

Exceptional points and double poles of the S matrix

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Exceptional points and double poles of the S matrix are both characterized by the coalescence of a pair of eigenvalues. In the first case, the coalescence causes a defect of the Hilbert space. In the second case, this is not so as shown in previous papers. Mathematically, the reason for this difference is the biorthogonality of the eigenfunctions of a non-Hermitian operator that is ignored in the first case. The consequences for the topological structure of the Hilbert space are studied and compared with existing experimental data.

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I. INTRODUCTION

Information on the topological structure of the Hilbert space can be obtained from a study of its singularities. Berry [1] showed that geometric phases appear when a diabolic point is surrounded by varying adiabatically external parameters of a quantum system. Manifestations of this phase factor have been considered and proven experimentally already in 1980s in many different fields of physics, e.g., Ref. [2]. In 1994, it has been studied also by using microwave resonators: the sign change of the wave function has been found after a cyclic excursion around a diabolic point in the space of shapes of the resonator [3].

Other singularities are exceptional points [4], which appear in the complex Λ plane of the eigenvalues $\mathcal{E}_k(\Lambda)$ of the Hamiltonian $H = H_0 + \Lambda H_1$. Their positions are characteristic of the Hamiltonian H , once H_0 and H_1 are given [5–7] (which both are assumed to be real and symmetric). The exceptional points are characterized by the coalescence of a pair of eigenvalues, i.e., $\mathcal{E}_l(\Lambda_{\text{EP}}) = \mathcal{E}_k(\Lambda_{\text{EP}})$. When the corresponding eigenfunctions are assumed to be orthogonalized in the standard manner, it follows that $\psi_l(\Lambda_{\text{EP}}) = \psi_k(\Lambda_{\text{EP}})$. This means, that $\psi_k(\Lambda_{\text{EP}})$ cannot be normalized at $\Lambda = \Lambda_{\text{EP}}$, since the orthogonality conflicts with the normalization requirement. As a consequence, an exceptional point is characterized by the fact that the rank of the associated matrix $H_0 + \Lambda_{\text{EP}} H_1$ drops by 1 at $\Lambda = \Lambda_{\text{EP}}$ and the two wave functions coalesce into one. This implies a defect of the underlying Hilbert space [4].

In Ref. [8], the topological structure of exceptional points is studied experimentally by using a microwave resonator. The exceptional point is surrounded by varying adiabatically external parameters of the system. As a result, the eigenvalues and eigenvectors are exchanged while encircling an exceptional point, but one of the eigenvectors undergoes a sign change which can be discerned in the field patterns. From these results, the authors draw the conclusion that the exceptional points can clearly be distinguished from other topological singularities such as diabolic points.

In describing physical processes, the exceptional points lead to problems. First, the splitting of the Hamiltonian H into H_0 and H_1 cannot be done arbitrarily. For a fixed H_0 , the part H_1 is well defined since it describes the coupling of the states of the system (described by H_0) via the environment (continuum of decay channels) into which it is embed-

ded [9]. Second, the property $\mathcal{E}_l(\Lambda_{\text{EP}}) = \mathcal{E}_k(\Lambda_{\text{EP}})$ is characteristic of a double pole of the S matrix. Here, $\mathcal{E}_k = E_k - i/2\Gamma_k$ is the complex pole of the resonance state k with energy E_k and width Γ_k . The S matrix describes physical processes, and no hints at all to defects of the Hilbert space are known at a double pole. For numerical examples, see the results of calculations performed in a schematical model [10] and for atoms [11,12].

Theoretical studies have shown that the topological structure of avoided level crossings is directly related to the topological structure of double poles of the S matrix being branch points in the complex plane [13]. The transition from a double pole of the S matrix to an avoided level crossing by varying a parameter occurs continuously. The avoided level crossings are directly related to the diabolic points [1]. Thus, the topological structure of a double pole of the S matrix and that of a diabolic point are related to one another.

