PHYSICAL REVIEW LETTERS

VOLUME 85 | 9 OCTOBER 2000 | NUMBER 15

Off-Diagonal Geometric Phases

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(Received 5 November 1999)

We investigate the adiabatic evolution of a set of nondegenerate eigenstates of a parametrized Hamiltonian. Their relative phase change can be related to geometric measurable quantities that extend the familiar concept of Berry phase to the evolution of more than one state. We present several physical systems where these concepts can be applied, including an experiment on microwave cavities for which off-diagonal phases can be determined from published data.

PACS numbers: 03.65.Bz

Consider the adiabatic evolution of a set of nondegenerate normalized eigenstates $|\psi_i(\mathbf{s})\rangle$ of a parametrized Hamiltonian $H(\mathbf{s})$. The idea that, with a suitable definition, the phase of the scalar product $\langle\psi_j(\mathbf{s}_1)\,|\,\psi_j(\mathbf{s}_2)\rangle$ contains a geometric, measurable contribution dates back to Pancharatnam's pioneering work [1]. In particular, when $\mathbf{s}_1 = \mathbf{s}_2$ and the state $|\psi_j(\mathbf{s})\rangle$ is transported adiabatically along a closed loop, the existence of a nontrivial phase factor was discovered and put on a firm basis by Berry [2]. Since then, considerable work has been devoted to interpretation [3–7], generalization [8–13], and experimental determination [14–18] of these geometric phase factors. Surprisingly, for $\mathbf{s}_1 \neq \mathbf{s}_2$, the phase relation of $\langle\psi_j(\mathbf{s}_1)\,|\,\psi_k(\mathbf{s}_2)\rangle$ between two *different* eigenstates has not been equally well investigated so far [19].

This is even more surprising if one considers that, for some pair of points $\mathbf{s}_1$ and $\mathbf{s}_2$, it may occur that $|\psi_j(\mathbf{s}_2)\rangle = e^{i\alpha}|\psi_j(\mathbf{s}_1)\rangle$ $(k \neq j)$. This implies that both scalar products $\langle\psi_j(\mathbf{s}_1)\,|\,\psi_j(\mathbf{s}_2)\rangle$ and $\langle\psi_k(\mathbf{s}_1)\,|\,\psi_k(\mathbf{s}_2)\rangle$ vanish, and, as well known, the usual Pancharatnam-Berry phase on any path connecting $\mathbf{s}_1$ to $\mathbf{s}_2$ is undefined for the states k and j. The only phase information left is thus contained in the cross scalar products $\langle\psi_j(\mathbf{s}_1)\,|\,\psi_k(\mathbf{s}_2)\rangle$.

In this Letter we determine the measurable and geometric phase factors associated with the off-diagonal matrix elements $\langle\psi_j(\mathbf{s}_1)\,|\,\psi_k(\mathbf{s}_2)\rangle$ of the operator describing the evolution along a general open path in the parameter space that connect $\mathbf{s}_1$ to $\mathbf{s}_2$. We find a set of independent off-diagonal phase factors that exhaust the geometrical phase information carried by the basis of eigenstates along the path. Analogously to the familiar Berry phase, the value of these phases depend on the presence of degeneracies of the energy levels in the parameters' space. The formalism is then applied to an experiment on quantum billiards [17], where the off-diagonal phase factors can be extracted directly from published experimental data.

In order to introduce the off-diagonal geometric phases, it is convenient to consider the usual definition of the geometric phase of one normalized state $|\psi_j(\mathbf{s})\rangle$ in terms of parallel transport [2,4,8,9]. Given any path Γ that joins $\mathbf{s}_1$ to $\mathbf{s}_2$, the state parallel-transported along it is defined by

$$|\psi_j^{\parallel}(\mathbf{s}_2)\rangle = \exp\left\{-\int_\Gamma d\mathbf{s}\cdot\langle\psi_j(\mathbf{s})\,|\,\nabla_s\psi_j(\mathbf{s})\rangle\right\}|\psi_j(\mathbf{s}_2)\rangle\,. \tag{1}$$

