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Degeneracy and crossing of resonance energy surfaces

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Abstract. We investigate the accidental degeneracy of resonances mixed by a Hermitian interaction. We give general expressions for the codimension in parameter space of any degeneracy of resonances. In the case of a degeneracy of two resonances which produces only one simple pole in the S matrix, the codimension is four for time reversal invariant interactions and six when the quantum system is not time reversal invariant. Close to this type of degeneracy the corresponding energy surfaces are two double cones lying in orthogonal subspaces with a common vertex at a double diabolic point. When the degeneracy of two resonances leads to one simple plus one double pole of S the codimension is two irrespective of the time reversal invariant character of the quantum system. Close to this type of degeneracy, the energy surfaces are a hyperbolic cone and a sphere which lie in orthogonal subspaces and touch one another at all points on a diabolic circle.

1. Introduction

Accidental degeneracy and level crossings, true or avoided, are important for the understanding of a wide variety of quantum phenomena [1]. For instance, a quantum system acquires a geometric phase—the Berry phase—when transported adiabatically around a path in parameter space [2–4]. This phase is of special importance in cases where the path includes an accidental degeneracy, sometimes called a diabolic point, i.e. a point in parameter space where two neighbouring eigenenergy surfaces with the same symmetry touch one another. Near an accidental degeneracy one often describes the behaviour of the system in terms of the well known Landau–Zener effect [5, 6] which is the enhanced transition amplitude between two adiabatic levels at an avoided level crossing. For a recent review of the nuclear Landau–Zener effect see Thiel [7]. Accidental degeneracies and level crossings are also important for the understanding of the statistical properties of nuclear spectra [8, 9] and the onset and properties of quantum chaos [1].

Although most of the information on statistical properties of nuclear spectra, as well as the effects due to interference of nuclear states, is obtained from resonances, i.e. metastable quantum states, virtually all the existing literature has been concerned with stable states of closed systems driven by Hermitian Hamiltonians [1, 8, 9].

In a statistical approach to nuclear scattering and reactions, bound states of a chaotic system are coupled to one or more decay channels with arbitrary coupling strength between bound states and continua [10]. In this theoretical framework Rotter [11, 12] investigated numerically the problem of cross-section fluctuations arising from avoided resonance overlapping. The statistical theory of nuclear spectra was extended from bound to unstable states by Sokolov and Zelevinsky [13, 14] but without considering the effect of degeneracy of resonances in an explicit way.

It is only very recently that von Brentano [15–17] examined the generalization of the level repulsion theorem from von Neumann and Wigner [18] from bound states to a system of two interacting resonances.

In this work we will be concerned with the degeneracy of resonances and the behaviour of the energy surfaces in a parameter space in the neighbourhood of a degeneracy. In section 2, we generalize the level repulsion theorem from bound states to resonances and calculate the minimum number of free real parameters in the mixing Hamiltonian necessary to produce a degeneracy. In the next section we formulate the problem of accidental degeneracy of two resonances in parameter space. In section 4 we discuss the shape of the energy surfaces close to a crossing for the two possible types of two-resonance degeneracy found in section 2. We end our paper with a summary of our results and some conclusions.

2. Codimension of resonance degeneracies

Consider a complex quantum system, for instance, a highly excited atomic nucleus near an excitation energy E . Let the system have m open reaction channels and n resonance states in the given energy region. A general phenomenological expression for the S matrix is [10, 14, 19]

$$S(E) = U_1 \{ \mathbf{1} - i\mathbf{W}[E - \mathbf{H}]^{-1}\mathbf{W}^\dagger \} U_2^\dagger. \quad (1)$$

In this expression, the $n \times n$ matrix \mathbf{H} plays the role of an effective non-Hermitian Hamiltonian in the internal space,

$$\mathbf{H} = H - i\frac{1}{2}\mathbf{W}^\dagger\mathbf{W}. \quad (2)$$

The Hermitian matrix H consists of the Hamiltonian terms and the shift functions. The $m \times n$ matrix \mathbf{W} is the matrix of the decay amplitudes which contains the interaction matrix elements that couple the channels to the levels. The form of the anti-Hermitian part of \mathbf{H} ensures the unitarity of S . When the mean spacing between resonances is small in comparison with the mean spacing between channel thresholds and E is far from any threshold, both matrices are smooth functions of the energy. In a small region in the complex energy plane the regular variation of these quantities is negligible and we will take them as constants.

The poles of the S matrix are the eigenvalues of the complex matrix \mathbf{H} . When the interactions are time reversal invariant, the channel states and the inner basis may be chosen in such a way as to make the S matrix and the matrix \mathbf{H} symmetric. When the interactions are not time reversal invariant no relations exist among the matrix elements of \mathbf{H} other than those due to the Hermiticity of H and $\mathbf{W}^\dagger\mathbf{W}$.

Usually, the description of a collision or reaction process is made in terms of well defined kinematic and dynamic laws and a number of real, linearly independent 'external' parameters whose numerical values are not given by the theory. Therefore, we may consider the S matrix embedded in a population of S matrices smoothly parametrized by a set of N external parameters which take values in some domain of a manifold or parameter space. In the representation of (1), this implies that \mathbf{H} is also embedded in a population of complex matrices smoothly parametrized by a set of N real external parameters, and all the complex matrix elements H_{ij} are functions of the real parameters (X_1, X_2, \dots, X_N) .

We may now turn to the question of the accidental degeneracy of two resonances, and we ask: how many parameters must one vary, in general, to obtain a coincidence of two poles of S ?

We will show that two possibilities present themselves:

(i) When the coincidence of two resonance energies produces one simple pole in S . Then, for interactions which are not time reversal invariant at least six real external parameters must be varied. When the interactions are time reversal invariant, at least four real external parameters must be specified.

(ii) When the degeneracy of two resonance energies produces one simple pole plus one double pole of S at the degenerate resonance energy. Then, at least two real external parameters should be varied independently of the time reversal invariant character of the interactions.

To show this, we count the free real parameters in an n -dimensional complex matrix \mathbf{H} with and without two equal eigenvalues. The difference in these two numbers is the codimension of the degeneracy in parameter space.

2.1. Systems which are not time reversal invariant

In order to count the number of free real parameters in an n -dimensional, square complex matrix \mathbf{H} , it is convenient to recall some results from matrix theory [20-22].

