_\beta \rangle = \delta_{\alpha\beta}$. We can expand H in this basis $H = \sum_\alpha x^\alpha Q_\alpha$. It is convenient to normalize H by the condition $\langle H, H \rangle = 1$. This results in the x^α satisfying $\sum_\alpha x^\alpha x^\alpha = 1$, which describes a sphere S^4 in five dimensions.

At some points of S^4 , H has doubly degenerate levels and these points are said to belong to \mathcal{D} . Let us arrange the

eigenvalues in decreasing order so that $\lambda_1 \geq \lambda_2 \geq \lambda_3$, the equalities holding only at points of \mathcal{D} . If $\lambda_1 = \lambda_2 > \lambda_3$, we say that the point belongs to \mathcal{D}^+ and if $\lambda_1 > \lambda_2 = \lambda_3$ we say that the point belongs to \mathcal{D}^- . The eigenvalues of H satisfy two identities $\lambda_1 + \lambda_2 + \lambda_3 = 0$ and $\lambda_1^2 + \lambda_2^2 + \lambda_3^2 = 1$ (from tracelessness and normalization of H) and can be parametrized by an angle ψ , $0 \leq \psi \leq \pi/3$: $\lambda_1 = \sqrt{2/3} \cos \psi$, $\lambda_2 = \sqrt{2/3} \cos(\psi - 2\pi/3)$, and $\lambda_3 = \sqrt{2/3} \cos(\psi + 2\pi/3)$. Note that $\psi = 0$ at points of \mathcal{D}^- and $\psi = \pi/3$ at points of \mathcal{D}^+ .

Given a closed curve in the space of perturbations (which before normalization is five dimensional) which does not pass through points of \mathcal{D} , the standard Berry phase lore would instruct us to diagonalize H along the curve and transport its eigenvectors by continuity to compute the phase change as the system is cyclically perturbed. The general problem of computing the phase is greatly simplified if one restricts attention to great circles on S^4 , which is well motivated experimentally. In an actual experiment [5], one does not always explore the full five-dimensional parameter space. One needs to vary at least two parameters to effect a cyclic evolution and see a Berry phase. Following Ref. [7], we will restrict ourselves to a two-dimensional parameter space (x, y) , chosen so that $(0, 0)$ represents the triply degenerate Hamiltonian $H = 0$. Expanding the Hamiltonian $H(x, y)$ in a Taylor expansion about the degenerate point, we find

$$H(x, y) = fx + gy + O(x^2, y^2), \quad (1)$$

where $f = \frac{\partial H}{\partial x}(0, 0)$ and $g = \frac{\partial H}{\partial y}(0, 0)$. Thus the perturbations span a two-dimensional plane in the space of 3×3 traceless symmetric matrices. The intersection of this plane with the sphere S^4 is a great circle (or geodesic) on S^4 . The great circle can be specified by giving two (non-antipodal) points on it. We choose (F, G) , an orthonormal basis in the (f, g) plane, and write

$$H(\theta) = \cos\theta F + \sin\theta G, \quad (2)$$

where θ varies from 0 to 2π and $\langle F, G \rangle = 0$. If $H(\theta)$ is nondegenerate for all θ , one can uniquely follow the eigenvectors of $H(\theta)$ as a function of θ , and the adiabatic Berry phase γ_i of the state $|i\rangle$ is well defined. From [7] it follows that $\gamma_2 = 1$ and $\gamma_1 = \gamma_3 = \gamma = \pm 1$. Without loss of generality, we can suppose that F is in diagonal form: $F = \lambda_1|1\rangle\langle 1| + \lambda_2|2\rangle\langle 2| + \lambda_3|3\rangle\langle 3|$, since this can be arranged by using the eigenvectors of F as an orthonormal basis. The problem posed in Ref. [7] is as follows: given the pair (F, G) , compute the topological phase γ for the great circle $H(\theta)$. This problem was solved in Ref. [7] in the case where G is of a special ‘‘bipartite’’ form. Another special case where the answer is known is when F and G share a common eigenvector. By projecting orthogonal to this eigenvector, one can reduce this case to the two-state topological phase. Then the projection of H can be expanded in terms of the Pauli matrices as $\cos\theta \sigma_z + \sin\theta \sigma_x$ and its eigenvectors clearly reverse sign as θ goes from 0 to 2π . For a general pair (F, G) there does not at present

exist a simple rule to determine the topological phase. This is the purpose of this Letter. We give the general solution to this problem below.

Regard F as the ‘‘north pole’’ of S^4 . Geodesics through F are characterized by $G \in S^3$, where G lies in the ‘‘equator’’ of S^4 . We will first locate all points in S^3 which lead to geodesics passing through \mathcal{D} . We refer to these as ‘‘degenerate’’ points and they form a set $\mathcal{B} \in S^3$. Regarded as a function of G , the topological phase can change only when G passes through \mathcal{B} , when the phase becomes ill defined. Thus \mathcal{B} divides S^3 into regions, each of which has the same topological phase. Our next step is to locate the set \mathcal{B} in S^3 and thus split S^3 into regions of constant topological phase.

