Branch points in the complex plane and geometric phases

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Laser-induced degenerate states (LIDS) are equivalent to double poles of the *S* matrix that are branch points in the complex plane (BPCP). These branch points cause geometric phase changes by encircling them adiabatically around a closed circuit by varying certain parameters. They cause also the well-known phase changes appearing by encircling a diabolic point (DP) being a singularity associated with level repulsion. In both cases, the wave functions are exchanged, $\tilde{\Phi}_i \to \pm i \tilde{\Phi}_{j\neq i}$, at the critical value of the parameter where the states avoid crossing. Such a critical point is passed twice by encircling a DP but only once by surrounding a BPCP. As a consequence, the phase changes are different in both cases. A second surrounding restores the wave functions including their phases in both cases (when the BPCP is well isolated from others and the time of encircling is shorter than the lifetime of the two states). The different interference pictures appearing in surrounding LIDS adiabatically in opposite directions on a closed circuit represent a completion of the work by Berry.

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I. STRUCTURES IN THE CONTINUUM AND POLES OF THE *S* MATRIX

The interest in the topological structure of the Hilbert space and geometric phases has advanced since the pioneering paper by Berry [1]. Best known are the diabolic points (DP), e.g., [2]. They are singularities associated with level repulsions (called avoided level crossings or anticrossings) that occur by variation of a certain parameter.

When a DP is encircled adiabatically in the parameter space, a geometric phase appears [1]. Some years ago, the appearance of such a geometric phase has been studied experimentally on two-dimensional microwave resonators by surrounding a DP where the parameter space is the space of shapes of the resonator [3]. While the results for a well-separated DP showed the expected Berry phase, the results for not-separated DP are much more complicated and could be understood only recently [4,5]. Geometric phases in dissipative systems may be complex [6–8]. In [8], the geometric phase of the wave function of the hydrogen atom for a closed circuit in a three-parameter space is calculated in the framework of the Floquet theory where the three physical parameters are the individual intensities of the two components of the bichromatic light beam and the relative phase of these components.

Besides the DP, other singularities in different fields of physics are discussed. Most interesting are the singularities of the mapping from parameter space to the Hilbert space. These singularities are in the continuum into which dissipative systems are embedded. An example are the laser-induced degenerate states (LIDS), see the review [9], which appear as structures in the continuum (resonances in the cross section). It is clear that any structure in the continuum is related to the poles of the *S* matrix that provide the energies and widths of the resonance states, see, e.g., [10]. They are the eigenvalues of an effective Hamilton operator H^{eff} that appears in the function space of discrete states when it is embedded in a continuum of decay channels. The effective Hamiltonian is non-Hermitian since it is defined in a subspace of the function space whose eigenstates can decay into the complementary subspace. An essential point is the biorthogonality of the eigenfunctions of H^{eff} due to which the right and left eigenfunctions, $\tilde{\Phi}_R^{\mathrm{rt}}$ and $\tilde{\Phi}_R^{\mathrm{lt}}$, respectively, are different from one another. For symmetrical H^{eff}, it is [10]

$$\langle \tilde{\Phi}_R^{\mathrm{lt}} | \tilde{\Phi}_{R'}^{\mathrm{rt}} \rangle = \langle \tilde{\Phi}_R^{*} | \tilde{\Phi}_{R'} \rangle = \delta_{RR'} \tag{1}$$

where $\tilde{\Phi}_R^{\mathrm{rt}} \equiv \tilde{\Phi}_R$ and $\tilde{\Phi}_R^{\mathrm{lt}} = \tilde{\Phi}_R^{*}$. Equation (1) provides the biorthogonality relations

$$\langle \tilde{\Phi}_R | \tilde{\Phi}_R \rangle = \mathrm{Re}(\langle \tilde{\Phi}_R | \tilde{\Phi}_R \rangle) = \langle \tilde{\Phi}_{R'} | \tilde{\Phi}_{R'} \rangle$$

