REVISTA MEXICANA DE FÍSICA S **52** (1) 97–105 ENERO 2006

Local topology and universal unfolding of the energy surfaces at a crossing of unbound states

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Recibido el 19 de enero de 2005; aceptado el 5 de marzo de 2005

We show that when an isolated doublet of unbound states of a physical system becomes degenerate, the eigenenergy surfaces have an algebraic branch point of rank one and branch cuts in its real and imaginary parts starting at the same exceptional point but extending in opposite directions in parameter space. Associated with this singularity in parameter space, the scattering matrix, $S_\ell(E)$, and the Green's function, $G_\ell^{(+)}(k;r,r')$, have one double pole in the unphysical sheet of the complex energy plane. We characterize the universal unfolding or deformation of a typical degeneracy point of two unbound states in parameter space by means of a universal 2-parameter family of functions which is contact equivalent to the pole position function of the isolated doublet of resonances at the exceptional point and includes all small perturbations of the degeneracy condition up to contact equivalence. The rich phenomenology of crossings and anticrossings of energies and widths, as well as the sudden change in shape of the $S(E)-$matrix pole trajectories, observed in an isolated doublet of resonances when one control parameter is varied, is fully explained in terms of the topological properties of the energy hypersurfaces close to the degeneracy point.

Keywords: Resonances; nonrelativistic scattering theory; multiple resonances; Berry's phase.

Demostramos que, cuando un doblete aislado de estados no-ligados de un sistema físico está degenerado, las superfices de la autoenergía tienen un punto ramal de rango uno y cortes ramales en las partes real e imaginaria que empiezan en el mismo punto exceptional pero se extienden en direcciones opuestas en el espacio de parámetros. Asociado a esta singularidad en el espacio de parámetros, la matriz de dispersión, $S(E)$, y la función de Green, $G_\ell(k;r,r')$, tienen un polo doble en la hoja no física del plano complejo de la energía. Caracterizamos el despliegue universal o deformación de un punto de degeneración de dos estados no ligados típico, en el espacio de los parámetros, por medio de una familia universal de funciones que depende de dos parámetros y que es equivalente por contacto a la función de posición del polo del doblete aislado de resonancias en el punto excepcional e incluye todas las perturbaciones pequeñas de las condiciones de degeneración, hasta equivalencia por contacto. La rica fenomenología de cruces y anticruces de energías y semianchuras, así como el cambio repentino de la forma de las trayectoria de los polos de la matriz $S(E)$, que se observa en un doblete aislado de resonancias cuando un parámetro de control se hace variar, se explica completamente en términos de las propiedades topológicas de las hipersuperficies de la energía cerca del punto de la degeneración.

Descriptores: Resonancias; Teoría de la dispersión; Resonancias dobles; Fases geométricas y topológicas.

PACS: 25.70.Ef; 03.65.Nk; 33.40.+f; 03.65.Bz

1. Introduction

In this paper, we will be concerned with some physical and mathematical aspects of the mixing and degeneracy of two unbound energy eigenstates in an isolated doublet of resonances of a quantum system depending on two control parameters.

Unbound decaying states are energy eigenfunctions of a time reversal invariant Hamiltonian describing non dissipative physics in a situation in which there are no particles incident [1]. This boundary condition makes the corresponding energy eigenvalues complex, $\mathcal{E}_n = E_n - i(1/2)\Gamma_n$, with $E_n > \Gamma_n > 0$ [1].

Commonly, unbound energy eigenstates are regarded as a perturbation with the physics essentially unchanged from the bound states case, except for an exponential decay. But, unbound state physics differs radically from bound state physics in the presence of degeneracies, that is, coalescence of eigenvalues, as will be shown below.

In the case of bound states of a Hermitian Hamiltonian depending on parameters, the energy eigenvalues are real and, when a single parameter is varied, the two level mixing leads to the well known phenomenon of energy level repulsion and avoided level crossing. In their celebrated theorem [2], J. von Neumann and E.P.Wigner explained that, in the absence of symmetry, true degeneracies or crossings require the variation of at least a number of parameters equal to the codimension of the degeneracy which, in the general case, is three. A few years later, E. Teller showed that "if the parameters are X, Y and Z, the two degenerating levels correspond to the two sheets of an elliptic double cone in the (X, Y, Z, E) space near the degeneracy" [3], this is the diabolic crossing scenario [4] of the levels $\mathcal{E}_\pm$. for a recent review on diabolical conical intersections, see D.R. Yarkoni [5].