Any complex, n -dimensional, square matrix \mathbf{H} may always be brought to a Jordan canonical form \mathbf{E} by means of a similarity transformation,

$$\mathbf{H} = \mathbf{K}\mathbf{E}\mathbf{K}^{-1}. \tag{3}$$

In general, the matrix \mathbf{K} is not unique. If \mathbf{V} is a square, non-singular matrix which commutes with \mathbf{E} , substitution of \mathbf{KV} for \mathbf{K} in (3) leaves \mathbf{H} invariant. Therefore, if we call $par(\mathbf{H})$ the number of independent real parameters in \mathbf{H} ,

$$par(\mathbf{H}) = par(\mathbf{K}) + par(\mathbf{E}) - par(\mathbf{V}). \tag{4}$$

In this subsection we will consider the case of a system driven by interactions which are not time reversal invariant, then \mathbf{H} is, in general, non-symmetric. In this case, \mathbf{K} has, in general, n^2 different complex matrix elements. Therefore,

$$par(\mathbf{K}) = 2n^2. \tag{5}$$

When \mathbf{H} has ν ($\nu \leq n$) different eigenvalues, E_1, E_2, \dots, E_ν , with multiplicities $\mu_i(E_i)$, the Jordan canonical form \mathbf{E} is the direct sum of ν square Jordan blocks \mathbf{E}_i . Each Jordan block \mathbf{E}_i is the sum of a diagonal matrix, $E_i \mathbf{I}_{\mu_i \times \mu_i}$, and a nilpotent matrix \mathbf{N}_{μ_i} . The nilpotent matrix \mathbf{N}_{μ_i} has no free parameters. Hence, each Jordan block \mathbf{E}_i has only one complex free parameter, namely the eigenvalue E_i . Therefore, the number of free real parameters in \mathbf{E} is 2ν

$$par(\mathbf{E}) = 2\nu. \tag{6}$$

A square, complex matrix \mathbf{V} which commutes with the Jordan canonical matrix \mathbf{E} is the direct sum of ν square blocks \mathbf{V}_i of dimension μ_i [21,22]. Each block \mathbf{V}_i commutes with the corresponding block \mathbf{E}_i . The form of the block \mathbf{V}_i and the number of different, non-vanishing matrix elements in \mathbf{V}_i is determined by the number and length of the cycles (degree of the invariant factors $\neq 1$ of $\det[E\mathbf{I} - \mathbf{H}]$) of generalized eigenvectors of \mathbf{H} which belong to the eigenvalue E_i . If E_i has k_i cycles of lengths $\ell_1(E_i) \geq \ell_2(E_i) \geq \dots \geq \ell_{k_i}(E_i)$, the number of free real parameters in the block \mathbf{V}_i is given by ([21,22])

$$par(\mathbf{V}_i) = 2 \sum_{s=1}^{k_i} (2s - 1)\ell_s(E_i). \tag{7}$$

Hence, the number of different, non-vanishing, real parameters in the matrix \mathbf{V} is

$$par(\mathbf{V}) = 2 \sum_i \left[\sum_{s=1}^{k_i} (2s-1) \ell_s(E_i) \right]. \quad (8)$$

Substitution of (8), (6) and (5) in (4) gives the number of linearly independent, free real parameters in the complex, square, non-symmetric matrix \mathbf{H} as

$$par(\mathbf{H}) = 2 \left\{ n^2 + \nu - \sum_i \left[\sum_{s=1}^{k_i} (2s-1) \ell_s(E_i) \right] \right\} \quad (9)$$

where n is the dimension of \mathbf{H} , ν is the number of different eigenvalues of \mathbf{H} and $\ell_1(E_i) \geq \ell_2(E_i) \geq \dots \geq \ell_{k_i}(E_i)$ are the lengths of the k_i cycles of generalized eigenvectors of \mathbf{H} which belong to the eigenvalue E_i .

A general expression for the codimension $C(\mathbf{H}_{deg})$ of the degeneracy of any number of interacting resonances of a system driven by interactions which are not time reversal invariant is obtained subtracting $par(\mathbf{H}_{deg})$, as given in (9), from $2n^2$, which is the number of free real parameters of \mathbf{H} when all the eigenvalues of \mathbf{H} are different,

$$C(\mathbf{H}_{deg}) = 2 \left\{ \sum_i \left[\sum_{s=1}^{k_i} (2s-1) \ell_s(E_i) \right] - \nu \right\}. \quad (10)$$

2.2. Time reversal invariant system

Let us now consider the case of a system driven by time reversal invariant interactions, in this case the matrix \mathbf{H} is symmetric, and we write (3) as

$$\mathbf{H} = \mathbf{O} \mathbf{E} \mathbf{T} \mathbf{O}^T \quad (11)$$

where \mathbf{O}^T is the transposed of the matrix \mathbf{O} , and \mathbf{T} is a real n -dimensional, square, symmetric matrix such that

$$\mathbf{E} = \mathbf{T} \mathbf{E}^T \mathbf{T} \quad (12)$$

where \mathbf{E}^T is the transpose of \mathbf{E} , and

$$\mathbf{T}^2 = \mathbf{1}. \quad (13)$$

The matrix \mathbf{T} has no free parameters. The matrix $\mathbf{T} \mathbf{O}^T$ is the inverse of the matrix \mathbf{O} and satisfies the relations

$$\mathbf{O}^T \mathbf{O} = \mathbf{T} \quad (14)$$

and

$$\mathbf{O} \mathbf{T} \mathbf{O}^T = \mathbf{1}. \quad (15)$$

The matrix $\mathbf{O}^T\mathbf{O}$ is obviously symmetric, hence the matrix equation (14) is equivalent to a set of $\frac{1}{2}n(n + 1)$ linearly independent scalar equations. Since \mathbf{O} is non-singular, equation (15) may be derived from (14) and adds no further constraints on \mathbf{O} . Then,

$$par(\mathbf{O}) = n(n - 1). \tag{16}$$

As in the previous case, the matrix \mathbf{O} is not unique. Let \mathcal{V} be a square, non-singular matrix which commutes with \mathbf{E} and satisfies the condition

$$\mathcal{V}\mathbf{T}\mathcal{V}^T\mathbf{T} = \mathbf{1} \tag{17}$$

then substitution of $\mathbf{O}\mathcal{V}$ for \mathbf{O} in (11) leaves \mathbf{H} invariant.