The problem is now the following. The double pole of the S matrix and the exceptional point are both characterized by the coalescence of two eigenvalues of a non-Hermitian Hamilton operator at a certain value of a parameter. Nevertheless, their topological structures are different: according to Ref. [8], the topological structure of an exceptional point differs from that of a diabolic point, while the topological structure of the double pole is related to that of the diabolic point, as discussed above [13]. The question arises, therefore, what differences exist between the exceptional points and the double poles of the S matrix, which could cause their different topological structures.

In order to find an answer to this question, the Schrödinger equation has to be solved in the whole function space containing everything, i.e., discrete and continuous states. By using a projection operator technique, an effective Hamiltonian can be derived from this Schrödinger equation which describes the system (Q subspace) after embedding it into the continuum of decay channels (P subspace) [9]. Its eigenvalues and eigenfunctions are complex. The eigenvalues coincide with the poles of the S matrix. The eigenfunctions are related to the wave functions of the resonance states by a Lippmann-Schwinger-like relation [14]. They are biorthogonal. At the double pole of the S matrix, the Hilbert space has no defect due to the biorthogonality of the wave functions. The S matrix behaves smoothly by varying parameters also when the double pole is met [13].

It is the aim of the present paper to derive the phase

changes of the wave functions that appear after surrounding a double pole of the S matrix parametrically. In Sec. II, the relation between the eigenvalues of the effective Hamiltonian operator and the poles of the S matrix is discussed, while in Sec. III the relation between double poles and avoided level crossings is discussed. The double poles of the S matrix are branch points in the complex plane. At these points, the wave functions of the two states are exchanged, $\psi_1 \rightarrow \pm i\psi_2$. This causes a mixing of the wave functions in the region of avoided level crossings. In Sec. IV, the phase changes appearing after surrounding a diaboloic point and a double pole of the S matrix are derived and compared with experimental results. They agree with all data for isolated crossings of two states that are published in Refs. [3,8]. Conclusions on the topological structure of the function space are drawn in the last section.

II. EFFECTIVE HAMILTONIAN AND POLES OF THE S MATRIX

After embedding a system into the continuum of decay channels, the discrete states of the system turn over in resonance states with a finite lifetime. The Hamiltonian of the system becomes effectively non-Hermitian with complex eigenvalues $\mathcal{E}_k = E_k - i/2\Gamma_k$, where the width Γ_k is inversely proportional to the lifetime.

The relation between the poles of the S matrix and the complex eigenvalues \mathcal{E}_k can be derived from the Schrödinger equation,

$$(H - E)\Psi_E = 0, \quad (1)$$

with the Hamilton operator H and the set $\{\Psi_E\}$ of wave functions containing the discrete states of the system as well as the scattering wave functions of the environment into which the system is embedded. The operator H is Hermitian.

In a first step, two sets of equations have to be solved:

$$(H^{\text{cl}} - E_k^{\text{cl}})\Phi_k^{\text{cl}} = 0 \quad (2)$$

and

$$\sum_{c'} (H^{cc'} - E)\xi_E^{c'(+)} = 0, \quad (3)$$

where H^{cl} describes the system with the discrete states k and $H^{cc'}$ the continuum with coupled decay channels c . Then, the two projection operators are defined by

$$Q = \sum_k |\Phi_k^{\text{cl}}\rangle\langle\Phi_k^{\text{cl}}|, \quad P = \sum_c \int dE |\xi_E^{c(+)}\rangle\langle\xi_E^{c(+)}| \quad (4)$$

and H^{cl} is identified with $QHQ \equiv H_{QQ}$ and $H^{cc'}$ with $PHP \equiv H_{PP}$. The two other terms of $H = H_{QQ} + H_{PP} + H_{QP} + H_{PQ}$ describe the coupling between the two subspaces. The solutions of coupled channel equations with source term

$$\sum_{c'} (H^{cc'} - E)\langle\xi_E^{c'(+)}|\omega_k\rangle = -\langle\xi_E^{c(+)}|H_{PQ}|\Phi_k^{\text{cl}}\rangle \quad (5)$$

provide the wave functions ω_k that contain the coupling between the two subspaces.