In the case of unbound states, the energy eigenvalues are complex, this fact opens a rich variety of possibilities, namely, crossings and anticrossings of energies and widths. Novel effects have been found which attracted considerable theoretical [6–8] and recently, also experimental interest [9, 10]. Furthermore, a joint crossing of energies and widths produces a true degeneracy of resonance energy eigenvalues in a physical system depending on only two real parameters [7] and gives rise to the occurrence of a double pole of the scattering matrix in the complex energy plane.

A number of examples of double poles of the scattering matrix brought about when the resonant states can be manipulated by external control parameters, have been mentioned in the literature. Lassila and Ruuskanen [11] pointed out that Stark mixing in an atom can display double pole decay. Knight [12] examined the decay of Rabi oscillations in two level system with double poles. Kylstra and Joachain [13,14] discussed double poles of the S-matrix in the case of laser-assisted electron-atom scattering.

The crossing and anticrossing of energies and widths of two interacting resonances in a microwave cavity were carefully measured by P. von Brentano, who also discussed the generalization of the von Neumann-Wigner theorem from bound to unbound states [15–17].

Examples of double poles in the scattering matrix of simple quantum mechanical systems have also been recently described. The formation of resonance double poles of the scattering matrix in a two-channel model with square well potentials was described by Vanroose *et al.* [18]. Hernández *et al.* [19] investigated a one channel model with a double $\delta-$barrier potential and showed that a double pole of the $S-$matrix can be induced by tuning the parameters of the model. A generalization of the double barrier potential model to the case of finite width barriers was proposed and discussed by W. Vanroose [20].

The problem of the characterization of the singularities of the energy surfaces at a degeneracy of unbound states arises naturally in connection with the topological phase of unbound states which was predicted by Hernández, Jáuregui and Mondragón [21–23], and later and independently by W.D. Heiss [24], and which was recently meassured by the Darmstadt group [25, 26]. The energy surfaces representing the resonance energy eigenvalues close to a degeneracy of unbound states in the scattering of a beam of particles by a finite double barrier potential was numerically computed by Hernández, Jáuregui and Mondragón [27]. Korsch and Mossman [28] made a detailed investigation of degeneracies of resonances in a symmetric double $\delta-$well in a constant Stark field. Keck, Korsch and Mossman [29] extended and generalized the discussion of the Berry phase of resonance states, from the case of unbound states of a Hermitian Hamiltonian given in [21–23] to the case of unbound states of non-Hermitian Hamiltonians.

The general theory of Gamow or resonant eigenfunctions associated with multiple poles of the scattering matrix and Jordan blocks in the spectral representation of the resolvent operator in a rigged Hilbert space was developed by Antoniou, Gadella and Pronko [30], A. Bohm *et al.* [31] and Hernández, Jáuregui and Mondragón [1].

2. Resonance energy eigenvalue surfaces close to degeneracy

In this communication, we will consider the resonance energy eigenvalues of a radial Schrödinger Hamiltonian, $H_r^{(\ell)}$, with a potential $V(r; x_1, x_2)$ which is a short ranged function of the radial distance, r, and depends on at least two external control parameters (x_1, x_2). When the potential $V(r; x_1, x_2)$ has two regions of trapping, the physical system may have isolated doublets of resonances which may become degenerate for some special values of the control parameters. For example, a double square barrier potential has isolated doublets of resonances which may become degenerate for some special values of the heights and widths of the barriers [19, 20, 27].

In the case under consideration, the regular and physical solutions of the Hamiltonian are functions of the radial distance, r, the wave number, k, and the control parameters (x_1, x_2). When necessary, we will stress this last functional dependence by adding the control parameters (x_1, x_2) to the other arguments after a semicolon.