This fixes the phase of the state along the path in the unique way satisfying $\langle\psi_j^{\parallel}(\mathbf{s})\,|\,\psi_j^{\parallel}(\mathbf{s}+\delta)\rangle = 1 + O(\delta^2)$ for $\delta \to 0$, i.e., having maximal projection on the "previous" state. The *geometric* phase factor is then defined simply in terms of the scalar product along the parallel evolution:

$$\gamma_j^{\Gamma} \equiv \Phi(U_{jj}^{\Gamma}) = \Phi[\langle\psi_j^{\parallel}(\mathbf{s}_1)\,|\,\psi_j^{\parallel}(\mathbf{s}_2)\rangle]\,, \tag{2}$$

where $\Phi(z) = z/|z|$ for complex $z \neq 0$. γ_j^{Γ} is univocally determined by the sequence Γ_j of states $|\psi_j(\mathbf{s})\rangle$, with $\mathbf{s}$ varying along Γ. Indeed, γ_j^{Γ} is unchanged by a local "gauge" transformation,

$$|\psi_j(\mathbf{s})\rangle \to |\psi_j(\mathbf{s})\rangle \exp[i\varphi_j(\mathbf{s})], \tag{3}$$

and by any reparametrization of the sequence of states Γ_j. It is thus a geometric, measurable quantity.

In a similar way, we define [20] the phase factors associated with the off-diagonal elements of the parallel-evolution operator U^Γ:

$$\sigma_{jk}^\Gamma \equiv \Phi(U_{jk}^\Gamma) = \Phi[\langle \psi_j^\parallel(\mathbf{s}_1) | \psi_j^\parallel(\mathbf{s}_2)\rangle]. \tag{4}$$

Liue γ_j^Γ, the phase factor σ_{jk}^Γ is independent of the path parametrization. However, σ_{jk}^Γ depends on the relative phase of the two vectors $|\psi_j\rangle$ and $|\psi_k\rangle$ at $\mathbf{s}_1$. Indeed, under the gauge transformation (3), σ_{jk}^Γ transforms as follows:

$$\sigma_{jk}^\Gamma \to \sigma_{jk}^\Gamma \exp i[\varphi_k(\mathbf{s}_1) - \varphi_j(\mathbf{s}_1)]. \tag{5}$$

This shows that σ_{jk}^Γ is arbitrary, thus nonmeasurable. In order to define a gauge-invariant quantity, we combine two σ's in the following product:

$$\gamma_{jk}^\Gamma = \sigma_{jk}^\Gamma \sigma_{kj}^\Gamma. \tag{6}$$

This new phase factor γ_{jk}^Γ is determined uniquely by the trajectories Γ_j and Γ_k of $|\psi_j\rangle$ and $|\psi_k\rangle$ in the Hilbert space. The finding of the measurable geometric quantity γ_{jk}^Γ is the central result of this Letter.

A simple geometric interpretation for γ_{jk}^Γ can be obtained in analogy with that for the Pancharatnam phase. Consider the path of state j in the space of rays (where two states differing only for a complex factor are identified). If $|\psi_j(\mathbf{s}_1)\rangle$ is not orthogonal to $|\psi_j(\mathbf{s}_2)\rangle$, there exists a unique geodesic path G_{jj} going from $|\psi_j(\mathbf{s}_2)\rangle$ to $|\psi_j(\mathbf{s}_1)\rangle$, along which the geometric phase factor is unity. Then, trivially, the open-path geometric factor γ_j^Γ equals the phase factor on the circuit composed by Γ_j and G_{jj} (see Fig. 1) [9,11]. Once reduced to a closed path, using Stokes' theorem, one can write γ_j^Γ in terms of the integral of Berry's local-gauge-invariant two-form on any surface S_j is bounded by $\Gamma_j + G_{jj}$ [2,9,12].