The number of different, non-vanishing real parameters in the matrix \mathcal{V} may be obtained by subtracting the number of linearly independent constrictions implicit in the matrix equation (17) from the general expression (7) for the number of real parameters in a matrix \mathbf{V} which commutes with \mathbf{E} . To count the number of linearly independent scalar equations equivalent to (17), we notice that, if \mathcal{V} commutes with \mathbf{E} , then $\mathbf{T}\mathcal{V}^T\mathbf{T}$ and $\mathcal{V}\mathbf{T}\mathcal{V}^T\mathbf{T}$ also commute with \mathbf{E} . Hence, the matrices $\mathbf{T}\mathcal{V}^T\mathbf{T}$ and $\mathcal{V}\mathbf{T}\mathcal{V}^T\mathbf{T}$ have the same block structure as \mathbf{V} , with submatrices of the same type as those occurring in the blocks \mathbf{V}_i of \mathbf{V} . The left-hand side of equation (17) is invariant under the operations of transposition and left and right multiplication by \mathbf{T} . From the definition of \mathbf{T} (12) it may be seen that the operation of transposition and left and right multiplication by \mathbf{T} leaves the diagonal submatrices in each block \mathcal{V}_i invariant while the off-diagonal submatrices below the diagonal are transformed in those above the diagonal, and *vice versa*. Therefore, the matrix equation (17) is equivalent to a set of as many linearly independent scalar equations as there are different, non-vanishing matrix elements in the diagonal and supradiagonal submatrices in all the blocks \mathbf{V}_i of \mathbf{V} . A straightforward count gives this last number for each block \mathbf{V}_i as $\sum_{s=1}^{k_i} s\ell_s(E_i)$ [22]. Hence, the number of real independent parameters in the block \mathcal{V}_i is

$$par(\mathcal{V}_i) = par(\mathbf{V}_i) - 2 \sum_{s=1}^{k_i} s\ell_s(E_i). \tag{18}$$

Substitution of the expression (7) for $par(\mathbf{V}_i)$ in (18) gives

$$par(\mathcal{V}_i) = 2 \sum_{s=1}^{k_i} (s - 1)\ell_s(E_i). \tag{19}$$

Adding the contributions of all blocks \mathcal{V}_i , we obtain the number of independent real parameters in \mathcal{V}

$$par(\mathcal{V}) = 2 \sum_i \sum_{s=1}^{k_i} (s - 1)\ell_s(E_i). \tag{20}$$

Collecting the results in (4), (6), (16) and (20), we obtain the number of independent free real parameters in the n -dimensional, square complex symmetric matrix \mathbf{H}

$$par(\mathbf{H}) = n^2 + n - 2(n - \nu) - 2 \sum_{i=1}^{\nu} \sum_{s=1}^{k_i} (s - 1)\ell_s(E_i) \tag{21}$$

the notation in this expression is as in equation (9).

The codimension $C(\mathbf{H}_{deg})$ of the degeneracy of any number of interacting resonances of a system driven by time reversal invariant interactions is obtained by subtracting $par(\mathbf{H}_{deg})$, as given in (21), from $n(n + 1)$ which is the number of free real parameters of the complex symmetric matrix \mathbf{H} when all the eigenvalues of \mathbf{H} are different. In this way we obtain

$$C(\mathbf{H}_{deg}) = 2 \left[(n - \nu) + 2 \sum_l \sum_{s=1}^{k_l} (s - 1) \ell_s(E_l) \right] \tag{22}$$

where n is the dimension of \mathbf{H} , ν is the number of different eigenvalues of \mathbf{H} , $k_i(E_i)$ is the number and $\ell_1(E_i) \geq \dots \geq \ell_{k_i}(E_i)$ the lengths of the cycles of generalized eigenvectors of \mathbf{H} which correspond to the eigenvalue E_i .

Although the expressions (10) and (22) are general enough to discuss the properties of accidental degeneracies of any number of resonances, in the following we will restrict the discussion to accidental degeneracies of two resonances. An accidental degeneracy of two resonances occurs when two eigenvalues of \mathbf{H} coincide and all the others are different from these two and different from each other. Then, one block, say \mathbf{E}_1 , in the Jordan canonical form \mathbf{E} , is of rank two, and all the others, $\mathbf{E}_3, \mathbf{E}_4, \dots, \mathbf{E}_n$, are of rank one. Two possibilities arise according to whether or not the block of rank two is diagonal.

2.3. Resonance degeneracy leading to one pole of S

Let us examine first the case when the Jordan canonical form \mathbf{E} is diagonal; the eigenvalues E_n may be arranged in two groups, so that the two equal eigenvalues are in the outlined square

$$\mathbf{E} = \begin{pmatrix} E_1 & 0 & & & \\ 0 & E_1 & & & \\ & & E_3 & & \\ & & & \ddots & \\ & & & & E_n \end{pmatrix}. \tag{23}$$

\mathbf{E} has $\nu = n - 1$ different eigenvalues and n linearly independent eigenvectors.

The matrix $[E - \mathbf{H}]^{-1}$ may be written as

$$[E - \mathbf{H}]^{-1} = \frac{|1\rangle\langle 1| + |2\rangle\langle 2|}{E - E_1} + \sum_{i=3}^n \frac{|i\rangle\langle i|}{E - E_i} \tag{24}$$

where the vectors $|1\rangle, |2\rangle, \dots, |n\rangle$ are the columns in \mathbf{K} (or \mathbf{O}) and the vectors $\langle 1|, \langle 2|, \dots, \langle n|$ are the rows in \mathbf{K}^{-1} (or \mathbf{O}^T). All these vectors are right or left eigenvectors of \mathbf{H} but the numerator of the first term on the right-hand side of (24) is defined only up to an arbitrary similarity (or complex orthogonal) transformation. As may be seen from (24) and (1), the poles of the S matrix which become degenerate fuse into one simple pole. Hence, we may call this type of degeneracy, resonance degeneracy into one simple pole of S or resonance degeneracy of rank one.

From (23) it is apparent that the first Jordan block in \mathbf{E} has two cycles of length one

$$k_1 = 2 \quad \ell_1(E_1) = \ell_2(E_1) = 1 \tag{25}$$

all the other Jordan blocks in \mathbf{E} have one cycle of eigenvectors of length one

$$k_i = 1 \quad \ell_1(E_i) = 1 \quad 3 \leq i \leq n. \tag{26}$$

Substitution of (25) and (26) in expressions (10) and (22) gives the codimension of the rank-one degeneracy as six when \mathbf{H} is non-symmetric and four when \mathbf{H} is symmetric. This result may also be expressed as follows: the minimum number of external parameters that should be varied to produce a degeneracy of two resonances leading to one simple pole in the S matrix is four or six depending on whether the quantum system is time reversal invariant or not.