$$A_R \equiv \langle \tilde{\Phi}_R | \tilde{\Phi}_R \rangle \geqslant 1$$

$$\langle \tilde{\Phi}_R | \tilde{\Phi}_{R'\neq R} \rangle = i\,\mathrm{Im}(\langle \tilde{\Phi}_R | \tilde{\Phi}_{R'\neq R} \rangle) = -\langle \tilde{\Phi}_{R'\neq R} | \tilde{\phi}_R \rangle$$

$$B_R^{R'\neq R} \equiv |\langle \tilde{\Phi}_R | \tilde{\Phi}_{R'\neq R} \rangle| \geqslant 0. \tag{2}$$

Due to these relations, some nonlinear terms appear in the Schrödinger equation that vanish with $A_R \to 1$, $B_R^{R'} \to 0$ [10].

In [10], the relation between the effective Hamiltonian H^{eff} and the *S* matrix is derived that holds for isolated as well as for overlapping resonances. Especially, it holds also for two resonance states whose eigenvalues are the same, i.e., at a double pole of the *S* matrix. It is shown further that the relation (1) holds also at a double pole of the *S* matrix. Here, the two wave functions are linearly dependent,

$$\tilde{\Phi}_R^{\mathrm{bp}} \to \pm i \tilde{\Phi}_{R'\neq R}^{\mathrm{bp}}, \tag{3}$$

as shown analytically [10] as well as numerically for LIDS [11]. Nevertheless, the orthonormality relation (1) can be fulfilled because $A_R \to \infty$ and $B_R^{R'} \to \infty$ in approaching the double pole [10]. Since the *S* matrix contains the product of the wave functions $\tilde{\Phi}_R$ according to the orthonormality condition (1) [10], a smooth behavior around the double pole of the S matrix is expected in all experimentally relevant values. The double poles of the S matrix are second-order branch points in the complex plane (BPCP) [10,12]. They appear as LIDS in laser-induced continuum structures in atoms [11,13]. They cause, among others, some stabilization of atoms (called adiabatic stabilization [9] or resonance trapping [11,13]), i.e., a decrease of the ionization rate with increasing intensity of the laser.

In some other studies of singularities, the properties of exceptional points are investigated [14] that are, according to their definition, related to avoided level crossings. They are shown to be also BPCP [10,12]. Surrounding exceptional points in the parameter space, phase changes are expected to appear [15] and found in a microwave cavity experiment [16], indeed. The phase changes observed in encircling a DP and an exceptional point are caused by the *same* topological structure of the Hilbert space [17].

The phenomenon of avoided level crossing is traced as a function of a certain parameter in calculations on microwave billiards [18] as well as on atoms [11,13]. While two interacting discrete levels avoid always crossing, resonance states can cross, under certain conditions, in the complex plane. The transition from an avoided level crossing to a real crossing in the complex plane (where the S matrix has a double pole) takes place smoothly, at least in laser-induced continuum structures in atoms where the double pole of the S matrix appears as LIDS [11,13].

In other studies, the influence of the BPCP is traced up to the discrete states of quantum systems. In [19,20], the BPCP (called hidden crossings) are shown to influence the spectra of atoms. The position of the BPCP is clearly determined by the (Hermitian) Hamiltonian of the system and its relation to the (Hermitian) Hamiltonian of the residual system ("spectroscopic factors") [12]. The relation between a BPCP and the avoided crossings of discrete states is traced as a function of a certain parameter in [10,12]. As a result, a BPCP causes an avoided crossing of discrete states in the same manner as it does it for resonance states. Further, a nontrivial influence of nonisolated BPCP on the mixing of the discrete states could be stated.

All these studies show that avoided crossings of discrete and resonance states are caused by singularities of the mapping from the parameter space to the Hilbert space. Although the number of BPCP is of measure zero, their influence on physically relevant values and the level dynamics is large. It can be expressed by nonlinear terms in the Schrödinger equation that are related to the biorthogonal terms A_R and $B_R^{R'}$ defined by Eq. (2) [10]. Experimentally, it can be studied by means of the LIDS.