We first characterize the degenerate set \mathcal{D} in S^4 . Clearly, $\mathcal{D} = \mathcal{D}^+ \cup \mathcal{D}^-$, which are disjoint sets. The points of \mathcal{D}^\pm can be written as $D_{\hat{n}}^\pm = \pm \frac{1}{\sqrt{6}}(1 - 3|\hat{n}\rangle\langle \hat{n}|)$, where $|\hat{n}\rangle$ is some unit ket vector (the nondegenerate eigenvector of D). Since $|\hat{n}\rangle$ and $-|\hat{n}\rangle$ define the same $D_{\hat{n}}^\pm$, \mathcal{D} is the disjoint union of two $\mathcal{R}\mathcal{P}^2$ s. To find the degenerate set \mathcal{B} is easy: the plane containing the vectors F and $D_{\hat{n}}^\pm$ intersects the sphere S^4 in a great circle. The intersection of this great circle with the equator of S^4 is simply the projection of $D_{\hat{n}}^\pm$ orthogonal to F , suitably normalized:

$$B_{\hat{n}}^\pm = \frac{D_{\hat{n}}^\pm - (D_{\hat{n}}^\pm, F)F}{[(D_{\hat{n}}^\pm, D_{\hat{n}}^\pm) - (D_{\hat{n}}^\pm, F)^2]^{1/2}}. \quad (3)$$

When G is equal to any of these points $B_{\hat{n}}^\pm$, the topological phase is ill defined. These are the degenerate points in S^3 . Let us compute their coordinates explicitly. Choose matrices Q_α (similar parametrizations appear in [10–12]):

$$Q_0 = \frac{1}{\sqrt{6}} \text{diag}(2, -1, -1),$$

$$Q_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad Q_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

$$Q_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad Q_4 = \frac{1}{\sqrt{2}} \text{diag}(0, 1, -1).$$

F is diagonal and therefore a linear combination of Q_0 and Q_4 : $F = \cos\psi Q_0 + \sin\psi Q_4$. Let us define $E = -\sin\psi Q_0 + \cos\psi Q_4$, a diagonal matrix orthogonal to F . In the basis (F, E, Q_1, Q_2, Q_3) , we find that $G = g_4 E + g_1 Q_1 + g_2 Q_2 + g_3 Q_3$, where the g 's satisfy $g_1^2 + g_2^2 + g_3^2 + g_4^2 = 1$, which describes S^3 . Similarly expanding the degenerate points $B_{\hat{n}}^\pm$ in this basis $B_{\hat{n}}^\pm = b_4 E + b_1 Q_1 + b_2 Q_2 + b_3 Q_3$, we find, by explicit computation,

$$b_1 = \mp \sqrt{3} \frac{n_2 n_3}{\sqrt{1 - c^2}}, \quad b_2 = \mp \sqrt{3} \frac{n_1 n_3}{\sqrt{1 - c^2}},$$

$$b_3 = \mp \sqrt{3} \frac{n_2 n_1}{\sqrt{1 - c^2}}, \quad b_4 = \pm \frac{s}{\sqrt{1 - c^2}}, \quad (4)$$

where $c = \sqrt{3/2}\langle \hat{n}|F|\hat{n}\rangle$ and $s = -\sqrt{3/2}\langle \hat{n}|E|\hat{n}\rangle$. By defining angles $\psi_1 = \psi$, $\psi_2 = \psi - 2\pi/3$, and $\psi_3 = \psi + 2\pi/3$, c and s can be expressed as $c = \sum_i \cos\psi_i n_i^2$; $s = \sum_i \sin\psi_i n_i^2$.

Since G and $-G$ represent the same geodesic oppositely traversed, it is clear that they have the same topological phase. Also, reversing the sign of two of (g_1, g_2, g_3) amounts to a π rotation about one of the principal axes of F . This is merely a similarity transformation of the pair (F, G) and does not alter the topological phase. By such phase preserving transformations, one can arrange for (g_1, g_2, g_3) to be non-negative. (g_4 can have either sign.) It is easily seen from (4) that points of S^3 where (g_1, g_2) or (g_2, g_3) vanish are degenerate points. Points of S^3 where (g_1, g_3) vanish are [13] in \mathcal{B} if $g_4 < g_4^c = -[1 - 3/4 \csc^2(\psi + \pi/3)]^{1/2}$. If $g_4 > g_4^c$, the topological phase is well defined, and F and G have a common eigenvector $(0, 1, 0)$ and the topological phase is then -1 . Points with two or more of (g_1, g_2, g_3) vanishing will be excluded from the following discussion.

