Geometric Phases and Multiple Degeneracies in Harmonic Resonators

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(26 April 2000)

In a recent experiment Lauber et al. have deformed cyclically a microwave resonator and have measured the adiabatic normal-mode wavefunctions for each shape along the path of deformation. The nontrivial observed cyclic phases around a 3-fold degeneracy were accounted for by Manolopoulos and Child within an approximate theory. However, open-path geometrical phases disagree with experiment. By solving exactly the problem, we find unsuspected extra degeneracies around the multiple one that account for the measured phase changes throughout the path. It turns out that proliferation of additional degeneracies around a multiple one is a common feature of quantum mechanics.

Geometric phases may show up whenever the system under study depends on several parameters and is transported adiabatically around a closed path in parameters space [1]. Such phases have been predicted and observed in many different systems [1–6]. In particular, the cyclic phases observed by Lauber et al. [3] for a deformed microwave resonator have been recently accounted for within an approximate theory [6]. However, the closed-path phases are not the only interesting observable quantities: for an open-path evolution, the phase of the projection of a parallel-transported [3] eigenstate on the initial eigenstate is equally well defined [3,11] whenever these two states are not orthogonal. The experiment of Ref. [6] measures also such phase relations for a number of intermediate points along the path. These phases can be compared with the theoretical outcome of the calculation of Ref. [6]. We observe that the two sets of values disagree at half loop. The geometrical nature of these phases implies that the approximation of Ref. [6] is missing the topological structure of the simple system at hand.

To find what is missing, we push the perturbative expansion of Ref. [6] to higher order and demonstrate the presence of unsuspected extra degeneracies which account for the phase discrepancies. We show that similar “satellite” degeneracies close to a multiple degeneracy appear as a systematic, predictable feature of the Laplace operator in distorted domains: they can therefore arise in a broad range of undulatory phenomena, including acoustics, optics and quantum mechanics.

In Ref. [6] Lauber et al. follow the adiabatic evolution of three eigenstates of a microwave resonator driven along a loop in the two-dimensional space of deformations around the rectangular geometry. We indicate with \( r = (r \cos \theta, r \sin \theta) \) the external parameter representing the displacement of the right upper corner of the cavity from the rectangular position \((a, b) = (\sqrt{3}, 1)\) [3] at which the eigenstates \( |\psi_1\rangle = |2, 4\rangle, |\psi_2\rangle = |5, 3\rangle \) and \( |\psi_3\rangle = |7, 1\rangle \) become degenerate [with \( n_x, n_y \)] we indicate the wavefunctions \( 2 \sin(n_x x / a) \sin(n_y y / b) / \sqrt{a b} \) in the rectangle. We define the angle \( \theta \) so that it goes from 0 to \( 2\pi \) following the path of distortions used in the experiment. In Fig. 1 we report a sequence of adiabatic eigenfunctions \( |\psi_1(\theta)\rangle \) from the original pictures of Ref. [6].

![Figure 1](image)

**FIG. 1.** The observed initial \((\theta = 0)\), intermediate \((\theta = \pi)\) and final \((\theta = 2\pi)\) eigenstates of the microwave cavity deformed following adiabatically the path of Ref. [6].

The cyclic phase factors \( \gamma_1(2\pi) = -1, \gamma_2(2\pi) = +1 \) and \( \gamma_3(2\pi) = -1 \) are easily identified in Fig. 1 from the recurrence of the pattern and the sign changes at \( \theta = 0 \) and \( 2\pi \). Similarly, the sign change of the central state \( |\psi_2(\theta)\rangle \) at \( \theta = \pi \) tells us that its Berry-Pancharatnam open-path phase factor is \( \gamma_2(\pi) = -1 \).