2.4. Resonance degeneracy leading to one simple and one double pole of S

Let us now consider the case when two eigenvalues of \mathbf{H} coincide and its Jordan canonical form is non-diagonal.

$$\mathbf{E} = \begin{pmatrix} E_1 & 0 & & & \\ 0 & E_1 & & & \\ & & E_3 & & \\ & & & \ddots & \\ & & & & E_n \end{pmatrix}. \tag{27}$$

As in the previous case, \mathbf{E} has $\nu = n - 1$ different eigenvalues but now it has only $n - 1$ linearly independent eigenvectors. A complete set of n linearly independent vectors may be obtained adding to the set of eigenvectors one generalized eigenvector corresponding to E_1 .

In this case, the matrix $[E - \mathbf{H}]^{-1}$ may be written as

$$[E - \mathbf{H}]^{-1} = \frac{|1\rangle\langle\hat{1}| + |\hat{1}\rangle\langle 1|}{(E - E_1)} + \frac{|1\rangle\langle 1|}{(E - E_1)^2} + \sum_{i=3}^n \frac{|i\rangle\langle i|}{(E - E_i)} \tag{28}$$

where $|1\rangle$ and $\langle 1|$ are right and left eigenvectors of \mathbf{H} corresponding to E_1 , but $\langle\hat{1}|$ and $|\hat{1}\rangle$ are left and right generalized eigenvectors of \mathbf{H} also corresponding to E_1 . The vectors $|1\rangle, |\hat{1}\rangle, |3\rangle, \dots, |n\rangle$ are the columns of \mathbf{K} (or \mathbf{O}) in that order, while the vectors $\langle\hat{1}|, \langle 1|, \langle 3|, \dots, \langle n|$ are the rows of \mathbf{K}^{-1} (or \mathbf{TO}^T) in that order. All the vectors appearing on the right-hand side of (28) are uniquely defined.

From (28) and (1), it follows that, in this case the poles of the S matrix which become degenerate fuse into one simple and one double pole. Hence, we may call this type of degeneracy, resonance degeneracy into one simple and one double pole or resonance degeneracy of rank two.

From (27), it is evident that the first Jordan block in \mathbf{E} has only one cycle of eigenvectors of length two

$$k_1 = 1 \quad \ell_1(E_1) = 2 \tag{29}$$

all the other Jordan blocks in \mathbf{E} have one cycle of length one,

$$k_i = 1 \quad \ell_1(E_i) = 1 \quad 3 \leq i \leq n. \tag{30}$$

These values, when substituted in (10) and (22), give the codimension of a rank-two degeneracy as two when \mathbf{H} is both symmetric and non-symmetric. It follows that the minimum number of external parameters that should be varied to produce a degeneracy of two resonances leading to one simple and one double pole in the S matrix is two, independently of the time reversal invariant character of the interactions.

3. Accidental degeneracy in parameter space

In the absence of symmetry, degeneracies are called accidental for the lack of an obvious reason to explain why two energy eigenvalues, E_1 and E_2 , of a typical Hamiltonian should coincide. If one embeds the Hamiltonian \mathbf{H} in a population of Hamiltonians $\mathbf{H}(X_i)$ smoothly parameterized by N 'external parameters' $\{X_1, X_2, \dots\}$, then degeneracy in the absence of symmetry is a geometric property of the hypersurfaces representing the real or complex energy eigenvalues in an $(N + 2)$ -dimensional Euclidean space with Cartesian coordinates $\{X_1, X_2, \dots, \text{Re } E, \text{Im } E\}$. Suppose that, for some set of values of the external parameters, the complex energies E_1 and E_2 coincide, all other energies being different from each other, then, for this set of $\{X_i\}$ values of the external parameters, the hypersurfaces corresponding to E_1 and E_2 touch one another. A small change in the external parameters about these values will produce small changes in all the other hypersurfaces which, however, will remain well separated. If we are only interested in the behaviour of the energy hypersurfaces in the immediate neighbourhood of the crossing, we may suppose that we already know the correct eigenvectors of \mathbf{H} for all complex eigenenergies except for the two energy hypersurfaces the crossing of which we want to investigate. Using for these last two, two vectors which are not eigenvectors but which are chosen to be orthogonal to each other and to all the other eigenvectors we obtain a complete basis to represent \mathbf{H} . In this basis the effective Hamiltonian \mathbf{H} will be diagonal except for the elements H_{12} and H_{21} . The diagonal elements H_{11} and H_{22} are, in general, not equal; H_{12} and H_{21} will also be different from zero. Therefore, in the following, we need consider only a pair of unstable states of the system, close in energy, which are mixed by the 2×2 effective Hamiltonian $H_{2 \times 2}$. To simplify the discussion it will be convenient to measure the energies from \mathcal{E} , the centroid of the diagonal energy terms, defined as,

$$\mathcal{E} = \frac{1}{2}(H_{11} + H_{22}). \quad (31)$$

Then,

$$H_{2 \times 2} = \mathcal{E} \mathbf{1}_{2 \times 2} + \mathcal{H} \quad (32)$$

and

$$\mathcal{H} = \begin{pmatrix} \Delta & H_{12} \\ H_{21} & -\Delta \end{pmatrix} \quad (33)$$

where

$$\Delta = \frac{1}{2}(H_{11} - H_{22}). \quad (34)$$

It is convenient to write \mathcal{H} in terms of the Pauli matrix valued vector $(\sigma_x, \sigma_y, \sigma_z)$ as

$$\mathcal{H} = (\mathbf{R} - i\frac{1}{2}\mathbf{\Gamma}) \cdot \boldsymbol{\sigma} \quad (35)$$

where \mathbf{R} and $\mathbf{\Gamma}$ are real vectors with Cartesian components

$$X_i = \frac{1}{2} \text{Re}[\text{Tr}(\mathcal{H}\sigma_i)] \quad (36)$$

and

$$\Gamma_i = -\text{Im}[\text{Tr}(\mathcal{H}\sigma_i)]. \quad (37)$$

The eigenvalues of \mathcal{H} are given by

$$\epsilon_{\pm} = \pm \sqrt{(R - i\frac{1}{2}\Gamma)^2} \quad (38)$$

and the corresponding poles of the S matrix are given by

$$E_{1,2} = \mathcal{E} \mp \epsilon. \quad (39)$$

From (39) we see that E_1 and E_2 coincide when ϵ vanishes. Hence, from (38), the condition for accidental degeneracy of two resonances may be written as

$$\sqrt{R_d^2 - \frac{1}{4}\Gamma_d^2 - iR_d \cdot \Gamma_d} = 0. \quad (40)$$

Now, since real and imaginary parts of ϵ should vanish, we get the pair of equations

$$R_d^2 - \frac{1}{4}\Gamma_d^2 = 0 \quad (41)$$

$$R_d \cdot \Gamma_d = 0. \quad (42)$$

These equations admit two types of solution according to whether or not \mathbf{H} is a diagonal at the degeneracy.