We now introduce new coordinates (v_1, v_2, v_3) given by

$$v_1 = Ag_2^2g_3^2, \quad v_2 = Ag_3^2g_1^2, \quad v_3 = Ag_1^2g_2^2, \quad (5)$$

where

$$A = (g_1^2g_2^2 + g_2^2g_3^2 + g_1^2g_3^2)^{-1}.$$

The v 's are positive and satisfy $v_1 + v_2 + v_3 = 1$, which defines a triangular region. Let us define the following Cartesian coordinates in the plane $v_1 + v_2 + v_3 = 1$:

$$C = \sum_i v_i \cos\psi_i, \quad S = \sum_i v_i \sin\psi_i. \quad (6)$$

Let g_4 be held fixed. Then $g_1^2 + g_2^2 + g_3^2 = 1 - g_4^2 = r^2$ and (g_1, g_2, g_3) determine a point in the C - S plane via (5) and (6). As (g_1, g_2, g_3) vary over permissible values, (C, S) describe an equilateral triangle Δ . The orientation of this triangle relative to the C axis is controlled by the eigenvalue parameter ψ of F . We now locate the degenerate points in Δ . These points are given parametrically by Eq. (4). The v coordinates of these points are $v_1 = n_1^2$, $v_2 = n_2^2$, and $v_3 = n_3^2$. As (n_1, n_2, n_3) range over permissible values ($n_1, n_2, n_3 > 0, n_1^2 + n_2^2 + n_3^2 = 1$), (C, S) describe all the points in Δ . The degenerate points of Δ are located by requiring that $b_4 = g_4$. Using the last of Eqs. (4) it follows that these points describe an ellipse in the C - S plane: $C^2 + S^2/(1 - r^2) = 1$ with eccentricity determined by g_4 . The part of the ellipse inside Δ consists of two segments (Fig. 1). The degenerate points consist of the lower segment (for $g_4 > 0$) and the upper segment (for $g_4 < 0$). These clearly split up the triangle into two regions with constant topological phase. When $g_4 = 0$, the ellipse degenerates to a straight line parallel to the C axis. As g_4 approaches 1, the ellipse expands to the unit circle. By slightly perturbing the matrix $G = Q_2$ so that it is represented in the figure, we see that the correct assignments are as shown in the figure. This figure and the algorithm given below for using it are the main results of this paper.

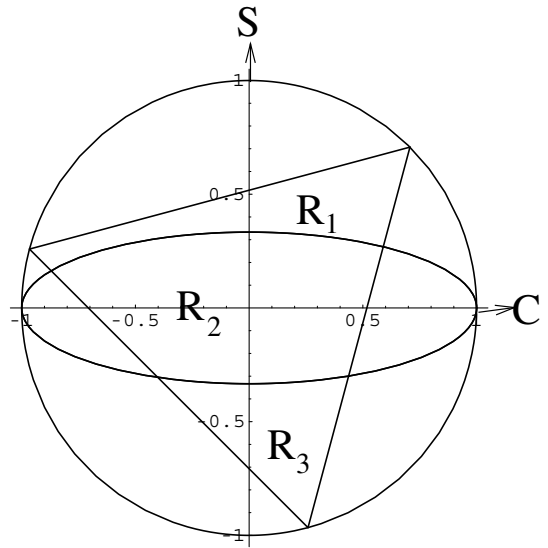


FIG. 1. Any point (g_1, g_2, g_3) gets mapped to one of the three regions, R_1 , R_2 , and R_3 , within the triangle. The topological phase is -1 in R_1 , $-\text{sgn}(g_4)$ in R_2 , and $+1$ in R_3 . The ellipse and circle correspond to $g_4 = 1/3$ and 1, respectively, and the triangle corresponds to $\psi = \pi/4$.

The algorithm is as follows: (i) Given two 3×3 symmetric, perturbation matrices (f, g) , add a multiple of the identity to make them trace-free and choose linear combinations (F, G) which are normalized and orthogonal: $\text{Tr}(FF) = \text{Tr}(GG) = 1$, $\text{Tr}(FG) = 0$.

(ii) Diagonalize F and write G in the basis in which F is diagonal. Determine the eigenvalue parameter ψ and construct E .

(iii) Expand G in the basis (E, Q_1, Q_2, Q_3) and determine (g_1, g_2, g_3, g_4) [e.g., $g_2 = \text{Tr}(GQ_2)$]. Apply appropriate rotations so that g_1, g_2, g_3 are positive.

(iv) Draw an equilateral triangle Δ in the (C, S) plane with vertices $(\cos\psi_1, \sin\psi_1)$, $(\cos\psi_2, \sin\psi_2)$, and $(\cos\psi_3, \sin\psi_3)$, where $\psi_1 = \psi$ and $\psi_{2,3} = \psi \mp 2\pi/3$.