Consider now *two* states j and k evolving along Γ_j and Γ_k in the space of rays. We generate all possible oriented loops by connecting the extremal points with geodesics. As Fig. 1 shows, only the three loops $\Gamma_j + G_{jj}$, $\Gamma_k + G_{kk}$, and $\Gamma_j + G_{jk} + \Gamma_k + G_{kj}$ can be generated. The first two loops give the usual phase factors γ_j^Γ and γ_k^Γ, while the third one corresponds to γ_{jk}^Γ. In this way, γ_{jk}^Γ can be calculated, in analogy to γ_j^Γ, as the integral of Berry's two-form over a surface S_{jk} bounded by this four-legs loop. The complementarity of γ_{jk}^Γ and γ_j^Γ is evident from this geometric picture. In complete analogy with the usual Berry phase, this expression in terms of a surface integral also proves the sensitivity of γ_{jk}^Γ to the presence of degeneracies of the two energy level i and j in the parametric Hamiltonian associated with the above paths. However, given the open path Γ and the energy levels involved, there is no general rule to determine a closed loop in parameter's space entangled with a degenerate submanifold. Whenever this loop can be found, γ_{jk}^Γ is a direct probe of the presence and position of degeneracies.

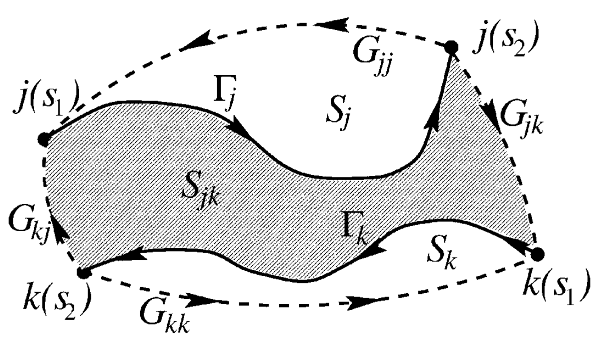

FIG. 1. States $|\psi_j(\mathbf{s})\rangle$ and $|\psi_k(\mathbf{s})\rangle$ follow the (solid) paths Γ_j and Γ_k along the evolution in rays space. Geodesics G_{jj}, G_{kk}, G_{jk}, and G_{kj} (dashed) lead back from the evolved states $|\psi_j(\mathbf{s}_2)\rangle |\psi_k(\mathbf{s}_2)\rangle$ to the initial ones $|\psi_j(\mathbf{s}_1)\rangle |\psi_k(\mathbf{s}_1)\rangle$. Integration of Berry's two-form over the shaded surface S_{jk} yields the off-diagonal phase γ_{jk}^Γ.

The simplest system to illustrate the concept of off-diagonal geometric phase is a spin-$\frac{1}{2}$ aligned to a slowly rotating magnetic field $\mathbf{B}$ in (say) the xz plane. The polar angle θ of $\mathbf{B}$ parametrizes a circular path in the two-dimensional space of the magnetic fields. For any value of θ, the columns of the matrix

$$U(\theta) = \begin{pmatrix} \cos\frac{\theta}{2} & \sin\frac{\theta}{2} \\ -\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix} \tag{7}$$

represent the parallel-transported eigenvectors $|\psi_j(\theta)\rangle$ on the initial basis $|\psi_1(0)\rangle = |\downarrow\rangle, |\psi_2(0)\rangle = |\uparrow\rangle$. Thus, the familiar Pancharatnam-Berry phase factor of the state $|\psi_j(\theta)\rangle$ evolving from $\theta = 0$ to θ_f is given by the diagonal matrix element $\gamma_j(\theta_f) = \Phi(U_{jj}(\theta_f)) \times \Phi[\langle\psi_j(0)\rangle | \psi_j(\theta_f)\rangle]$. The single off-diagonal term is $\gamma_{12} = \Phi(\sin\theta_f/2)\Phi(-\sin\theta_f/2) \equiv -1$ for any $\theta_f \neq 0, 2\pi$. For generic θ, γ_1, γ_2, and γ_{12} are all equally important. For $\theta = \pi$, γ_{12} carries all the geometric phase contents of the eigenstates, while γ_1 and γ_2 are undefined. At $\theta = 2\pi$ the roles are exchanged. In this sense, the off-diagonal phase factor γ_{12} constitutes the counterpart of γ_j, when the latter is undefined.