In the first case \mathcal{H} should vanish at the degeneracy and (41) and (42) are only satisfied if both R_d and Γ_d vanish for the same set of values of the external parameters. In this case, (41) and (42) define a point in parameter space. In the second case, when (41) and (42) are satisfied for non-vanishing R_d and Γ_d these equations define a circle in parameter space. In this case \mathcal{H}_d does not vanish at the degeneracy and the corresponding \mathbf{H}_d is equivalent to a Jordan canonical form with one Jordan block of rank two and all other Jordan blocks of rank one. (Miniatura *et al* [23] derived a set of conditions similar to our second case for the occurrence of an accidental degeneracy of a non-Hermitian Hamiltonian which drives an unstable atomic state which decays by photon emission.)

In the case of stable states, $\Gamma = 0$, and we recover the usual condition for accidental degeneracy of bound states

$$|R_d| = 0 \quad (43)$$

which defines a point in parameter space. The diabolic geometry which characterizes accidental degeneracies of stable states makes it natural to refer to the degeneracies themselves as diabolic points [1, 12]. In the next section, it will be shown that in the case of accidental degeneracies of unstable states we are also justified in calling the point or circle defined by equations (41) and (42) the diabolic point or diabolic circle and, by extension, to refer to the degeneracies of unstable states themselves as diabolic points or diabolic circles, according to which type of solution we have in mind.

4. Energy surfaces

The energy surface in parameter space is defined by equation (38). From this equation, the real and imaginary parts of the energy are given by

$$\text{Re } \epsilon_{\pm} = \pm \frac{1}{2} \{ [(R^2 - \frac{1}{4}\Gamma^2)^2 + (R \cdot \Gamma)^2]^{1/2} + (R^2 - \frac{1}{4}\Gamma^2) \}^{1/2} \quad (44)$$

and

$$\text{Im } \epsilon_{\pm} = \mp \left[\frac{1}{2} \left[(R^2 - \frac{1}{4}\Gamma^2)^2 + (R \cdot \Gamma)^2 \right]^{1/2} - (R^2 - \frac{1}{4}\Gamma^2) \right]^{1/2}. \quad (45)$$

These equations define two hypersurfaces in parameter space. We are interested in the shape of the energy surfaces in the immediate neighbourhood of a crossing resulting from the accidental degeneracy of two resonant states.

We shall first consider the accidental degeneracy of two resonant states leading to one simple pole in the S matrix. In this case the conditions for accidental degeneracy, equations (41) and (42), are satisfied for vanishing R and Γ , as shown in section 3. The effective Hamiltonian should have at least four independent free parameters to produce this type of degeneracy. There are only three independent parameters in R , hence Γ cannot be a fixed vector. Furthermore, since Γ and R should vary independently of each other it is not convenient to represent Γ as a vector in the same Euclidean space \mathcal{E}_3 as R . Therefore, in this case, we will understand equations (44) and (45) as defining the energy hypersurface in an eight-dimensional Euclidean space, \mathcal{E}_8 , with Cartesian coordinates $\{X, Y, Z, u, v, w, \text{Re } \epsilon, \text{Im } \epsilon\}$. The coordinates (u, v, w) are the Cartesian components of Γ , while (X, Y, Z) are the Cartesian components of R . In this way, the crossing should take place at the origin, i.e. at the point $R = 0$ and $\Gamma = 0$.

When the Hermitian and anti-Hermitian parts of \mathcal{H} commute the problem simplifies. From

$$[R \cdot \sigma, \frac{1}{2}\Gamma \cdot \sigma] = i(R \times \Gamma) \cdot \sigma$$

we see that, when $R \cdot \sigma$ and $\Gamma \cdot \sigma$ commute, $R \times \Gamma$ vanishes and $R \cdot \Gamma$ is equal to $R\Gamma$. Then, the equations of the energy, (44) and (45), take the simple form

$$\text{Re } \epsilon_{\pm} = \pm |R| = \pm \sqrt{X^2 + Y^2 + Z^2} \quad (46)$$

and

$$\text{Im } \epsilon_{\pm} = \mp \frac{1}{2} |\Gamma| = \mp \frac{1}{2} \sqrt{u^2 + v^2 + w^2}. \quad (47)$$

In this particularly simple case the two hypersurfaces representing the real and imaginary parts of the energy are double cones lying in orthogonal subspaces with the vertices at the origin.

In general $R \cdot \sigma$ and $\Gamma \cdot \sigma$ do not commute, so to study the behaviour of the energy hypersurfaces close to the crossing point we will approach the origin of the coordinates keeping $(\hat{R} \cdot \hat{\Gamma})/(R\Gamma)$ fixed and letting R and Γ go to zero in such a way that the ratio R/Γ is constant.

We consider first the case when

$$R < \frac{1}{2}\Gamma \quad (48)$$

then the energy equations (44) and (45) may be written as

$$\text{Re } \epsilon_{\pm} = \pm \frac{1}{2} |\Gamma| \left[\frac{1}{2} \{ (1 - \eta)^2 + 4\eta(\hat{R} \cdot \hat{\Gamma})^2 \}^{1/2} + (1 - \eta) \right]^{1/2} \quad (49)$$

and

$$\text{Im } \epsilon_{\pm} = \mp \frac{1}{2} |\Gamma| \left[\frac{1}{2} \{ (1 - \eta)^2 + 4\eta(\hat{R} \cdot \hat{\Gamma})^2 \}^{1/2} - (1 - \eta) \right]^{1/2} \quad (50)$$

with

$$\eta = \left(\frac{2R}{\Gamma}\right)^2 \tag{51}$$

and \hat{R} and $\hat{\Gamma}$ are unit vectors. Expanding the right-hand sides of (49) and (50) in powers of η and keeping only the first term, we get

$$\text{Re } \epsilon_{\pm} \simeq \pm(\hat{R} \cdot \hat{\Gamma})|R| = \pm(\hat{R} \cdot \hat{\Gamma})\sqrt{X^2 + Y^2 + Z^2} \tag{52}$$

and

$$\text{Im } \epsilon_{\pm} \simeq \mp\frac{1}{2}|\Gamma| = \mp\frac{1}{2}\sqrt{u^2 + v^2 + w^2}. \tag{53}$$