The energy eigenvalues $\mathcal{E}_n = \left(\hbar^2/2m\right) k_n^2$ of the Hamiltonian $H_r^{(\ell)}$ are obtained from the zeroes of the Jost function, $f(-k; x_1, x_2)$ [32], where k_n is such that

$$f(-k_n; x_1, x_2) = 0. \tag{1}$$

When k_n lies in the fourth quadrant of the complex $k-$plane, $Rek_n > 0$ and $Imk_n < 0$, the corresponding energy eigenvalue, $\mathcal{E}_n$, is a complex resonance energy eigenvalue.

The condition (1) defines, implicitly, the functions $k_n(x_1, x_2)$ as branches of a multivalued function [32] which will be called the wave-number pole position function. Each branch $k_n(x_1, x_2)$ of the pole position function is a continuous, single-valued function of the control parameters. When the physical system has an isolated doublet of resonances which become degenerate for some exceptional values of the external parameters, (x_1^*, x_2^*), the corresponding two branches of the energy-pole position function, say $\mathcal{E}_n(x_1, x_2)$ and $\mathcal{E}_{n+1}(x_1, x_2)$, are equal (cross or coincide) at that point. As will be shown below, at a degeneracy of resonances, the energy hypersurfaces representing the complex resonance energy eigenvalues as functions of the real control parameters have an algebraic branch point of square root type (rank one) in parameter space.

2.1. Isolated doublet of resonances

Let us suppose that there is a finite bounded and connected region $\mathcal{M}$ in parameter space and a finite domain $\mathcal{D}$ in the fourth quadrant of the complex $k-$plane, such that, when $(x_1, x_2) \in \mathcal{M}$, the Jost function has two and only two zeroes, k_n and k_{n+1}, in the finite domain $\mathcal{D} \in \mathbf{C}$, all other zeroes of $f(-k; x_1, x_2)$ lying outside $\mathcal{D}$. Then, we say that the physical system has an isolated doublet of resonances. To make this situation explicit, the two zeroes of $f(-k; x_1, x_2)$, corresponding to the isolated doublet of resonances are explicitly factorized as

$$f(-k;x_1,x_2)=\left[\left(k-\frac{1}{2}(k_n+k_{n+1})\right)^2 -\frac{1}{4}\left(k_n-k_{n+1}\right)^2\right] g_{n,n+1}(k,x_1,x_2). \quad (2)$$

When the physical system moves in parameter space from the ordinary point (x_1,x_2) to the exceptional point (x_1^*,x_2^*), the two simple zeroes, $k_n(x_1,x_2)$ and $k_{n+1}(x_1,x_2)$, coalesce into one double zero $k_d(x_1^*,x_2^*)$ in the fourth quadrant of the complex $k-$plane.

If the external parameters take values in a neighbourhood of the exceptional point $(x_1^*,x_2^*)\in\mathcal{M}$ and $k\epsilon\mathcal{D}$, we may write

$$g_{n,n+1}(k;x_1,x_2)\approx g_{n,n+1}(k_d,x_1^*,x_2^*)\neq 0. \quad (3)$$

Then,

$$\left[k-\frac{1}{2}\left(k_n(x_1,x_2)+k_{n+1}(x_1,x_2)\right)\right]^2 -\frac{1}{4}\left(k_n(x_1,x_2)-k_{n+1}(x_1,x_2)\right)^2 \approx \frac{f(-k;x_1,x_2)}{g_{n,n+1}(k_d;x_1^*,x_2^*)}, \quad (4)$$

the coefficient $[g_{n,n+1}(k_d;x_1^*,x_2^*)]^{-1}$ multiplying $f(-k;x_1,x_2)$ may be understood as a finite, non-vanishing, constant scaling factor.

The vanishing of the Jost function defines, implicitly, the pole position function $k_{n,n+1}(x_1,x_2)$ of the isolated doublet of resonances. Solving eq.(2) for $k_{n,n+1}$, we get

$$k_{n,n+1}(x_1,x_2)=\frac{1}{2}\left(k_n(x_1,x_2)+k_{n+1}(x_1,x_2)\right) +\sqrt{\frac{1}{4}\left(k_n(x_1-x_2)-k_{n+1}(x_1,x_2)\right)^2} \quad (5)$$

with $(x_1,x_2)\in\mathcal{M}$. Since the argument of the square-root function is complex, it is necessary to specify the branch. Here and thereafter, the square root of any complex quantity F will be defined by

$$\sqrt{F}=|\sqrt{F}|\exp\left(i\frac{1}{2}argF\right), \quad 0\leq argF\leq 2\pi \quad (6)$$

so that $|\sqrt{F}|=\sqrt{|F|}$ and the $F-$ plane is cut along the real axis.