Using the completeness relation $P + Q = 1$, one obtains for the solution of the whole problem [9]

$$\Psi_E^c = \xi_E^{c(+)} + \frac{1}{\sqrt{2\pi}} \sum_{k=1}^N \tilde{\Omega}_k \frac{\tilde{\gamma}_k^c}{E - \tilde{E}_k + \frac{i}{2}\tilde{\Gamma}_k}. \quad (6)$$

Here,

$$\tilde{\Omega}_k = \tilde{\Phi}_k + \tilde{\omega}_k = (1 + G_P^{(+)}H_{PQ})\tilde{\Phi}_k \quad (7)$$

is the wave function of the resonance state k , $G_P^{(+)} = P(E - H_{PP})^{-1}P$ is the Green function in the P subspace, $\tilde{\omega}_k$ is determined by Eq. (5) with Φ_k^{cl} replaced by $\tilde{\Phi}_k$, and

$$\tilde{\gamma}_k^c(E) = \sqrt{2\pi}\langle\tilde{\Phi}_k^*|H_{QP}|\xi_E^{c(+)}\rangle = \sqrt{2\pi}\langle\xi_E^{c(+)}|H_{PQ}|\tilde{\Phi}_k\rangle. \quad (8)$$

Further, $\tilde{\Phi}_k$ is the eigenfunction and $\tilde{\mathcal{E}}_k = \tilde{E}_k - i/2\tilde{\Gamma}_k$ is the eigenvalue of the effective Hamiltonian

$$\mathcal{H} = H_{QQ} + H_{QP}G_P^{(+)}H_{PQ}, \quad (9)$$

which describes the system after embedding it into the continuum of decay channels. \mathcal{H} is non-Hermitian, its eigenvalues and eigenvectors are complex. The eigenfunctions are biorthogonal,

$$\langle\tilde{\Phi}_k^*|\tilde{\Phi}_l\rangle = \delta_{k,l}, \quad (10)$$

where $\tilde{\Phi}_k^{\text{right}} \equiv \tilde{\Phi}_k$ and $\tilde{\Phi}_k^{\text{left}} = \tilde{\Phi}_k^*$ [13,15]. As a consequence,

$$\langle\tilde{\Phi}_k|\tilde{\Phi}_l\rangle = \text{Re}(\langle\tilde{\Phi}_k|\tilde{\Phi}_k\rangle); \quad A_k \equiv \langle\tilde{\Phi}_k|\tilde{\Phi}_k\rangle \geq 1,$$

$$\langle\tilde{\Phi}_k|\tilde{\Phi}_{l \neq k}\rangle = i \text{Im}(\langle\tilde{\Phi}_k|\tilde{\Phi}_{l \neq k}\rangle) = -\langle\tilde{\Phi}_{l \neq k}|\tilde{\Phi}_k\rangle;$$

$$B_k^{l \neq k} \equiv |\langle\tilde{\Phi}_k|\tilde{\Phi}_{l \neq k}\rangle| \geq 0. \quad (11)$$

Using Eqs. (6) and (7) and the Lippmann-Schwinger equation for the scattering wave functions, one gets for the resonance part of the S matrix [9,13],

$$S_{cc'}^{(\text{res})} = i \sum_{k=1}^N \frac{\tilde{\gamma}_k^c \tilde{\gamma}_k^{c'}}{E - \tilde{E}_k + \frac{i}{2}\tilde{\Gamma}_k}. \quad (12)$$

The $\tilde{\gamma}_k^c$ are the coupling matrix elements of the resonance states to the continuum. $S_{cc'}^{(\text{res})}$ describes the resonance part of the S matrix also in the overlapping regime. The interferences between the resonance states are taken into account by diagonalizing the effective Hamiltonian \mathcal{H} . Due to the unitarity of the S matrix, the $\tilde{\gamma}_k^c$, \tilde{E}_k , and $\tilde{\Gamma}_k$ are energy dependent functions. The relation $\tilde{\Gamma}_k = \Sigma(\tilde{\gamma}_k^c)^2$ holds only for isolated resonances. In the overlapping regime, the energy dependence of both functions is different, as a rule. For numerical examples, see Ref. [16].