Interference experiments [18] have measured the noncyclic Pancharatnam-Berry phases γ_j in the spin-$\frac{1}{2}$ system. In a similar way, one can envisage a spin-rotation experiment to measure by interference σ_{12} and σ_{21} for an arbitrary fixed gauge at the starting point. The dependence on the gauge chosen cancels out in the product γ_{12}, which, for this simple system, must equal -1 for any rotation angle $\theta \neq 2\pi$. Essentially any experiment [5,16,18] sensitive to open-path diagonal geometric phases can be generalized to observe off-diagonal phases. In systems of larger dimensionality, several off-diagonal phase factors can be defined, and they may assume different values on different paths.

The definition (6) of the off-diagonal phase factors γ^Γ can be generalized to the simultaneous evolution of more than two orthonormal states. Consider, for example,

n orthonormal eigenstates $|\psi_j(\mathbf{s})\rangle$ (ordered by increasing energy) of a parametrized Hermitian Hamiltonian matrix $H(\mathbf{s})$, representing a physical system. Observing the effect (5) of a gauge change on the σ^Γ_{jk} phase factors, we note that *any cyclic product* of σ's is gauge invariant. It is then natural to generalize Eq. (6) by defining

$$\gamma^{(l)\Gamma}_{j_1 j_2 j_3 \ldots j_l} = \sigma^\Gamma_{j_1 j_2} \sigma^\Gamma_{j_2 j_3} \cdots \sigma^\Gamma_{j_{l-1} j_l} \sigma^\Gamma_{j_l j_1} . \tag{8}$$

For $l = 1$, Eq. (8) reduces to the familiar definition (2) of the Pancharatnam-Berry diagonal phase factor $\gamma^\Gamma_j = \gamma^{(1)\Gamma}_j = \sigma^\Gamma_{jj}$. The two-indexes $\gamma^{(2)\Gamma}_{jk}$ phase factors coincide with those introduced by Eq. (6). Larger l describe more complex phase relations among off-diagonal components of the eigenstates at the end points of Γ. The same geometrical construction of a closed path done for $\gamma^{(2)}$ extends to $\gamma^{(l)}$ with $l > 2$.

We note that any cyclic permutation of all the indexes $j_1 j_2 j_3 \ldots j_l$ is immaterial. Moreover, if one index is repeated, the associated $\gamma^{(l)}$ can be decomposed into the product $\gamma^{(l_1)}\gamma^{(l_2)}$'s with $l_1 + l_2 = l$. We can thus reduce to consider the $\gamma^{(l)}$with no repeated indexes, which means, in particular, $l \le n$.

One can readily verify that the number of $\gamma^{(l)}$'s left grows with n faster than n^2. Since n^2 is the number of the constituent σ_{jk}'s, not all the $\gamma^{(l)}$'s can be independent. We shall now find a complete set of independent $\gamma^{(l)}$'s, under the condition that $U^\Gamma_{jk} \neq 0$ for all j and k. Clearly, the n Pancharatnam-Berry diagonal phase factors $\gamma^{(1)}_j$ are all independent, since any diagonal σ_{jj} enters only $\gamma^{(1)}_j$. On the other hand, the off-diagonal $\gamma^{(l)}$'s are interrelated by the following exact equalities [they can be verified substituting explicitly the definition (8)]:

$$\gamma^{(l)}_{i\{j\}k\{m\}} = \gamma^{(l')}_{i\{j\}k}\gamma^{(l'')}_{k\{m\}i}\gamma^{(2)^*}_{ik} \qquad (l \ge 4), \tag{9}$$

$$\gamma^{(3)}_{jkm}\gamma^{(3)}_{jmk} = \gamma^{(2)}_{jk}\gamma^{(2)}_{km}\gamma^{(2)}_{jm}, \tag{10}$$

$$\gamma^{(3)}_{ijm}\gamma^{(2)^*}_{mj}\gamma^{(3)}_{jkm} = \gamma^{(3)}_{ijk}\gamma^{(2)^*}_{ki}\gamma^{(3)}_{ikm}. \tag{11}$$