In the following, the differences occurring after a full surrounding of a (well-isolated) DP and a (well-isolated) BPCP in the parameter space under adiabatic conditions will be illustrated under the assumption that the encircling time is shorter than the lifetimes of both resonance states. The phase changes received by encircling the two points are different, generally, but prove the *same* topological structure of the Hilbert space. The two experimental data complete one another therefore in a valuable manner. While the phases of the two wave functions change in the same manner, $\Phi_R \to -\Phi_R$ (Berry phase), in surrounding a DP under adiabatic conditions, those in surrounding a BPCP change differently, $\Phi_R \to \pm i \Phi_{R' \neq R}$. These differences should be visible in the interference picture obtained after surrounding a LIDS.

II. TWO-BY-TWO HAMILTONIAN MATRIX

Let us illustrate the avoided level crossing and its relation to a BPCP by means of the complex two-by-two Hamiltonian matrix

$$\mathcal{H} = \begin{pmatrix} e_1(a) & 0 \\ 0 & e_2(a) \end{pmatrix} - \begin{pmatrix} \frac{1}{2}\gamma_1(a) & \omega \\ \omega & \frac{1}{2}\gamma_2(a) \end{pmatrix}. \quad (4)$$

The unperturbed energies e_k and widths γ_k $(k=1,2)$ of the two states depend on the parameter a to be tuned in such a manner that the two states may cross in energy (and/or width) when $\omega=0$. The two states interact only via the nondiagonal matrix elements ω that may be complex, in general [10]. They are assumed, in the following, to be independent of the parameter a. The eigenvalues of $\mathcal{H}$ are

$$\mathcal{E}_{i,j} \equiv E_{i,j} - \frac{i}{2}\Gamma_{i,j} = \frac{\epsilon_1+\epsilon_2}{2} \pm \frac{1}{2}\sqrt{(\epsilon_1-\epsilon_2)^2+4\omega^2} \quad (5)$$

with i, $j=1$, 2 and $\epsilon_k \equiv e_k - (i/2)\gamma_k$ $(k=1,2)$. According to Eq. (5), two interacting discrete states (with $\gamma_k=0$) always avoid crossing since ω and $(\epsilon_1-\epsilon_2)$ are real in this case. Equation (5) shows also the generic property that resonance states with nonvanishing widths γ_k avoid crossing since

$$F(a,\omega) \equiv (\epsilon_1-\epsilon_2)^2 + 4\omega^2 \quad (6)$$

is different from zero for all a (with the exception of a few values the number of which is of measure zero). Only when $F(a,\omega)=0$ at $a=a^{\mathrm{cr0}}$ (and $\omega=\omega^{\mathrm{cr}}$), the states cross, i.e., $\mathcal{E}_1=\mathcal{E}_2$. In such a case, the S matrix has a double pole. It can further be seen from Eq. (5) that the crossing point is a BPCP of second order due to the square root appearing in the expression for the eigenvalues. The critical value a^{cr0} of the parameter a is determined by the values $(\omega)^2$ and $(\epsilon_1-\epsilon_2)^2$ but not by the signs of these values. According to Eq. (5), the position of the BPCP is in the complex plane at the point $X \equiv (1/2)\{\epsilon_1(a^{\mathrm{cr0}}) + \epsilon_2(a^{\mathrm{cr0}})\}$.