As can be seen from Eq. (12), the poles of the S matrix are determined by the eigenvalues $\tilde{\mathcal{E}}_k$ of the effective Hamiltonian (9) after solving the fixed-point equations $\mathcal{E}_k = \tilde{\mathcal{E}}_k(E = E_k)$ [13]. As an example, resonances of a microwave cavity are studied experimentally in the overlapping regime [17]. The results show the phenomenon of resonance trapping and are described well by Eq. (12) with the effective Hamiltonian (9).

III. DOUBLE POLES OF THE S MATRIX AND AVOIDED LEVEL CROSSINGS

The relation between double poles of the S matrix and avoided level crossings can be illustrated best by means of a simple two-level model. Let us consider the complex two-by-two Hamiltonian matrix

$$\mathcal{H} = \begin{pmatrix} e_1(\lambda) - \frac{i}{2}\gamma_1 & \omega \\ \omega & e_2(\lambda) - \frac{i}{2}\gamma_2 \end{pmatrix}, \quad (13)$$

where e_k and γ_k ($k=1,2$) are the unperturbed energies and widths, respectively, of the two states. The e_k are assumed to depend on the parameter λ in such a manner that the two states may cross in energy at λ^{cr} when $\omega=0$. The two states interact only via ω , which is assumed in the following to be independent of the parameter λ (as the γ_k). The eigenvalues of \mathcal{H} are

$$E_{\pm} - \frac{i}{2}\Gamma_{\pm} = \frac{1}{2} \left[(e_1 + e_2) - \frac{i}{2}(\gamma_1 + \gamma_2) \right] \pm \frac{1}{2}\sqrt{F}, \quad (14)$$

with

$$F = \left[(e_1 - e_2) - \frac{i}{2}(\gamma_1 - \gamma_2) \right]^2 + 4\omega^2. \quad (15)$$

When $F(\lambda, \omega) = 0$ at $\lambda = \lambda^{\text{cr}}$ (and $\omega = \omega^{\text{cr}}$), the S matrix has a double pole.

According to Eq. (15), $F = F_R + iF_I$ is generally a complex number. For illustration, let us discuss the case with real ω . Then $e_1 = e_2$ at $\lambda = \lambda^{\text{cr}}$ and we have to differentiate between three cases

$$F_R(\lambda, \omega) > 0 \rightarrow \sqrt{F_R} = \text{real}, \quad (16)$$

$$F_R(\lambda, \omega) = 0 \rightarrow \sqrt{F_R} = 0, \quad (17)$$

$$F_R(\lambda, \omega) < 0 \rightarrow \sqrt{F_R} = \text{imaginary}. \quad (18)$$

The first case gives the avoided level crossing in energy with an exchange of the two wave functions at λ^{cr} . The second case corresponds to the double pole of the S matrix. In the third case, the two levels cross freely in energy and the two states are *not* exchanged at the critical value λ^{cr} [13]. In Ref. [18], the two cases $F_R > 0$ and $F_R < 0$ are studied experimentally in a microwave cavity and called *overcritical* and *sub-*

critical coupling, respectively. The more complicated cases with complex ω are considered in Ref. [19].

The example with real ω illustrates nicely the relation between a double pole of the S matrix and avoided or even free crossings of two levels in the complex plane. The double pole is a branch point in the complex plane. The number of these branch points is of measure zero, but their influence on the dynamics of quantum systems can be traced in many avoided level crossings. While the wave functions of the two states are exchanged just at the double pole of the S matrix and are unmixed at any value of the parameter different from the critical one, this is not so at an avoided level crossing. In this case, the wave functions remain mixed in a certain range of the parameter around the critical value. This fact has a strong influence on the mixing of all the wave functions of a system when the level density is high, and different avoided level crossings appear at values of the parameter inside this range. For the results of numerical studies, see Ref. [13].

The biorthogonality relation (10) holds everywhere, including at the double pole of the S matrix. The reason is that $A_{k \rightarrow \infty}; B_k^l \rightarrow \infty$ [Eq. (11)] and that $\langle \tilde{\Phi}_k^* | \tilde{\Phi}_l \rangle$ is the difference between two infinitely large numbers (but not their sum). This difference may be 0 (for $l \neq k$) or 1 (for $l = k$). Thus, the orthogonality and normalization requirements do not conflict with one another and the Hilbert space has no defect at all. For the results of numerical studies, see Ref. [13].