In Eq. (9), $\{j\}$ indicates a set of one or more indexes, and l', l'' ($<l$) count the indexes in the corresponding γ. Combining relations (9)–(11), any $\gamma^{(l)}$'s may be expressed in terms of three categories: the n diagonal phases $\gamma^{(1)}_j$, the $n(n-1)/2$ quadratic $\gamma^{(2)}_{j<k}$'s, and the $(n-1)(n-2)/2$ cubic $\gamma^{(3)}_{1<j<k}$. These $n^2 - n + 1$ factors are indeed functionally independent combinations of the σ's: we verified that the Jacobian determinant $|\partial\gamma_{\{j\}}/\partial\sigma_{km}|$ is nonzero. The number of independent phases can be easily understood: it amounts to the n^2 phases of U^Γ_{jk} minus the arbitrary $n-1$ relative phases among the n eigenstates at a given point $\mathbf{s}$.

We restrict now the particular case of a path joining a pair of points $\mathbf{s}^P_1\mathbf{s}^P_2$ such that the n eigenstates at the final point are a permutation P of the initial eigenstates, i.e.,

$$\begin{cases} H(\mathbf{s}^P_1) = \sum_j E_j|\psi_j\rangle\langle\psi_j|, \\ H(\mathbf{s}^P_2) = \sum_j E'_j|\psi_{P_j}\rangle\langle\psi_{P_j}|, \end{cases} \tag{12}$$

where E_j and E'_j are in increasing order as usual. The only well-defined σ^Γ's are the n phase factors $\sigma^\Gamma_{jP_j}$. When the permutation is nontrivial ($P_j \neq j$), the familiar Berry-Pancharatnam phase factor associated with state j is undefined. For this special case the only well-defined geometric phases are the off-diagonal ones. One can classify them according to standard group theory. Any permutation P can be decomposed univocally into c cycles of lengths $l_1, l_2, \ldots, l_c$ [21]. To each cycle i, it is possible to associate one $\gamma^{(l_i)\Gamma}_{\{j\}}$, the l_i indexes $\{j\}$ following the corresponding cycle. These phase factors involve only nonzero U^Γ_{jk} and are thus well defined. In contrast, all other $\gamma^{(l)\Gamma}$'s are undefined. In Table I, for each permutation P of the eigenstates we report the corresponding well-defined $\gamma^{(l)}$ for $n \le 4$.

For these paths permuting the eigenvectors, the determinant $|U^\Gamma|$ of the overlap matrix is related to the product of the σ's. The equality $|U^\Gamma| = 1$ becomes therefore

$$\prod_{j=1}^{n} \sigma^\Gamma_{jP_j} = (-1)^P . \tag{13}$$

The third column of Table I summarizes this condition in terms of the $\gamma^{(l)}$'s. In the special case of a *real symmetric*

TABLE I. All possible geometric phase factors $\gamma^{(l)}$ defined in Eq. (8), for an arbitrary path joining a point $\mathbf{s}_1$ to $\mathbf{s}_2$, such that the eigenvectors of $H(\mathbf{s}_2)$ are permuted according to P with respect to those of $H(\mathbf{s}_1)$. The last column lists the number of the possible combinations of values (± 1) that the $\gamma^{(l)}$ factors can take in the special case of a real $H(\mathbf{s})$. The stars mark the permutations induced by relation (14), observed at the half-loop of Ref. [17] for $n = 2$ and 3.