As can be seen from Eq. (6), $F=F_R+iF_I$ is generally a complex number,

$$F_R(a,\omega) = (e_1-e_2)^2 - \tfrac{1}{4}(\gamma_1-\gamma_2)^2 + 4(\omega_R^2-\omega_I^2), \quad (7)$$

$$F_I(a,\omega) = (e_1-e_2)(\gamma_1-\gamma_2) + 8\omega_R\omega_I, \quad (8)$$

where $\omega=\omega_R+i\omega_I$ (and ω_R, ω_I are real values). At a double pole of the S matrix, both parts F_R and F_I are zero at the critical value a_R^{cr0} of the parameter a. When only the real or the imaginary part of $\sqrt{F}$ is zero at the critical value a_R^{cr}, then the two levels do not cross in the complex plane. In such a case, they cross freely in width but not in energy or

TABLE I. Level crossing and critical coupling.

ω	$\sqrt{F}$	Energy	Width	Coupling
Real	Real	Avoided crossing	Free crossing	Overcritical
Real	Imag	Free crossing	No crossing	Subcritical
Imag	Real	No crossing	Free crossing	Subcritical
Imag	Imag	Free crossing	Avoided crossing	Overcritical

vice versa. Some combinations with $\omega=\omega_R$ and $\omega=\omega_I$ are shown in Table I. The difference between *avoided crossing* and *no crossing* will be illustrated by means of two special cases with $F_I=0$ where the critical value a^{cr} (for a certain fixed value $\omega=\omega^{\mathrm{cr}}$) is determined by the crossing of the unperturbed energies e_i or widths γ_i.

(i) $\omega_I=0$ (the coupling is real, $\omega=\omega_R$), γ_i independent of the parameter a. Then $e_1=e_2$ and

$$F_R^{(\mathrm{i})}(a,\omega)=-\tfrac{1}{4}(\gamma_1-\gamma_2)^2+4\omega_R^2 \tag{9}$$

at a^{cr}. According to the value of F_R, we have to differentiate between three cases

$$F_R(a,\omega)>0\rightarrow\sqrt{F_R}=\text{real}, \tag{10}$$

$$F_R(a,\omega)=0\rightarrow\sqrt{F_R}=0, \tag{11}$$

$$F_R(a,\omega)<0\rightarrow\sqrt{F_R}=\text{imaginary}. \tag{12}$$

The first case is the well-known level repulsion in energy (*avoided crossing in energy*) with an exchange of the two states that is accompanied by a free (true) crossing of the widths at a^{cr}. The second case corresponds to the double pole of the *S* matrix. In the third case, the two levels cross freely in energy, the difference of the widths does never become zero (*no crossing in width*) and the two states are not exchanged at the critical value a^{cr}. Examples from numerical studies are shown in [10], Figs. 1 and 2. The two cases $F_R>0$ and $F_R<0$ have been studied experimentally in a microwave cavity [21]. Here, the first case is called *overcritical* coupling, the second one *critical* coupling, and the third one *subcritical* coupling (Table I).

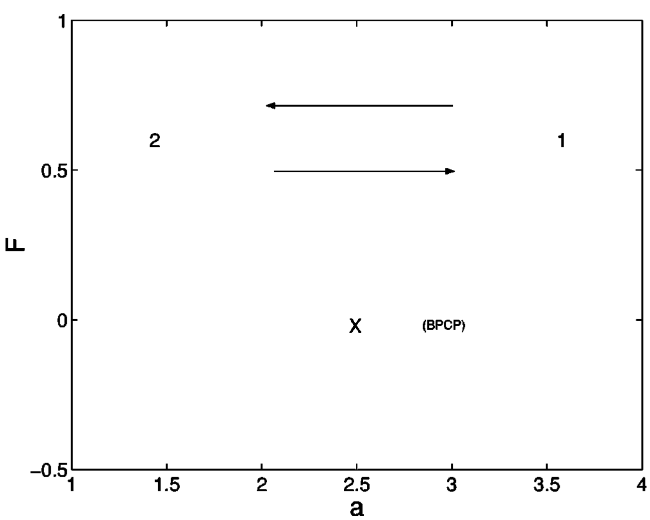

FIG. 1. One possible way of encircling the DP lying at $F>0$. For real ω, $F>0$ is the overcritical region with an avoided level crossing in energy at $a=a^{\mathrm{cr}}$. The BPCP lying at $F=0$ is denoted by *X*. *F* and *a* are in arbitrary units.