It should be mentioned here, that the biorthogonality of the $\{\tilde{\Phi}_k\}$ follows directly from the non-Hermiticity of \mathcal{H} . Only for the eigenfunctions of a Hermitian operator holds $\tilde{\Phi}_k^{\text{left}} = \tilde{\Phi}_k^{\text{right}}$ [15]. Due to the symmetry of \mathcal{H} it holds $\tilde{\Phi}_k^{\text{left}} = \tilde{\Phi}_k^{\text{right}*}$ for its eigenfunctions what results in Eq. (10) for the biorthogonality relation.

Further analytical studies [13] have shown that the wave functions of the two states at the double pole of the S matrix are exchanged. It is

$$\tilde{\Phi}_k^{\text{bp}} \rightarrow \pm i \tilde{\Phi}_{l \neq k}^{\text{bp}} \quad (19)$$

in approaching the double pole of the S matrix. This result is confirmed by numerical studies on laser induced continuum structures in atoms [12].

The real and imaginary parts of the wave functions of two resonance states as a function of an external parameter increase limitless in approaching the double pole of the S matrix [13]. The sign of the imaginary part jumps at the double pole (when $\tilde{\Phi}_1 \rightarrow +i\tilde{\Phi}_2$). When the double pole is not met by varying the external parameter, but the levels avoid crossing at the critical value of the parameter, the real and imaginary parts remain finite but the jump of the sign remains. The wave function

$$\tilde{\Phi}_{\text{ch}} = a_1 \tilde{\Phi}_1 \pm ia_2 \tilde{\Phi}_2 \quad (20)$$

changes smoothly (without any jump of the sign of its components) for $a_2 \rightarrow a_1$ at the double pole of the S matrix or at the critical value of the parameter where the levels avoid crossing. For the results of a numerical study, see Ref. [13].

The diabolic points are related to avoided crossings of discrete levels. They occur by varying two independent parameters: at the diabolic point, two energy surfaces drawn over the plane of the two external parameters touch each other at one point forming a double cone.

IV. GEOMETRIC PHASES

Let us now consider the geometric phases appearing after encircling a diabolic point and a branch point in the complex plane (double pole of the S matrix), respectively. In any case, the paths of encircling are characterized by the value F , Eq. (15), which vanishes only at the branch point in the complex plane. Most interesting are states whose eigenvalues are near to the real axis. We can restrict our discussion therefore to real ω (see Sec. III).

For encircling the diabolic point or the branch point in the complex plane, two external parameters have to be varied. In the experiment of Ref. [3], the diabolic point is surrounded by varying the shape of the microwave resonator by means of two parameters but leaving the coupling strength to the antenna unchanged. Since the two levels considered avoid crossing, the whole path of encircling the diabolic point is in the overcritical regime. That means, the critical value of the parameter is passed twice, on the way forth as well as back, under overcritical conditions, and the wave functions are exchanged each time when the critical value of the parameter is reached. This is not so in the experiment of Ref. [8] where one of the two parameters is the coupling strength of the cavity to another one. Therefore, the critical value of the parameter is passed on the path of encircling the exceptional point (or branch point in the complex plane) only once under overcritical conditions. The other part of the path is in the subcritical regime where the wave functions are nowhere exchanged (see Sec. III).

In detail, the diabolic point is surrounded in the experiment of Ref. [3] in the regime of overcritical coupling along the whole way of encircling and λ^{cr} is passed twice in opposite directions,

$$(i) \Phi_k \rightarrow -i\Phi_l; \Phi_l \rightarrow +i\Phi_k, \text{ i.e.,}$$

$$\{\Phi_1, \Phi_2\} \rightarrow \{-i\Phi_2, +i\Phi_1\} \quad (21)$$

and (ii), on the way back, $\Phi_l \rightarrow -i\Phi_k; \Phi_k \rightarrow +i\Phi_l$, i.e.,

$$\{-i\Phi_2, +i\Phi_1\} \rightarrow \{-\Phi_1, -\Phi_2\}. \quad (22)$$

The phase change occurring after one surrounding the diabolic point is therefore

$$\{\Phi_1, \Phi_2\} \rightarrow \{-\Phi_1, -\Phi_2\}. \quad (23)$$

This corresponds to the geometric phase discussed by Berry [1].