n	P	Geometric phase factors	Condition $\lvert U^\Gamma\rvert = 1$	No. of cases
1	1	γ_1	$\gamma_1 = 1$	1
2	1 2	$\gamma_1\gamma_2$	$\gamma_1\gamma_2 = 1$	2
	2 1 *	γ_{12}	$\gamma_{12} = -1$	1
3	1 2 3	$\gamma_1\gamma_2\gamma_3$	$\gamma_1\gamma_2\gamma_3 = 1$	4
	2 1 3	$\gamma_{12}\gamma_3$	$\gamma_{12}\gamma_3 = -1$	2
	3 2 1 *	$\gamma_{13}\gamma_2$	$\gamma_{13}\gamma_2 = -1$	2
	1 3 2	$\gamma_{23}\gamma_1$	$\gamma_{23}\gamma_1 = -1$	2
	2 3 1	γ_{123}	$\gamma_{123} = 1$	1
	3 1 2	γ_{132}	$\gamma_{132} = 1$	1
4	1 2 3 4	$\gamma_1\gamma_2\gamma_3\gamma_4$	$\gamma_1\gamma_2\gamma_3\gamma_4 = 1$	8
	2 1 3 4	$\gamma_{12}\gamma_3\gamma_4$	$\gamma_{12}\gamma_3\gamma_4 = -1$	4
	[5 similar]	$\cdots$		4
	4 3 2 1 *	$\gamma_{12}\gamma_{34}$	$\gamma_{12}\gamma_{34} = 1$	2
	[2 similar]	$\cdots$		2
	2 3 1 4	$\gamma_{123}\gamma_4$	$\gamma_{123}\gamma_4 = -1$	2
	[7 similar]	$\cdots$		2
	2 3 4 1	γ_{1234}	$\gamma_{1234} = 1$	1
	[5 similar]	$\cdots$		1

Hamiltonian $H(\mathbf{s})$, all σ's, and thus all $\gamma^{(l)}$'s, equal either $+1$ or -1. For this simple but relevant situation, the last column of Table I reports the number of combinations of values that the $\gamma^{(l)}$'s may take, as allowed by the condition (13).

The above arguments on the permutational symmetry remain valid even if Eq. (12) is only approximate, provided that $|U^{\Gamma}_{j,P_j}| \gg n \max_{(k \neq P_j)} |U^{\Gamma}_{jk}|$ for all j. This extends the interest of the permutational case to a finite domain of the parameters' space around the point where Eq. (12) holds exactly or, more in general, to any region where the inequality on U^{Γ}_{jk} holds. For example, an approximate permutation occurs when the energy levels of a Hamiltonian $H(\mathbf{s})$ undergo a sequence of sharp avoided crossings along the path. At each avoided crossing, the two involved eigenstates, to a good approximation, exchange. As a result, there exist sizable regions between two avoided crossings where the eigenvectors are an approximate permutation of the starting ones.

Probably the simplest example of a nontrivial permutation of the Hamiltonian eigenstates occurs when the relation

$$H(\mathbf{s}_1) = -H(\mathbf{s}_2) \tag{14}$$

holds at the ends of the path. This symmetry is verified exactly by the spin-$\frac{1}{2}$ system, where it determines the swap of the eigenstates between $\theta = 0$ and $\theta = \pi$. Relation (14) holds also, approximately, in very common situations. Suppose, for example, that a point, say, $\mathbf{s} = 0$, locates an n-fold degeneracy, and consider the perturbative expansion around there:

$$H(\mathbf{s}) = \mathbf{s} \cdot \mathbf{H}^{(1)} + \dots . \tag{15}$$

[$\mathbf{H}^{(1)}$ is a vector of Hermitian numerical matrices.] In the sufficiently small neighborhood of the degeneracy, where the linear term accounts for the main contribution to the energy shifts, pairs of opposite points ($\mathbf{s}_1, \mathbf{s}_2 = -\mathbf{s}_1$) satisfy the relation (14). The permutation of the eigenstates associated with (14) is composed by $n/2$ 2-cycles for even n, or by $(n - 1)/2$ 2-cycles plus one 1-cycle for odd n: the corresponding γ's are marked by stars in Table I.