(v) Let $r^2 = 1 - g_4^2$. Draw an ellipse $C^2 + S^2/(1 - r^2) = 1$. The sign of g_4 tells us which of the two segments of the ellipse contains the degenerate points.

(vi) Using Eqs. (5) and (6) locate (g_1, g_2, g_3) in the C - S plane and read off the topological phase from the diagram: the phase is -1 for R_1 , $-\text{sgn}(g_4)$ in R_2 , and $+1$ in R_3 .

This completely solves the problem posed in [7]. Since our formalism involves a Taylor expansion of the Hamiltonian around the triple degeneracy, we would expect the theory to agree with experiments that explore a region of parameter space close to the degeneracy. If the perturbations are such that the pair (F, G) describe a degenerate point, then neither the theory nor the experiment will produce a definite answer for the topological phase: the adiabatic approximation breaks down. Generically, for most shapes of cavities, G will not be close to a degenerate point and the first order theory applies in a region around the triple degeneracy.

For perturbed rectangular cavities the first order theory predicts a symmetry for the wave functions. Let us start with the observation that the unperturbed system has a discrete symmetry: reflection about a line normal to the long side [14] and bisecting the cavity (P). The eigenstates of the unperturbed system can be chosen to have a definite P parity. It can be easily seen [15] that the first order perturbations can be decomposed into nonzero even (F) and odd (G) parts satisfying $\text{Tr}(FG) = 0$. Constructing $H(\theta) = \cos\theta F + \sin\theta G$, we see that $PH(\theta)P = H(2\pi - \theta)$. Thus if $H(\theta)|\Psi_i(\theta)\rangle = E_i(\theta)|\Psi_i(\theta)\rangle$, $|\Psi_i(2\pi - \theta)\rangle = \sigma_i P|\Psi_i(\theta)\rangle$, where $\sigma_i = \pm 1$ is constant by continuity. This relation between the wave functions at θ and $2\pi - \theta$ is what we refer to as mirror symmetry. Setting $\theta = 0$ and using $|\Psi_i(2\pi)\rangle = \gamma_i|\Psi_i(0)\rangle$, where γ_i is the topological phase, we find that σ_i is the product of the topological phase and the parity of the i th state.

For the experiment of Lauber *et al.* [5], it turns out that F corresponds to $\psi = \cos^{-1}(23/26)$ and $G \approx (0.995, 0.101, 0, 0)$. G is not actually a degenerate point but it is very close to one. The point in \mathcal{B} closest to G is $(0.997, 0.066, 0.048, -0.003)$. As a result, the small splittings in the first order Hamiltonian make the system very sensitive to second order perturbations. In fact these higher order terms are able to perturb the Hamiltonian into \mathcal{D} , which results in the appearance of two doubly degenerate “satellites” [8]. As correctly pointed out in Ref. [8], these must also be taken into account to predict the “open path” Berry phases [9]. Figure 4 of Ref. [8] shows the (shaded) regions in the parameter space where second order perturbations are important. These correspond to $\theta \approx \pi/2, 3\pi/2$. In the remaining regions first order theory applies and we would expect the mirror symmetry described in the preceding paragraph to be present. For the three states with quantum numbers $(n_x, n_y) = (7, 1)$, $(5, 3)$, and $(2, 4)$ the topological phase assignments are $\gamma_i = (-, +, -)$ and the parity assignments are $(+, +, -)$, which result in $\sigma_i = (-, +, +)$. The operation of reflecting the wave functions and multiplying them by σ_i relates the conjugate figures in [5]. This symmetry was noticed by Lauber *et al.* (see figure in [5]) experimentally. The mirror symmetry is particularly evident in the pairs $(1,16)$, $(2,15)$, $(8,9)$, and $(7,10)$, where the first order theory is expected to apply. For other pairs [e.g., the pairs $(4,13)$, $(5,12)$] in the vicinity of $\theta \approx \pi/2, 3\pi/2$ the symmetry is only approximate, as would be expected, since second order effects are important. Thus the first order theory is able to account for the experimentally observed approximate mirror symmetry in [5].

In summary, we have described a simple geometrical construction for representing the topological phases of a three-state system. The construction can be easily vi-

ualized and drawn on paper. For this reason it may serve as a useful tool to interpret experiments done on three-state topological phases. We have also given a theoretical framework which is closely related to experimental investigations of the topological phase. We are also able to understand the “mirror” symmetry of wave functions seen in the experiments of Lauber *et al.* In fact, the bipartite form of G noticed by [7] can be traced to this discrete symmetry. Of course, our work also encompasses situations where the unperturbed state has no discrete symmetries and F and G are general. We believe this work will be useful to the community of physicists interested in the three-state topological phase.

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