Let us compare now these results with those of the linear approximation [6]. The eigenstates of the 2-dimensional Laplacian operator represent the normal modes of this cavity. The secular problem in the deformed domain can be conveniently reduced [6] to the secular problem of the following differential operator

\[
H(r) = \sum_{i,j} \frac{\partial}{\partial u_i} M_{ij}(u, r) \frac{\partial}{\partial u_j} + D(u, r)
\]

with vanishing boundary conditions in an undistorted rectangular domain for the transformed variables \( u \). This form, given explicitly in Ref. [6], is particularly suitable to set up a perturbation theory in \( r \)

\[
H(r) = r H^{(1)}(\theta) + r^2 H^{(2)}(\theta) + \ldots
\]
since all the parametric dependence is now in the functions \(M_{ij}(\mathbf{u},r)\) and \(D(\mathbf{u},r)\). At first order it suffices to consider the subspace span by the three eigenstates of Lauber et al.’s experiment, and compute the 3 \(\times\) 3 matrices \(\mathcal{H}^{(1)}_{ij}(\theta) = \langle \psi_i | H^{(1)}(\theta) | \psi_j \rangle\). The form of this matrix, given in Ref. [3], is

\[
\mathcal{H}^{(1)}(\theta) = \cos \theta \ F + \sin \theta \ F',
\]

where \(F\) and \(F'\) are real symmetric numerical matrices. In a sufficiently small neighborhood of the 3-fold degeneracy, \(\mathcal{H}^{(1)}(\theta)\) accounts for the leading contribution to the energy shifts.

FIG. 2. The projection \(U_{23}(\theta) = \langle \psi_2(0) | \psi_3(\theta) \rangle\) calculated along the path of Lauber et al.’s experiment. Observation [3]: crosses (cf. Fig. 1).

Manolopoulos and Child [3] calculate the (real) transformation matrix \(U^{(1)}_{ij}(\theta) = \langle \psi_i(0) | \psi_j(\theta) \rangle\), which diagonalizes \(\mathcal{H}^{(1)}(\theta)\) parallel-transporting the eigenstates. In particular, \(U^{(1)}_{ii}(2\pi)\) is the cyclic geometric phase of state \(i\). Each calculated phase agrees with that observed experimentally. More generally, for any \(\theta\), \(U^{(1)}_{ii}(\theta)/|U^{(1)}_{ii}(\theta)|\) is the observable (open-path) Berry-Pancharatnam phase factor \(\gamma_i\). These phase factors are therefore represented by the signs of the curves of Fig. 2b of Ref. [3]. In Fig. 2 we report \(U^{(1)}_{22}(\theta)\) for the intermediate state \(|\psi_2\rangle\). Near \(\theta = \pi\), the discord with experiment is particularly evident: linear theory has \(U^{(1)}_{22}(\theta) \approx +1\), while experimentally \(\gamma_2(\pi) = -1\).

\[
\begin{array}{|c|c|c|}
\hline
\text{First order [3]} & \text{Experiment [3]} & \text{2nd order & BW} \\
\hline
\gamma_2 & +1 & -1 & -1 \\
\gamma_{13} & -1 & +1 & +1 \\
\hline
\end{array}
\]

TABLE I. Phase factors \(\gamma_2\) and \(\gamma_{13}\) for the open path \(\Gamma_1\) going from \(\theta = 0\) to \(\theta = \pi\) in the space of deformations.

Around \(\theta = \pi\), \(|U_{11}|\) and \(|U_{33}|\) are very small \((\ll 1)\): the interesting geometric phase information is contained in the off-diagonal part of the matrix \(U(\pi)\) [12]. In particular, in this case \(\gamma_{13}(\theta) \equiv U_{13}(\theta)U_{31}(\theta)/|U_{13}(\theta)U_{31}(\theta)|\) is the only observable phase associated to state 1 and 3, since \(|U_{13}(\theta)U_{31}(\theta)|\approx 1\). From Fig. 1 one can read \(U_{13}(\theta) \approx +1\), and \(U_{31}(\theta) \approx +1\). Thus the observed \(\gamma_{13} = +1\). We have verified that the linear theory of Ref. [3] gives instead \(\gamma_{13} = -1\).