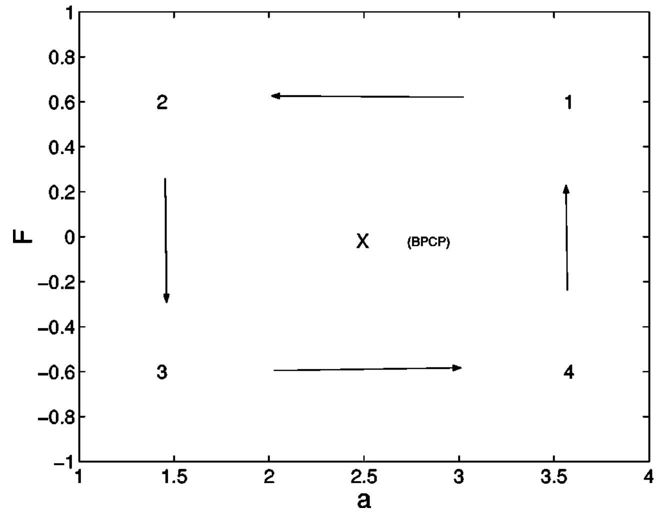

FIG. 2. One possible way of encircling the BPCP lying at $F=0$. For real ω, $F>0$ is the overcritical region with an avoided level crossing in energy at $a=a^{\mathrm{cr}}$ while $F<0$ is the subcritical region with free crossing in energy. The BPCP is denoted by *X*. *F* and *a* are in arbitrary units.

(ii) $\omega_R=0$ (the coupling is imaginary, $\omega=i\omega_I$), He_i, independent of the parameter a. Then $\gamma_1=\gamma_2$ and

$$F_R^{(\mathrm{ii})}(a,\omega)=(e_1-e_2)^2-4\omega_1^2 \tag{13}$$

at a^{cr}. According to the value of F_R, we have again the three cases (10)–(12) but describing now a different physical situation. The case with an exchange of the states at a^{cr} is Eq. (12) where the two levels repel in width (*avoided crossing in width*) and cross freely in energy. The second case corresponds again to the double pole of the *S* matrix. In the first case corresponding to Eq. (10), no exchange of the states takes place, the difference of their energies never becomes zero (*no crossing in energy*) and their widths cross freely. One can call the first case *subcritical* coupling, the second case *critical* coupling, and the third case *overcritical* coupling (Table I).

The two cases (i) and (ii) are physically different from one another. While the overcritical situation is characterized by Eq. (10) in (i), it is determined by the condition (12) in (ii). In the first case, the two levels repel in energy (''level repulsion'') but align their widths (''spreading of the transition strengths'') while in the latter case, they attract in energy (''cluster formation'') but repel in width (''formation of different time scales by means of resonance trapping'').

In microwave cavities, ω may be complex due to the coupling of the resonance states via the channels [10]. Under certain conditions ω_R is the dominant part while ω_I is dominant under other conditions [18]. The interplay between level repulsion caused by ω_R and cluster formation caused by ω_I is studied in laser-induced continuum structures in the adiabatic limit.[11,13] In this case, ω is given by the Rabi frequency. The cluster formation is accompanied by resonance trapping that may lead, under certain conditions, to a decrease of the ionization rate with increasing intensity of the laser beam (adiabatic stabilization or resonance trapping).

The two examples (i) and (ii) illustrate further that at the critical value a^{cr} the states are always exchanged when the coupling is overcritical. In the case of subcritical coupling, no exchange occurs. The exchange is related, in any case, to a BPCP that appears as a double pole of the S matrix when the condition of the critical coupling is fulfilled [10,12]. The two wave functions can be normalized according to Eq. (1) in the whole function space including the BPCP although they are linearly dependent at the BPCP according to Eq. (3). The point is that $(\tilde{\Phi}_i)^2$ is, at a^{cr}, the *difference* of two infinitely large numbers that may be 0 or 1. All physically relevant values contain the wave functions in a combination according to the orthonormality condition (1). They do *not* contain any singularities caused by the $|\tilde{\Phi}_i|^2$ at the BPCP, i.e., by the relations (2) at a^{cr} (which are sums of two infinitely large numbers).