Equation (5) relates the wave number-pole position function of the doublet of resonances to the wave number-pole position functions of the individual resonance states in the doublet.

2.2. The analytical behaviour of the pole-position function at the exceptional point

The derivatives of the functions

$$1/2(k_n(x_1,x_2)+k_{n+1}(x_1,x_2))$$

and

$$1/4\big(k_n(x_1,x_2)-k_{n+1}(x_1,x_2)\big)^2$$

are finite at the exceptional point. They may be computed from the Jost function with the help of the implicit function theorem [33],

$$\left[\left(\frac{\partial\left(k_n(x_1,x_2)-k_{n+1}(x_1,x_2)\right)^2}{\partial x_1}\right)_{x_2}\right]_{k=k_d} = \frac{-8}{\left[\left(\frac{\partial^2 f(-k;x_1,x_2)}{\partial k^2}\right)_{x_1^*,x_2^*}\right]_{k=k_d}} \left[\left(\frac{\partial f(-k;x_1,x_2)}{\partial x_1}\right)_{x_2}\right]_{k_d}, \quad (7)$$

$$\frac{1}{2}\left[\left(\frac{\partial\left(k_n(x_1,x_2)+k_{n+1}(x_1,x_2)\right)}{\partial x_1}\right)_{x_2}\right]_{k_d} = \frac{-1}{\left[\left(\frac{\partial^2 f(-k;x_1,x_2)}{\partial k^2}\right)_{x_1^*,x_2^*}\right]_{k=d_d}} \times\left\{\left[\left(\frac{\partial^2 f(-k;x_1,x_2)}{\partial x_1\partial k}\right)_{x_2}\right]_{k=k_d} - \frac{1}{\left[\left(\frac{\partial^2 f(-k;x_1,x_2)}{\partial k^2}\right)_{x_1^*,x_2^*}\right]_{k=k_d}} \times\frac{1}{3}\left[\left(\frac{\partial^3 f(-k;x_1,x_2)}{\partial k^3}\right)_{x_1^*,x_2^*}\right]_{k=k_d}\left[\left(\frac{\partial f(-k;x_1,x_2)}{\partial x_1}\right)_{x_2}\right]_{k=k_d}\right\}. \quad (8)$$

From these results, the first terms in a Taylor series expansion of the functions $1/2\left(k_n(x_1,x_2)+k_{n+1}(x_1,x_2)\right)$ and $1/4\left(k_n(x_1,x_2)-k_{n+1}(x_1,x_2)\right)^2$ about the exceptional point (x_1^*,x_2^*), when substituted in eq.(5), give

$$\hat{k}_{n,n+1}(x_1,x_2)=k_d(x_1^*,x_2^*)+\Delta k_d(x_1,x_2)+\sqrt{\frac{1}{4}\left[c_1^{(1)}(x_1-x_1^*)+c_2^{(1)}(x_2-x_2^*)\right]} \quad (9)$$

for (x_1, x_2) in a neighbourhood of the exceptional point (x_1^*, x_2^*). This result may readily be translated into a similar assertion for the resonance energy-pole position function $\mathcal{E}_{n,n+1}(x_1, x_2)$ and the energy eigenvalues, $\mathcal{E}_n(x_1, x_2)$ and $\mathcal{E}_{n+1}(x_1, x_2)$, of the isolated doublet of resonances.