We now consider the case when

$$R > \frac{1}{2}\Gamma \tag{54}$$

we write the energy equations (44) and (45) in terms of

$$\zeta = \left(\frac{\Gamma}{2R}\right)^2 \tag{55}$$

$$\text{Re } \epsilon_{\pm} = \pm|R|\left[\frac{1}{2}\{(1 - \zeta)^2 + 4\zeta(\hat{R} \cdot \hat{\Gamma})^2\}^{\frac{1}{2}} + (1 - \zeta)\right]^{1/2} \tag{56}$$

and

$$\text{Im } \epsilon_{\pm} = \mp|R|\left[\frac{1}{2}\{(1 - \zeta)^2 + 4\zeta(\hat{R} \cdot \hat{\Gamma})^2\}^{1/2} - (1 - \zeta)\right]^{1/2} \tag{57}$$

we proceed as before, expanding the right-hand sides of (56) and (57) in powers of ζ and keeping only the first terms we obtain

$$\text{Re } \epsilon_{\pm} \simeq \pm|R| = \pm\sqrt{X^2 + Y^2 + Z^2} \tag{58}$$

and

$$\text{Im } \epsilon_{\pm} \simeq \mp\frac{1}{2}|\Gamma|(\hat{R} \cdot \hat{\Gamma}) = \mp\frac{1}{2}(\hat{R} \cdot \hat{\Gamma})\sqrt{u^2 + v^2 + w^2}. \tag{59}$$

Finally, when

$$R = \frac{1}{2}\Gamma \tag{60}$$

the energy equations (44) and (45) take the simple form

$$\text{Re } \epsilon_{\pm} = \pm|R|\sqrt{\frac{1}{2}(\hat{R} \cdot \hat{\Gamma})} = \pm\sqrt{\frac{1}{2}(\hat{R} \cdot \hat{\Gamma})}\sqrt{X^2 + Y^2 + Z^2} \tag{61}$$

and

$$\text{Im } \epsilon_{\pm} = \mp|\Gamma|\sqrt{\frac{1}{2}(\hat{R} \cdot \hat{\Gamma})} = \mp\sqrt{\frac{1}{2}(\hat{R} \cdot \hat{\Gamma})}\sqrt{u^2 + v^2 + w^2}. \tag{62}$$

From (52), (53), (58), (59), (61) and (62) it follows that, close to the crossing, the hypersurfaces representing the real and imaginary parts of the energy difference ϵ are double cones lying in orthogonal subspaces. The real part of the resonance energies E_1 and E_2 intersect conically in the subspace of \mathcal{E}_8 with Cartesian coordinates $\{X, Y, Z, 0, 0, 0, \text{Re } E, 0\}$. Explicit expressions for (X, Y, Z) in terms of the matrix elements of the Hermitian part of the mixing effective Hamiltonian are given in (36). The imaginary part of the resonance energies E_1 and E_2 also intersect conically but in a different subspace with Cartesian coordinates $\{0, 0, 0, u, v, w, 0, \text{Im } E\}$. The Cartesian coordinates (u, v, w) should be identified with $(\Gamma_x, \Gamma_y, \Gamma_z)$ as given in (37) in terms of the matrix elements of the anti-Hermitian part of the mixing effective Hamiltonian.

Therefore, in the case of a degeneracy of resonant states leading to one simple pole in the S matrix, any non-vanishing Hermitian or anti-Hermitian mixing interaction will move the resonance energies away from the degeneracy. There is energy level repulsion and also level width repulsion.

Let us now consider the case of a degeneracy of two resonant states leading to one simple and one double pole in the S matrix. In this case the condition for accidental degeneracy, equations (41) and (42), are satisfied for non-vanishing values of R and Γ and, as we saw in section 3, we need at least two free parameters in \mathcal{H} to bring about the degeneracy. For definiteness, we will keep the matrix W of the transition amplitudes fixed and let the parameters of the internal effective Hamiltonian \mathcal{H} vary. Then

$$W^\dagger W = \Gamma \cdot \sigma \quad (63)$$

is a constant matrix, and Γ is a fixed vector. To simplify the notation, it is convenient to make a rotation in parameter space such that the OZ axis is aligned with Γ .

In the case under consideration, equations (44) and (45) define two hypersurfaces in a five-dimensional Euclidean space, \mathcal{E}_5 , with Cartesian coordinates $\{X, Y, Z, \text{Re } \epsilon, \text{Im } \epsilon\}$. The hypersurfaces representing $\text{Re } \epsilon$ and $\text{Im } \epsilon$ are in orthogonal subspaces and touch one another only when both $\text{Re } \epsilon$ and $\text{Im } \epsilon$ vanish. It follows that the set of points in the energy hypersurfaces corresponding to a degeneracy are all in the subspace \mathcal{E}_3 with Cartesian coordinates $\{X, Y, Z, 0, 0\}$.

The equation

$$R \cdot \Gamma = 0 \quad (64)$$

defines a plane Π in \mathcal{E}_3 and a hyperplane $\hat{\Pi}$ in \mathcal{E}_5 with Cartesian coordinates $\{X, Y, 0, \text{Re } \epsilon, \text{Im } \epsilon\}$. When R is orthogonal to Γ , the equation

$$R^2 - \frac{1}{4}\Gamma^2 = 0 \quad (65)$$

for fixed Γ , defines a circle in the Π -plane. This is the diabolic circle.

In order to examine the energy hypersurface in the neighbourhood of the crossing, it is convenient to consider the hypersurface $\hat{\epsilon}$ resulting from the intersection of the ϵ -hypersurface and the $\hat{\Pi}$ -hyperplane. The equation of this hypersurface is obtained putting $R \cdot \Gamma = 0$ in (44) and (45). Then

$$\text{Re } \hat{\epsilon}_\pm = \pm \left[\frac{1}{2} \left[(R^2 - \frac{1}{4}\Gamma^2)^2 \right]^{1/2} + (R^2 - \frac{1}{4}\Gamma^2) \right]^{1/2} \quad (66)$$

and

$$\text{Im } \hat{\epsilon}_\pm = \mp \left[\frac{1}{2} \left[(R^2 - \frac{1}{4}\Gamma^2)^2 \right]^{1/2} - (R^2 - \frac{1}{4}\Gamma^2) \right]^{1/2}. \quad (67)$$

Hence, when $R^2 \geq \frac{1}{4}\Gamma^2$,

$$\operatorname{Re} \hat{\epsilon}_{\pm} = \pm(R^2 - \frac{1}{4}\Gamma^2)^{1/2} \quad (68)$$

and

$$\operatorname{Im} \hat{\epsilon}_{\mp} = 0. \quad (69)$$

Similarly, when $R^2 \leq \frac{1}{4}\Gamma^2$

$$\operatorname{Re} \hat{\epsilon}_{\pm} = 0 \quad (70)$$

and

$$\operatorname{Im} \hat{\epsilon}_{\pm} = \mp(\frac{1}{4}\Gamma^2 - R^2)^{1/2}. \quad (71)$$