The way of encircling the branch point in the complex plane itself passes from a region with overcritical coupling at λ^{cr} to another one with subcritical coupling at λ^{cr} . An ex-

change of the wave functions takes place only at overcritical coupling where the resonances avoid crossing. Thus, a first full surrounding gives

$$\{\Phi_1, \Phi_2\} \rightarrow \{-i\Phi_2, +i\Phi_1\} \quad (24)$$

and a second one (in the same direction) gives

$$\{-i\Phi_2, +i\Phi_1\} \rightarrow \{\Phi_1, +\Phi_2\}. \quad (25)$$

That means, surrounding the branch point in the complex plane twice restores the wave functions Φ_k including their phases. This corresponds to the result obtained for surrounding the diabolic point twice. In both cases, the wave functions including their phases are restored after a second encircling in the same direction:

$$\{\Phi_1, \Phi_2\} \Rightarrow \{\Phi_1, \Phi_2\}. \quad (26)$$

Encircling the branch point in the complex plane in the opposite direction gives

$$\{\Phi_1, \Phi_2\} \rightarrow \{+i\Phi_2, -i\Phi_1\}. \quad (27)$$

Since the experiment of Ref. [8] is not sensitive to the possible occurrence of a phase i of the wave function, the results (24) for one loop with a certain orientation of the path and the results (27) with the opposite orientation of the path agree with the experimental data given in Ref. [8]. There are no experimental data in Ref. [8] for the phase changes after a second loop.

An experimental study of interferences between atomic levels in a laser field is expected [19] to allow conclusions on the phase changes, including those after a second loop.

V. CONCLUDING REMARKS

In the present paper, the phase changes occurring after encircling parametrically an isolated diabolic point and a double pole of the S matrix (branch point in the complex plane) are calculated. The results are shown to agree with all experimental data that are published in Refs. [3,8].

The results of Ref. [3] point to the interesting fact that the phase changes after surrounding higher-order degeneracies are more complicated than those obtained after encircling a diabolic point. This result has given rise to further theoretical studies, e.g., Ref. [20].

The experimental results in Ref. [8] are interpreted by the authors on the basis of exceptional points. This interpretation leads to the conclusion that an exceptional point can clearly be distinguished from other topological singularities such as diabolic points. The authors claim the following: encircling the exceptional point a second time completely with the same orientation, one obtains $\{-\Phi_k, -\Phi_l\}$, while the next complete loop yields $\{-\Phi_l, \Phi_k\}$ and only the fourth loop restores fully the original pair $\{\Phi_k, \Phi_l\}$. The authors show experimental results only for one complete loop. No data are given for two or more loops.

The appearance of a phase change of both wave functions

after a second loop around the exceptional point, $\tilde{\Phi}_k \Rightarrow -\tilde{\Phi}_k$; $\tilde{\Phi}_l \Rightarrow -\tilde{\Phi}_l$, suggested in Ref. [8], does not agree with the result (26) obtained for a second complete loop around a branch point in the complex plane. According to result (26), the original pair $\{\tilde{\Phi}_k, \tilde{\Phi}_l\}$ is restored already after a second complete loop when it is completed with the same orientation. This result coincides with that obtained for a second loop around a diabolic point. It is an expression for the fact that diabolic points and branch points in the complex plane are related to one another as discussed in this paper.

The results for one loop cannot differentiate between the

two interpretations since the experiment is not sensitive to the possible occurrence of a phase i in the wave function. It can therefore not be concluded from the published experimental data whether or not the topological structure studied in Ref. [8] is different from that of a diabolic point. Further experimental studies are necessary, maybe on atoms in a laser field as suggested in Ref. [19].

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