2.3. Energy-pole position function

Let us take the square of both sides of Eq. (5), multiplying them by $(\hbar^2/2m)$ and recalling $\mathcal{E}_n = (\hbar^2/2m)\, k_n^2$, in the approximation of (9), we get

$$\hat{\mathcal{E}}_{n,n+1}(x_1, x_2) = \mathcal{E}_d(x_1^*, x_2^*) + \Delta\mathcal{E}_d(x_1, x_2) + \hat{\epsilon}_{n,n+1}(x_1, x_2), \quad (10)$$

where

$$\hat{\epsilon}_{n,n+1}(x_1, x_2) = \sqrt{\frac{1}{4}\left[(\vec{R}\cdot\vec{\xi}) + i(\vec{I}\cdot\vec{\xi})\right]} \quad (11)$$

The components of the real fixed vectors $\vec{R}$ and $\vec{I}$ are the real and imaginary parts of the coefficients $C_i^{(1)}$ of $(x_i - x_i^*)$ in the Taylor expansion of the function $1/4\,(\mathcal{E}_n(x_1, x_2) - \mathcal{E}_{n+1}(x_1, x_2))^2$ and the real vector $\vec{\xi}$ is the position vector of the point (x_1, x_2) relative to the exceptional point (x_1^*, x_2^*) in parameter space.

$$\vec{\xi} = \begin{pmatrix}\xi_1\\ \xi_2\end{pmatrix} = \begin{pmatrix}x_1 - x_1^*\\ x_2 - x_2^*\end{pmatrix} \quad (12)$$

$$\vec{R} = \begin{pmatrix}Re\, C_1^{(1)}\\ Re\, C_2^{(1)}\end{pmatrix}, \quad \vec{I} = \begin{pmatrix}Im\, C_1^{(1)}\\ Im\, C_2^{(1)}\end{pmatrix}. \quad (13)$$

The real and imaginary parts of the function $\hat{\epsilon}_{n,n+1}(x_1, x_2)$ are

$$Re\hat{\epsilon}_{n,n+1}(x_1, x_2) = \pm\frac{1}{2\sqrt{2}}\left[\sqrt[+]{\left(\vec{R}\cdot\vec{\xi}\right)^2 + \left(\vec{I}\cdot\vec{\xi}\right)^2} + \vec{R}\cdot\vec{\xi}\right]^{1/2} \quad (14)$$

$$Im\,\hat{\epsilon}_{n,n+1}(x_1, x_2) = \pm\frac{1}{2\sqrt{2}}\left[\sqrt[+]{\left(\vec{R}\cdot\vec{\xi}\right)^2 + \left(\vec{I}\cdot\vec{\xi}\right)^2} - \vec{R}\cdot\vec{\xi}\right]^{1/2} \quad (15)$$

and

$$sign\,(Re\epsilon_{n,n+1})\, sign\,(Im\epsilon_{n,n+1}) = sign\left(\vec{I}\cdot\vec{\xi}\right) \quad (16)$$

It follows from (14), that $Re\hat{\epsilon}_{n,n+1}(x_1, x_2)$ is a two branched function of (ξ_1, ξ_2) which may be represented as a two-sheeted surface S_R, in a three dimensional Euclidean space with cartesian coordinates $(Re\hat{\epsilon}_{n,n+1}, \xi_1, \xi_2)$. The two branches of $Re\hat{\epsilon}_{n,n+1}(\xi_1, \xi_2)$ are represented by two sheets which are copies of the plane (ξ_1, ξ_2) cut along a line where the two branches of the function are joined smoothly. The cut is defined as the locus of the points where the argument of the square- root function in the right hand side of (14) vanishes.

Therefore, *the real part of the energy-pole position function, $\mathcal{E}_{n,n+1}(x_1, x_2)$, as a function of the real parameters (x_1, x_2), has an algebraic branch point of square root type (rank one) at the exceptional point with coordinates (x_1^*, x_2^*) in parameter space, and a branch cut along a line, $\mathcal{L}_R$, that starts at the exceptional point and extends in the positive direction defined by the unit vector $\hat{\xi}_c$ satisfying.*

$$\vec{I}\cdot\hat{\xi}_c = 0 \quad \text{and} \quad \vec{R}\cdot\hat{\xi}_c = -|\vec{R}\cdot\hat{\xi}_c| \quad (17)$$