A similar reasoning can be applied to the path \(\Gamma_2\) leading back from \(\theta = \pi\) to \(\theta = 2\pi\). The observed and calculated phase changes for this second path are the same as those for path \(\Gamma_1\) going from \(\theta = 0\) to \(\theta = \pi\): they are summarized in Table I.

The failure of the linear approximation in predicting the correct geometrical phase factors suggests that it misses the topological structure of degeneracies in parameter space. In this Letter, we investigate this issue by considering both the next order in the expansion [3] and an exact numerical solution.

FIG. 3. Linear correction \(E^{(1)}_{ij}(\theta)\) [eigenvalues of \(H^{(1)}(\theta)\)] to the energies of the three states considered in the text as a function of \(\theta\).

The origin of the problem can be understood from inspection of Fig. 1. Indeed, close to \(\theta = \pi/2\) and \(3\pi/2\), the eigenenergies of \(H^{(1)}\) get pairwise very near (the minimum splittings being \(\sim 1\%\) of those in the \(\theta = 0\) direction). In this region, the linear approximation breaks down for \(r\) much smaller than in the (say) \(\theta = 0\) direction. Second-order terms can close the gaps inducing additional degeneracies in these directions, remaining dominant with respect to third- and higher-order ones. It is the smallness of the first-order splitting coefficient in this direction \(\theta = \pi/2\) and \(3\pi/2\) that makes this possible.

We compute therefore the second-order Hamiltonian correction [14]:

\[
\mathcal{H}^{(2)}_{ij} = \langle \psi_i | H^{(2)} | \psi_j \rangle + \sum_{k \neq 1,2,3} \frac{\langle \psi_i | H^{(1)} | \psi_k \rangle \langle \psi_k | H^{(1)} | \psi_j \rangle}{E_i - E_k},
\]

To calculate explicitly \(\mathcal{H}^{(2)}\), we cutoff the sum of Eq. [4] for \(|E_i - E_k| < E_{\text{max}}\). Convergence is achieved including \(\sim 10^2\) states. We have thus obtained the real symmetric numerical matrices \(G, G'\), and \(G''\)\(\in \mathcal{H}^{(2)}(\theta) = G + G' \cos 2\theta + G'' \sin 2\theta\). This second-order contribution adds to the linear Hamiltonian [3] to constitute the secular problem for the matrix

\[
r \mathcal{H}^{(1)}(\theta) + r^2 \mathcal{H}^{(2)}(\theta).
\]

We thus obtain the eigenvalues and eigenvectors of [5] as analytical functions of \(r\) and \(\theta\). Like in the linear case, the
If no degeneracies were present inside, the cyclic phase \( \gamma \) path phases inside the loop. Conical intersections of the second-order Hamiltonian (5) in first and second order calculations indicate additional symmetry. In other terms, the codimension of the degeneracy occur accidentally, i.e. not on account of symmetry. In this case, higher-order terms do not change the qualitative configuration of degenerate points and do not affect therefore the geometrical phases calculated at second order. However, without an upper bound on the higher-order terms, nothing guarantees that these terms do not displace significantly or even remove the degenerate points found at second order.

For this reason, we need to verify with a nonperturbative method the actual presence and position of the degeneracies. We thus resort to the numerical technique introduced by Berry and Wilkinson (BW) to solve the Laplace problem in two-dimensional domains. The advantage of this method is to reduce the two-dimensional differential equation to a one-dimensional integral equation for the normal derivative of the wavefunction at the boundary, which can be solved on a discrete mesh. We assess the presence of each degeneracy by encircling it with a loop in the parameters space and calculating the cyclic Berry phases of the involved states with the BW numerical method. Specifically, for the problem at hand we have calculated with the BW technique the Berry phases for the (discretized) loop \( \Gamma_1 - \Gamma_3 \) in Fig. 4 obtaining \( \gamma_1 = -1, \gamma_2 = -1, \) and \( \gamma_3 = +1 \). Similar procedure also confirms the presence of the degenerate point \( B \).