The DP is related to the avoided crossing of discrete levels belonging to the case (i) with the condition (10). The corresponding BPCP is beyond the function space considered. It is a hidden crossing. The DP is surrounded in the experiment [3], therefore, in the regime of overcritical coupling along the whole way of encircling and the BPCP itself is *not* encircled in this experiment.

III. ENCIRCLING OF ISOLATED DP AND BPCP

We will illustrate the surrounding of an isolated DP by means of adiabatically varying the parameter a in the Hamiltonian (4) and using the relation (3) at a^{cr} and Table I. The encircling is illustrated in Fig. 1 where $\omega \approx \omega_R$, case (i), is assumed. It causes the following changes: for the way from 1 to 2 with passing a^{cr} at overcritical coupling,

$$\begin{Bmatrix} \tilde{\Phi}_1 \\ \tilde{\Phi}_2 \end{Bmatrix} \to \begin{Bmatrix} -i\tilde{\Phi}_2 \\ i\tilde{\Phi}_1 \end{Bmatrix}, \tag{14}$$

and for the way back from 2 to 1 with passing a^{cr} at overcritical coupling,

$$\begin{Bmatrix} -i\tilde{\Phi}_2 \\ i\tilde{\Phi}_1 \end{Bmatrix} \to - \begin{Bmatrix} \tilde{\Phi}_1 \\ \tilde{\Phi}_2 \end{Bmatrix}. \tag{15}$$

The encircling of the DP gives a phase change by π of both wave functions that is caused by the hidden BPCP. Encircling it once more will restore the original wave functions $\tilde{\Phi}_i$ including their phases. Thus, the BPCP is a second-order branch point that is in agreement with the eigenvalue equation (5). The phase change occuring after the first surrounding of the DP, Eq. (15), corresponds to the well-known geometric phase discussed by Berry [1,3].

The way of encircling adiabatically the BPCP itself passes from a region with overcritical coupling at a^{cr} to another one with subcritical coupling at a^{cr}. For illustration see Fig. 2 where $\omega \approx \omega_R$, case (i), is assumed as in Fig. 1. The first surrounding causes the following changes: for the way from 1 to 2 with passing a^{cr} at overcritical coupling,

$$\begin{Bmatrix} \tilde{\Phi}_1 \\ \tilde{\Phi}_2 \end{Bmatrix} \to \begin{Bmatrix} -i\tilde{\Phi}_2 \\ i\tilde{\Phi}_1 \end{Bmatrix}; \tag{16}$$

for the way from 2 to 3 with transition from the overcritical to the subcritical coupling, no exchange occurs since a^{cr} will not be passed; for the way from 3 to 4 with passing a^{cr} at subcritical coupling, no exchange occurs at a^{cr}; for the way from 4 back to 1 with transition from the subcritical to the overcritical coupling, no exchange occurs since a^{cr} will not be passed. Thus, the wave functions are exchanged with phase changes of $\pi/2$ and $3\pi/2$, respectively.

The second surrounding is as follows: for the way from 1 to 2 with passing a^{cr} at overcritical coupling

$$\begin{Bmatrix} -i\tilde{\Phi}_2 \\ i\tilde{\Phi}_1 \end{Bmatrix} \to + \begin{Bmatrix} \tilde{\Phi}_1 \\ \tilde{\Phi}_2 \end{Bmatrix}, \tag{17}$$

and for the way from 2 to 3 with transition from the overcritical to the subcritical coupling, no exchange occurs since a^{cr} will not be passed; for the way from 3 to 4 with passing a^{cr} at subcritical coupling no exchange occurs at a^{cr}, and for the way from 4 back to 1 with transition from the subcritical to the overcritical coupling no exchange occurs since a^{cr} will not be passed. As a result, surrounding the BPCP adiabatically twice restores the wave functions $\tilde{\Phi}_i$ including their phases, see Eq. (17). The BPCP is a second-order branch point in correspondence with the eigenvalue equation (5).