In the final part of this Letter, we examine the deformed microwave resonators experiment of Ref. [17]. In a recent work [7] the diagonal, closed-path Berry phases were calculated for that system. Here we analyze the experiment of Ref. [17] as a transparent example of how off-diagonal $\gamma^{(2)}_{jk}$'s can be measured for open paths. For these systems, $\mathbf{s} = (s\cos\theta, s\sin\theta)$ parametrizes the displacement of one corner of the resonator away from the position of a conical intersection of the energy levels. Lauber *et al.* [17] investigate the Berry phase of these nearly degenerate states, when the distortion is driven through a loop $\theta = 0$ to 2π around the degenerate point. The distortion path is traced in small steps in θ, following adiabatically the real eigenfunctions. In Fig. 2 we report the initial ($\theta = 0$), halfway ($\theta = \pi$), and final ($\theta = 2\pi$) parallel-transported eigenfunctions from the original pictures of Ref. [17].

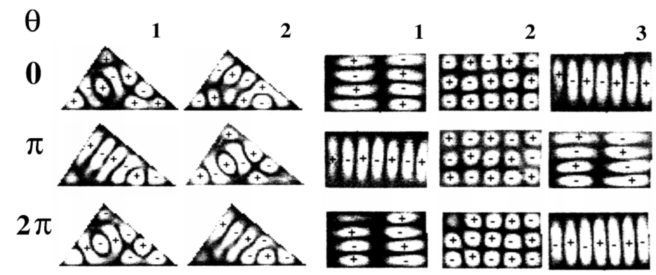

FIG. 2. The observed initial ($\theta = 0$), intermediate ($\theta = \pi$), and final ($\theta = 2\pi$) eigenstates of the microwave cavities deformed following adiabatically the path of Ref. [17]. Left: the two eigenstates of the triangular resonator. Right: the three eigenstates of the rectangular resonator.

The first case considered is that of a triangular cavity deformed around a twofold degeneracy: for small distortions, the system behaves similarly to a spin $\frac{1}{2}$. In particular, the Berry phases $\gamma^{(1)}_j$ at the end of the loop both equal -1 as expected for such a situation (cf. in Fig. 2 the recurrence of the pattern with changed sign at $\theta = 0$ and 2π). Because of the well approximate symmetry (14) at half path ($\theta = \pi$), the diagonal Berry phases are undefined there, but it is instead possible to determine the experimental value of $\gamma^{(2)}_{12}$ for this path. From inspection of Fig. 2 we determine $\sigma_{12} = 1, \sigma_{21} = -1$. This is consistent with the only possible value $\gamma^{(2)}_{12} = -1$ allowed in this spin-$\frac{1}{2}$-like case (see Table I). The same holds for the path going from $\theta = \pi$ to 2π.

The case of the rectangular resonator is more interesting. Here, three states intersect conically at $\mathbf{s} = 0$. The three Berry phases $\gamma^{(1)}_j$ at the end of the loop (-1, $+1$, and -1) are compatible with the determinant requirement of Table I. Figure 2 shows that empirically also this system satisfies the symmetry relation $H(\pi) = -H(0)$ at midloop. Thus, for the path $\theta = 0$ to π the only well-defined Pancharatnam-Berry phase is that of the central state $\gamma^{(1)}_2 = -1$. The upper and lower states exchange, giving $\sigma_{13} = 1$, $\sigma_{31} = 1$, and thus $\gamma^{(2)}_{13} = 1$. This is one of the two combinations of values allowed by the determinant rule $\gamma_{13}\gamma_2 = -1$ of Table I.

In conclusion, we have identified novel off-diagonal geometric phase factors, generalizing the (diagonal) Berry phase. The two sets of diagonal and off-diagonal geometric phases together exhaust the number of independent observable phase relations among n orthogonal states evolved along a path. We show that, in many common situations, the off-diagonal factors carry the relevant geometric phase information on the basis of eigenstates.

We thank Professor D. Dubbers, Dr. F. Faure, and Dr. A. F. Morpurgo for useful discussions.

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