At this stage, one may wonder if satellite degeneracies (i.e. degeneracies within the range of validity of perturbation theory, involving irrelevant components on states outside the multiplet) are present only in this specific distorted “quantum billiard”, or if they are a widespread feature. Consider, for example, the 3-fold degenerate multiplet \( \{ n_x, n_y \} = \{1, 3\}, \{4, 2\}, \) and \( \{5, 1\} \) in the same geometry \( a/b = \sqrt{3} \); in this case we find no satellite degeneracies in the neighborhood of the 3-fold one, where second-order perturbation theory holds. This is not surprising, since over the whole range \( 0 < \theta < 2\pi \), the first-order splittings vary much more slowly than those of Fig. 3. Thus, when the quadratic term becomes of the same order of the linear term, also higher-order terms are of comparable size.

If we could establish a general criterion to predict the occurrence of satellite degeneracies for the general case of a \( n \)-fold degenerate multiplet in a billiard of arbitrary side ratio \( a/b \), then we could easily realize practical classical/quantum systems with clustered conical degeneracies, and thus intricate patterns of parallel-transported wavefunctions. Satellite degeneracies are to be expected whenever (i) the smallest first-order gap \( \delta_1^{(1)} \) near \( \theta = \pi/2 \) is much smaller than those \( \delta_0^{(1)} \) at \( \theta = 0 \), and (ii) the
second-order matrix elements of $|\mathcal{H}^{(2)}(\pi/2)| \gg \delta^{(1)}_{\pi/2}$, so that for $r \sim \delta^{(1)}_{\pi/2}/|\mathcal{H}^{(2)}(\pi/2)| \ll 1$ first and second order terms are of the same magnitude and at the same time higher-orders are negligible.

We first look for the realization of condition (i). $\mathcal{H}^{(1)}(\theta)$ [Eq. (3)] determines the first-order splittings $\delta^{(1)}_\theta$. The diagonal matrix elements of $F$ determine the linear splittings $\delta^{(1)}_0$ since the off-diagonal elements either vanish or are much smaller. The diagonal matrix elements of $F'$ are instead all equal. Consequently, at $\theta = \pi/2$, the mixing and the splittings $\delta^{(1)}_{\pi/2}$ of the three states are governed by the off-diagonal elements of $F'$. A parity selection rule applies to these matrix elements: $F'_{\{n_x,n_y\}\{n'_x,n'_y\}}$ is zero when

$$(-1)^{n_x+n'_x} = (-1)^{n_y+n'_y} = 1.$$  \hfill (6)

In addition, the the nonzero elements (setting $a = b$ for the sake of an estimate) satisfy

$$|F'_{\{n_x,n_y\}\{n'_x,n'_y\}}| \leq \frac{2^{9/2} n_x n'_x n_y n'_y}{\left(1 - \left(\frac{n}{n_x^2}\right)^2\right)\left[1 - \left(\frac{n'_y}{n'}\right)^2\right]}.$$ \hfill (7)

For states widely separated in $n_x - n_y$ plane ($n_x/n'_x \ll 1$ and $n'_y/n_y \ll 1$) this coupling becomes very small. Small linear gaps occur at $\pi/2$ whenever a state $\{n_x,n_y\}$ in the degenerate multiplet is weakly coupled to the others, i.e. when all the off-diagonal matrix elements $F'_{\{n_x,n_y\}\{n'_x,n'_y\}}$ are much smaller than $\delta^{(1)}_0$. Indeed in Lauber’s multiplet the linear coupling between states $\{5,3\}$ and $\{7,1\}$ vanishes because of parity (3), and the coupling determining $\delta^{(1)}_{\pi/2}$ is $F'_{\{2,4\}\{7,1\}} \approx 0.9$, compared to $\delta^{(1)}_0 \approx 50$. As we saw, for the multiplet $\{1,3\}, \{4,2\}, \{5,1\}$ the ratio $\delta^{(1)}_{\pi/2}/\delta^{(1)}_0$ is much closer to one, and indeed, no satellite degeneracies appear there.