In the experiment [16], the BPCP is encircled once and a phase change of one of the wave functions has been observed. This result coincides with Eq. (16). Surrounding the BPCP in the opposite direction (i.e., from 2 to 1) changes the phase of the other wave function according to the experiment [16]. Such a result follows also theoretically. As in the case discussed above, the only changes between the wave functions take place by passing the critical value a^{cr} at overcritical coupling. This gives for the encircling of the BPCP in the opposite direction

$$\begin{Bmatrix} \tilde{\Phi}_1 \\ \tilde{\Phi}_2 \end{Bmatrix} \to \begin{Bmatrix} i\tilde{\Phi}_2 \\ -i\tilde{\Phi}_1 \end{Bmatrix}. \tag{18}$$

Thus, the theoretical results (16) and (18) agree with the experimental results presented in [16].

The relations (15) and (16) show that the phase changes of the wave functions are different in encircling a DP and the corresponding BPCP in the parameter space only once. In both cases, a second surrounding restores the original wave functions including their phases (which holds exactly of course only when the lifetimes of both states are long as compared to the time of encircling, i.e., in the adiabatic limit). This result is in correspondence to the fact that the BPCP is a second-order branch point.

Experimental studies with surrounding a DP and a BPCP have been performed, up to now, only on microwave resonators [3,16]. The results obtained are in agreement with the theoretical expectations discussed above (see [17]). The LIDS provide another example for the appearance of geometric phases when surrounded adiabatically in the parameter space. The different phase changes of the two wave functions after surrounding the LIDS in opposite directions are expected to influence the interference picture of measurable values. In any case, it will be restored to the original one after a second surrounding only.

It should be underlined here that all the results discussed above are obtained under the assumption that the system is adequately described by a two-state approximation, which includes that the considered BPCP is well separated from other BPCP in the neighborhood. This is surely true when the BPCP lies near to the real axis and the level density is low. As soon as two (or more) BPCP start to overlap in the complex plane, i.e., when the corresponding widths exceed the distance in energy between different BPCP, the changes of the wave functions under the influence of the BPCP are much more complicated, see [4,5]. Especially, the nonlinear effects arising from the BPCP are difficult to handle [10,12]. The other assumption stressed above is the adiabaticity that involves further that the lifetimes of both states are long as compared to the time of encircling the BPCP.

IV. SUMMARY

Summarizing, it can be stated the following.

(1) Well-isolated BPCP are second-order branch points. They can be studied by means of LIDS.

(2) The geometric phases appearing by surrounding a DP adiabatically in the parameter space are caused by a BPCP that is a hidden crossing when the consideration is restricted to the function space of discrete states.

(3) Encircling a DP adiabatically in the parameter space only once, the phases of both wave functions are changed by π, as discussed by Berry [1].

(4) Encircling a BPCP adiabatically in the parameter space only once, the two wave functions are exchanged with the phase changes $\pi/2$ and $3\pi/2$, respectively.

The results discussed in this paper show that the Berry phase is the sign of a BPCP that is hidden when the function space considered is restricted to the wave functions of discrete states. The BPCP are in the continuum, but their influence continues analytically into the function space of discrete states. Encircling adiabatically a LIDS in the parameter space will provide measurable values that differ, due to interference effects, from the original ones. Only a second surrounding will restore the original values (under the assumption that the states did not yet decay during the time of surrounding). An experimental study of this phenomenon would represent an interesting proof of the topological structure of the Hilbert space, including the mapping from the parameter space to the Hilbert space and the geometric phases.

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