A similar analysis shows that, *the imaginary part of the energy-pole position function, $Im\,\mathcal{E}_{n,n+1}(x_1, x_2)$, as a function of the real parameters (x_1, x_2), also has an algebraic branch point of square root type (rank one) at the exceptional point with coordinates (x_1^*, x_2^*) in parameter space, and also has a branch cut along a line, $\mathcal{L}_I$, that starts at the exceptional point and extends in the negative direction defined by the unit vector $\hat{\xi}_c$ satisfying eqs.(17).*

The branch cut lines, $\mathcal{L}_R$ and $\mathcal{L}_I$, are in orthogonal subspaces of a four dimensional Euclidean space with coordinates $(Re\epsilon_{n,n+1}, Im\epsilon_{n,n+1}, \xi_1, \xi_2)$, but have one point in common, the exceptional point with coordinates (x_1^*, x_2^*).

The individual resonance energy eigenvalues are conventionally asociated with the branches of the pole position function according to

$$\hat{\mathcal{E}}_m(\xi_1, \xi_2) = \mathcal{E}_d(0,0) + \Delta\mathcal{E}_{n,n+1}(\xi_1, \xi_2) + \sigma_R^{(m)}\frac{1}{2\sqrt{2}}\left[\sqrt[+]{(\vec{R}\cdot\vec{\xi})^2 + (\vec{I}\cdot\vec{\xi})^2} + (\vec{R}\cdot\vec{\xi})\right]^{1/2} + i\sigma_I^{(m)}\frac{1}{2\sqrt{2}}\left[\sqrt[+]{(\vec{R}\cdot\vec{\xi})^2 + (\vec{I}\cdot\vec{\xi})^2} - (\vec{R}\cdot\vec{\xi})\right]^{1/2}, \quad (18)$$

with $m = n, n+1$, and

$$\sigma_R^{(n)} = -\sigma_R^{n+1} = \frac{Re\mathcal{E}_n - Re\mathcal{E}_{n+1}}{|Re\mathcal{E}_n - Re\mathcal{E}_{n+1}|}, \quad (19)$$

$$\sigma_I^{(n)} = -\sigma_I^{n+1} = \frac{Im\mathcal{E}_n - Im\mathcal{E}_{n+1}}{|Im\mathcal{E}_n - Im\mathcal{E}_{n+1}|} \quad (20)$$

Along the line $\mathcal{L}_R$, excluding the exceptional point (x_1^*, x_2^*),

$$Re\mathcal{E}_n(x_1, x_2) = Re\mathcal{E}_{n+1}(x_1, x_2) \quad (21)$$

but

$$Im\mathcal{E}_n(x_1, x_2) \neq Im\mathcal{E}_{n+1}(x_1, x_2). \quad (22)$$

Similarly, along the line $\mathcal{L}_I$, excluding the exceptional point,

$$Im\mathcal{E}_n(x_1, x_2) = Im\mathcal{E}_{n+1}(x_1, x_2), \quad (23)$$

but

$$Re\mathcal{E}_n(x_1,x_2) \neq Re\mathcal{E}_{n+1}(x_1,x_2). \tag{24}$$

Equality of the complex resonance energy eigenvalues (degeneracy of resonances),

$$\mathcal{E}_n(x_1^*,x_2^*) = \mathcal{E}_{n+1}(x_1^*,x_2^*) = \mathcal{E}_d(x_1^*,x_2^*),$$

occurs only at the exceptional point with coordinates (x_1^*,x_2^*) in parameter space and only at that point.

In consequence, in the complex energy plane, the crossing point of two simple resonance poles of the scattering matrix is an isolated point where the scattering matrix has one double resonance pole.

Remark: In the general case, a variation of the vector of parameters causes a perturbation of the energy eigenvalues. In the particular case of a double complex resonance energy eigenvalue $\mathcal{E}_d(x_1^*,x_2^*)$, associated with a chain of length two of generalized Jordan-Gamow eigenfunctions [1], we are considering here, the perturbation series expansion of the eigenvalues $\mathcal{E}_n, \mathcal{E}_{n+1}$ about $\mathcal{E}_d$ in terms of the small parameter $|\xi|$, Eqs. (18)-(20), takes the form of a Puiseux series

$$\begin{aligned}\mathcal{E}_{n,n+1}(x_1,x_2) &= \mathcal{E}_d(x_1^*,x_2^*) \\ &+ |\xi|^{1/2}\sqrt{\frac{1}{4}\left[(\vec{R}\cdot\hat{\xi}) + i(\vec{I}\cdot\hat{\xi})\right]} \\ &+ \Delta\mathcal{E}_d(x_1,x_2) + O\left(|\xi|^{3/2}\right)\end{aligned} \tag{25}$$

with fractional powers $|\xi|^{j/2},\ j=0,1,2,...$ of the small parameter $|\xi|$ [33,35].