Let us examine these relations in more detail. To take advantage of the symmetry of the problem we introduce cylindrical coordinates in parameter space,

$$X = A \cos \phi = \frac{1}{2} \operatorname{Re}[H_{12} + H_{21}] \quad (72)$$

$$Y = A \sin \phi = -\frac{1}{2} \operatorname{Im}[H_{12} - H_{21}] \quad (73)$$

$$Z = \varpi = \frac{1}{2} \operatorname{Re}[H_{11} - H_{22}] \quad (74)$$

$$\Gamma_x = a \cos \chi = -\operatorname{Im}[H_{12} + H_{21}] \quad (75)$$

$$\Gamma_y = a \sin \chi = -\operatorname{Re}[H_{12} - H_{21}] \quad (76)$$

$$\Gamma_z = -\gamma = -\frac{1}{2} \operatorname{Im}[H_{11} - H_{22}]. \quad (77)$$

The orthogonality condition (42) may be expressed as

$$\varpi = \gamma^{-1} A a \cos(\phi - \chi) \quad (78)$$

then the difference $R^2 - \frac{1}{4}\Gamma^2$ becomes

$$R^2 - \frac{1}{4}\Gamma^2 = (A^2 - \frac{1}{4}\tilde{\gamma}^2)\{1 + \gamma^{-2}a^2 \cos^2(\phi - \chi)\} \quad (79)$$

with

$$\tilde{\gamma}^2 = \gamma^2 \frac{1 + a^2/\gamma^2}{1 + (a^2/\gamma^2) \cos^2(\phi - \chi)}. \quad (80)$$

According to (70) and (71) for each fixed value of $(\phi - \chi)$, when A is non-vanishing but smaller than $\frac{1}{2}\tilde{\gamma}$, $\hat{\epsilon}$ is purely imaginary, then

$$\operatorname{Re} E_1 = \operatorname{Re} E_2 = \operatorname{Re} \mathcal{E} \quad (81)$$

and

$$\operatorname{Im} E_{1,2} = -\frac{1}{2}\sigma \pm [(\frac{1}{4}\tilde{\gamma}^2 - A^2)\{1 + \gamma^{-2}a^2 \cos^2(\phi - \chi)\}]^{1/2} \quad (82)$$

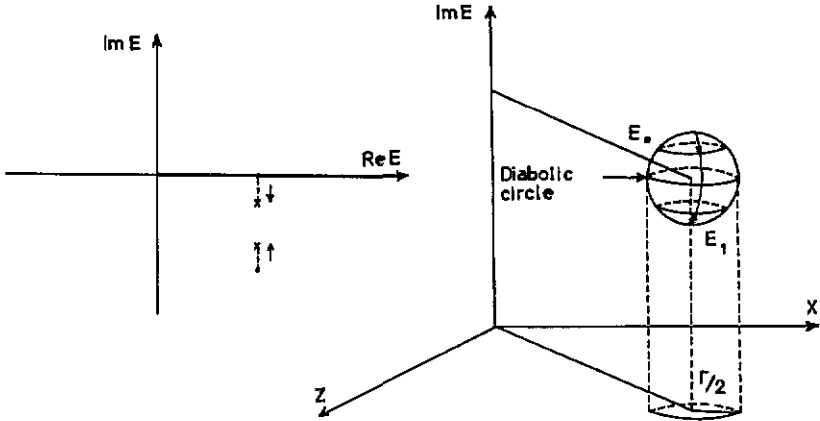


Figure 1. In the case of a degeneracy of two resonances leading to one simple and one double pole in the S matrix, the surface representing the imaginary part of the difference of the two energies in parameter space is a sphere. The upper and lower hemispheres represent the imaginary parts of the two neighbouring energies E_1 and E_2 . The diaboloic circle is the equator, where $\text{Im } E_1 = \text{Im } E_2$. In the regime of level width attraction $A^2 < \frac{1}{4}\tilde{\gamma}^2$. When the magnitude of the mixing interaction A increases from zero to some value smaller than $\frac{1}{2}\tilde{\gamma}$, the poles of the S matrix in the second sheet of the complex energy plane, initially at the position marked with dots, move along a straight line parallel to the imaginary axis to the final positions marked with crosses. In parameter space the system moves in the energy surface from the poles towards the equator along a meridian circle.

where $\sigma = -2\text{Im } \mathcal{E}$.

As long as $A^2 < \frac{1}{4}\tilde{\gamma}^2$, there is no degeneracy. When A increases, the difference between the two half-widths decreases. This is the regime of level width attraction [15, 16]. For each fixed value of A , we have two complex resonance energies, E_1 and E_2 , and two poles of the S matrix at the corresponding energies E_1 and E_2 in the unphysical sheet of the complex energy plane. When A increases, the poles of the S matrix approach each other moving along a straight line parallel to the imaginary axis, see figure 1.

In terms of parameter space, when $A < \frac{1}{4}\tilde{\gamma}$, $R^2 < \frac{1}{4}\Gamma^2$, and $\hat{\epsilon}$ is purely imaginary, equation (71) becomes the equation of a hypersphere of radius $\frac{1}{2}\Gamma$, see figure 1,

$$X^2 + Y^2 + Z^2 + (\text{Im } \hat{\epsilon})^2 = \frac{1}{4}\Gamma^2. \tag{83}$$

This sphere is embedded in the subspace \mathcal{E}_4 of \mathcal{E}_5 with Cartesian coordinates $\{X, Y, Z, 0, \text{Im } \epsilon\}$. The upper hemisphere represents $\hat{\epsilon}_-$ as a function of (X, Y, Z) . The lower hemisphere corresponds to $\hat{\epsilon}_+$. At the poles of the sphere, $A = 0$, the mixing interaction vanishes and the system is unperturbed.

At the equator, when

$$A = \frac{1}{2}\tilde{\gamma} \tag{84}$$

the energy difference $\hat{\epsilon}$ vanishes, the two energy eigenvalues are equal and the system becomes degenerate. Hence, the equator of the sphere is the diaboloic circle. In the complex energy plane, when (84) holds, the two poles of the S matrix collapse into one single pole and one double pole, located midway between the initial positions of the unperturbed poles.

When

$$A > \frac{1}{2}\tilde{\gamma} \tag{85}$$

the energy difference is purely real, and (68) becomes the equation of a hyperbolic cone of 'circular' cross section

$$X^2 + Y^2 + Z^2 - (\text{Re } \epsilon)^2 = \frac{1}{4}\Gamma^2 \quad (86)$$

when A increases, $\text{Re } \epsilon$ increases. This is the regime of level repulsion. In the complex energy plane, the corresponding poles of the S matrix repel one another and move away along a straight line parallel to the real axis, see figure 2.