We come now to condition (ii). The matrix elements of $\mathcal{H}^{(2)}(\pi/2)$ follow no selection rule. We have verified that these matrix elements are large: for instance $|\mathcal{H}^{(2)}_{\{n, n+1\}\{n+1, n\}}(\pi/2)| \sim n^3$. These matrix elements reduce rapidly as a function of the distance $(n_x - n'_x)^2 + (n_y - n'_y)^2$ between the states.

In conclusion, whenever in a degenerate multiplet one state is near some states (so that second-order coupling is large) for which selection rule (3) makes first order coupling vanish, and at the same time it is far from all remaining states (so that $\delta^{(1)}$ is small), one expects satellite degeneracies. This rule permits, for instance, to decide that the 3-fold multiplet $\{1,5\}, \{4,4\}, \{6,2\}$ for $a/b = \sqrt{5}/3$ has a structure of satellite degeneracies very similar to that of Lauber’s experiment, as we then verified by BW calculation.

An interesting case emerges from this analysis: when all off-diagonal matrix elements of $F'$ vanish because of selection rule (3), the linear perturbation does not remove the degeneracy at $\theta = \pi/2$. In this direction, the second-order term $\mathcal{H}^{(2)}$ is therefore the leading responsible for the splitting of the degenerate levels, which therefore “kiss” gently, instead of intersecting conically as usual. Many two-fold degenerate multiplets satisfy this condition (for example $\{2,4\}$ and $\{4,2\}$ for $a/b = 1$, or $\{2,3\}$ and $\{6,1\}$ for $a/b = 2$).

In this work, we have accounted for all experimental findings regarding the eigenstates of Lauber et al.’s deformed resonator. We have found that in deformed rectangular resonators additional degeneracies (with lower multiplicity) may appear very close to multiple degeneracies. These extra degeneracies are responsible for the observed pattern of geometric phases. These results rely only on the properties of the Laplace operator: for this reason they have a wide scope of applicability and are not restricted to simple microwave resonators.

We thank Dirk Dubbers for suggesting us to investigate this system and for useful discussions.

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1. M. V. Berry, Proc. R. Soc. Lond. A 392, 45 (1984).
2. R. Resta, Rev. Mod. Phys. 66, 899 (1994).
3. G. Delacrétaz, E. R. Grant, R. L. Whetten, L. Wöste, and J. W. Zwanziger, Phys. Rev. Lett. 56, 2598 (1986).
4. R. Tycko, Phys. Rev. Lett. 58, 2281 (1987).
5. H. Weinfurter and G. Badurek, Phys. Rev. Lett. 64, 1318 (1990).
6. H.-M. Lauber, P. Weidenhammer, and D. Dubbers, Phys. Rev. Lett. 72, 1004 (1994).
7. D. E. Manolopoulos and M. S. Child, Phys. Rev. Lett. 82, 2223 (1999).
8. J. Anandan and L. Stodolsky, Phys. Rev. D 35, 2597 (1987).
9. S. Pancharatnam, Proc. Ind. Acad. Sci. A 44, 247 (1956).
10. J. Samuel and R. Bhandari, Phys. Rev. Lett. 60, 2339 (1988).
11. A. G. Wagh, V. C. Rakhecha, P. Fischer, and A. Ioffe, Phys. Rev. Lett. 81, 1992 (1998); R. Bhandari, ibid. 83, 2080 (1999); A. G. Wagh et al., ibid. 83, 2090 (1999).
12. N. Manini and F. Pistolesi, quant-ph/9911083.
13. We fix the length-scale $b = 1$, and correspondingly the energy unit $b^{-2}$ throughout the paper.
14. L. D. Landau and E. M. Lifshitz, Quantum Mechanics (Pergamon, Oxford, 1976).
15. J. Von Neumann and E. P. Wigner, Phys. Z. 30 467 (1929).
16. M. V. Berry and M. Wilkinson Proc. R. Soc. Lond. A 392, 15 (1984).
17. A good convergence was reached with a mesh of 300 points on the boundary and Alice 1000 points along the discretized path in the parameters space.

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