3. Unfolding of the degeneracy point

Let us introduce a function $\hat{f}_{doub}(-k;\xi_1,\xi_2)$ such that

$$\begin{aligned}\hat{f}_{doub}(-k;\xi_1,\xi_2) &= \left[k - \left(k_d(0,0) + \Delta^{(1)}k_d(\xi_1,\xi_2)\right)\right]^2 \\ &- \frac{1}{4}\left((\vec{\mathcal{R}}\cdot\vec{\xi}) + i(\vec{\mathcal{I}}\cdot\vec{\xi})\right),\end{aligned} \tag{26}$$

and

$$\Delta^{(1)}k_d(x_1,x_2) = \sum_{i=1}^{2} d_i^{(1)}\xi_i \tag{27}$$

Close to the exceptional point, the Jost function $f(-k;\xi_1,\xi_2)$ and the family of functions $\hat{f}_{doub}(-k;\xi_1,\xi_2)$ are related by

$$f(-k;\xi_1,\xi_2) \approx \frac{1}{g_{n,n+1}(k_d;0,0)}\hat{f}_{doub}(-k;\xi_1,\xi_2) \tag{28}$$

the term $[g_{n,n+1}(k_d,0,0)]^{-1}$ may be understood as a non-vanishing scale factor.

Hence, the two-parameters family of functions $\hat{f}_{doub}(-k;\xi_1,\xi_2)$ is contact equivalent to the Jost function $f(-k;\xi_1,\xi_2)$ at the exceptional point. It is also an unfolding [34,36] of $f(-k;\xi_1,\xi_2)$ with the following features:

1. It includes all possible small perturbations of the degeneracy conditions

$$f(-k;\xi_1,\xi_2) = 0,$$

$$\left(\frac{\partial f(-k;\xi_1,\xi_2)}{\partial k}\right)_{k_d} = 0 \tag{29}$$

$$\left(\frac{\partial^2 f(-k;\xi_1,\xi_2)}{\partial k^2}\right)_{k_d} \neq 0 \tag{30}$$

up to contact equivalence.

2. It uses the minimum number of parameters, namely two, which is the codimension of the degeneracy [7]. The parameters are (ξ_1,ξ_2).

Therefore, $\hat{f}_{doub}(-k;\xi_1,\xi_2)$ *is a universal unfolding [34] of the Jost function* $f(-k;\xi_1,\xi_2)$ *at the exceptional point where the degeneracy of unbound states occurs.*

The vanishing of $\hat{f}_{doub}(-k;\xi_1,\xi_2)$ *defines the approximate wave number-pole position function*

$$\begin{aligned}\hat{k}_{n,n+1}(\xi_1,\xi_2) &= k_d + \Delta^{(1)}_{n,n+1}k_d(\xi_1,\xi_2) \\ &\pm\left[\frac{1}{4}\left(\vec{\mathcal{R}}\cdot\vec{\xi} + i\vec{\mathcal{I}}\cdot\vec{\xi}\right)\right]^{1/2}\end{aligned} \tag{31}$$

and the corresponding energy-pole position function $\hat{\mathcal{E}}_{n,n+1}(\xi_1,\xi_2)$ given in eq.(10).