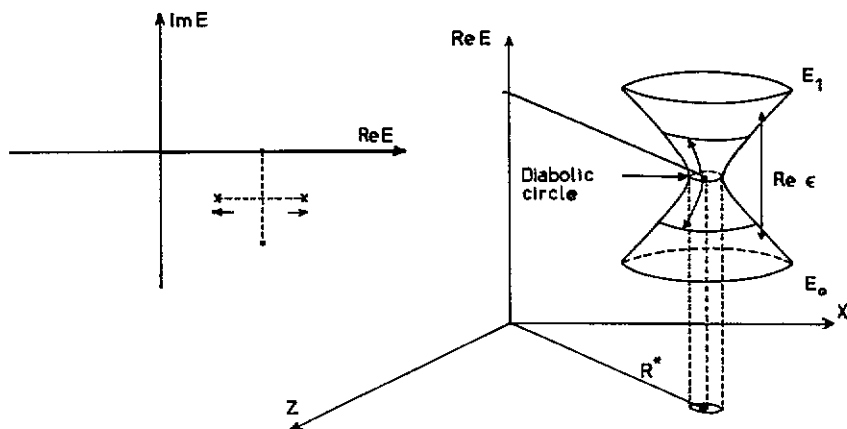


Figure 2. In the case of a degeneracy of two resonances leading to one simple and one double pole in the S -matrix, the surface representing the real part of the difference of the two energies in parameter space close to the degeneracy has the shape of a hyperbolic cone of circular cross section or diaboloic. At the narrowest cross section or waist of the diaboloic the two resonances are degenerate. The waist of the cone is the diaboloic circle. In the regime of level energy repulsion $A^2 > \frac{1}{4}\tilde{\gamma}^2$. When the magnitude of the mixing interaction A increases from the $\frac{1}{2}\tilde{\gamma}$ to some value larger than a $\frac{1}{2}\tilde{\gamma}$, the poles of the S matrix in the second sheet of the complex energy plane move away from the degeneracy along a straight line parallel to the real axis. In parameter space $\text{Re } E_2$ and $\text{Re } E_1$ move up and down respectively on the hyperbolic cone away from the diaboloic circle.

The narrowest cross section or 'waist' of the cone occurs when $\text{Re } \epsilon$ vanishes, i.e. when the two complex energy eigenvalues are equal and the two resonant states are degenerate. Hence, the waist of the cone is the diaboloic circle.

In brief, we have seen that the intersection of the energy hypersurface with the $\hat{\Pi}$ -hyperplane which contains the crossing points is a hypersurface which has two parts which lie in orthogonal subspaces. The surface representing the real part of the energy has the shape of an open sandglass or a diaboloic, with its waist at the diaboloic circle. The surface representing the imaginary part of the energy is a sphere with the equator at the diaboloic circle. The two surfaces are embedded in orthogonal subspaces but touch each other at all points in the diaboloic circle.

5. Results and conclusions

In order to study the conditions for the occurrence of an accidental degeneracy of two resonances, we considered explicitly the mixing of resonant states by a Hermitian interaction. We generalized the level repulsion theorem from bound states to a system of interacting

resonances and obtained the minimum number of free parameters in the mixing Hamiltonian necessary to produce a degeneracy of resonances in the absence of symmetry. We give general expressions for the codimension of any degeneracy of resonances in parameter space.

We find that two types of accidental degeneracy of two resonances may happen according to whether or not the effective complex Hamiltonian at the degeneracy may be brought to diagonal form by a similarity transformation.

In the first case, the number of free parameters in the mixing Hamiltonian necessary to produce a degeneracy is four when the mixing interaction is time reversal invariant and six when it is not. As in the case of degeneracies of bound states, in this case the two poles of the S matrix corresponding to the energies which become degenerate merge into one simple pole. The hypersurfaces representing the real and imaginary parts of the resonance energies in parameter space are double cones lying in orthogonal subspaces with their vertices located at the same point, which, for this reason, might be called a double diabolic point. In this case, the level energy difference and the level width difference of the mixed states are never smaller than the corresponding differences of the unmixed states. There is energy level repulsion and level width repulsion.

In the second case, the minimum number of free parameters in the effective Hamiltonian necessary to produce a degeneracy is two irrespective of the time reversal character of the interaction. The two poles of the S matrix corresponding to the energies which become degenerate fuse into one simple pole and one double pole at the degeneracy. Neighbouring energy surfaces are connected at all points in a circle with diameter equal to the difference in the half-widths of the unperturbed resonant states which are mixed. This is to be contrasted with the degeneracy of stable states in which case neighbouring surfaces are connected at a single conical or diabolic point. Close to the degeneracy, the energy surface has two parts lying in orthogonal subspaces. The surface representing the real part of the energy has the shape of an open sandglass or hyperbolic cone of circular cross section, its waist being at the diabolic circle. The surface of the imaginary part of the energy is a sphere with the equator at the diabolic circle. It has to be noted that, contrary to what happens in the bound state, in this type of resonance degeneracy, level energy repulsion does not always hold. When the spacing of the unperturbed levels is small, the finiteness of the widths removes the energy level repulsion and a purely off diagonal Hermitian interaction may produce level width attraction. This effect had been noted previously by von Brentano [15, 16].

Finally, let us notice that, for complex effective Hamiltonians, the codimension (two) of this type of resonance degeneracy is equal to the codimension of the degeneracies of bound states of a closed system driven by a real Hamiltonian. This feature might be related to the agreement between the short-distance behaviour of the nearest-neighbour spacing distribution derived from the study of irregular closed systems driven by Hermitian Hamiltonians [8, 9] and the nearest-neighbour spacing distribution obtained from the observation of series of resonances, i.e. metastable quantum states, in nuclear spectra [10]. If this were so, it might be an indication that accidental degeneracies of resonances leading to one simple plus one double pole in the S matrix might be the rule rather than the exception.

In the case just discussed, the topological structure of the energy surfaces at the complex energy crossing differs from that of bound-state crossings. The diabolic point obtained in the Hermitian case blows up into a diabolic circle and a sphere whose radius depends upon the magnitude of the difference of the unperturbed level widths and the magnitude of the anti-Hermitian part of the mixing interaction. This new feature gives rise to new and interesting effects [23, 24]. Elsewhere [24] we have discussed the generalization of Berry's

phase from bound to resonant states resulting from the different topological structure of the energy surfaces at the crossing of complex resonance energies.

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