Since the functions $\hat{\mathcal{E}}_n(\xi_1,\xi_2)$ and $\hat{\mathcal{E}}_{n+1}(\xi_1,\xi_2)$ are obtained from the vanishing of the universal unfolding $\hat{f}_{doub}(-k;\xi_1,\xi_2)$ of the Jost function $f(-k;\xi_1,\xi_2)$ at the exceptional point, we are justified in saying that, *the family of functions* $\hat{\mathcal{E}}_n(\xi_1,\xi_2)$ *and* $\hat{\mathcal{E}}_{n+1}(\xi_1,\xi_2)$*, given in eqs.(18) and (19-20), is a universal unfolding or deformation of a generic degeneracy or crossing point of two unbound state energy eigenvalues, which is contact equivalent to the exact energy-pole position function of the isolated doublet of resonances at the exceptional point, and includes all small perturbations of the degeneracy conditions up to contact equivalence .*

4. Crossings and anticrossings of resonance energies and widths

Crossings or anticrossings of energies and widths are experimentally observed when the difference of complex energy eigenvalues $\mathcal{E}_n(\xi_1,\bar{\xi}_2) - \mathcal{E}_{n+1}(\xi_1,\bar{\xi}_2) = \Delta E - i(1/2)\Gamma$ is measured as function of one slowly varying parameter, ξ_1, keeping the other constant, $\xi_2 = \bar{\xi}_2^{(i)}$. A crossing of energies occurs if the difference of real energies vanishes, $\Delta E = 0$, for some value $\xi_{1,c}$ of the varying parameter. An anticrossing of energies means that, for all values of the varying parameter, ξ_1, the energies differ, $\Delta E \neq 0$. Crossings and anticrossings of widths are similarly described.

The experimentally determined dependence of the difference of complex resonance energy eigenvalues on one control parameter, ξ_1, while the other is kept constant,

$$\hat{\mathcal{E}}_n(\xi_1, \bar{\xi}_2^{(i)}) - \hat{\mathcal{E}}_{n+1}(\xi_1, \bar{\xi}_2^{(i)}) = \hat{\epsilon}_{n,n+1}(\xi_1, \bar{\xi}_2^{(i)}) \tag{32}$$

has a simple and straightforward geometrical interpretation, it is the intersection of the hypersurface $\hat{\epsilon}_{n,n+1}(\xi_1, \xi_2)$ with the hyperplane defined by the condition $\xi_2 = \bar{\xi}_2^{(i)}$.

To relate the geometrical properties of this intersection with the experimentally determined properties of crossings and anticrossings of energies and widths, let us consider a point $(\xi_1, \bar{\xi}_2^{(i)})$ in parameter space away from the exceptional point. To this point corresponds the pair of non-degenerate resonance energy eigenvalues $\mathcal{E}_n(\xi_1, \bar{\xi}_2^{(i)})$ and $\mathcal{E}_{n+1}(\xi_1, \bar{\xi}_2^{(i)})$, represented by two points on the hypersurface $\hat{\epsilon}_{n,n+1}(\xi_1, \xi_2)$. As the point $(\xi_1, \bar{\xi}_2^{(i)})$ moves on a straight line path π_i in parameter space,

$$\pi_i : \xi_{1,i} \leq \xi_1 \leq \xi_{1,f}, \;\; \xi_2 = \bar{\xi}_2^{(i)} \tag{33}$$

the corresponding points, $\mathcal{E}_n(\xi_1, \bar{\xi}_2^{(i)})$ and $\mathcal{E}_{n+1}(\xi_1, \bar{\xi}_2^{(i)})$ trace two curving trajectories, $\hat{C}_n(\pi_1)$ and $\hat{C}_{n+1}(\pi_1)$ on the $\hat{\epsilon}_{n,n+1}(\xi_1, \xi_2)$ hypersurface. Since ξ_2 is kept constant at the fixed value $\bar{\xi}_2^{(i)}$, the trajectories (sections) $\hat{C}_n(\pi_i)$ and $\hat{C}_{n+1}(\pi_i)$, may be represented as three-dimensional curves in a space $\mathcal{E}_3$ with cartesian coordinates $(Re\epsilon, Im\epsilon, \xi_1)$, see Figs. 1, 2 and 3. The projections of the curves $\hat{C}_n(\pi_i)$ and $\hat{C}_{n+1}(\pi_i)$ on the planes $(Re\epsilon, \xi_1)$ and $(Im\epsilon, \xi_1)$ are

$$Re[\hat{C}_m(\pi_i)] = Re\hat{\mathcal{E}}_m(\xi_1, \bar{\xi}_2^{(i)}) \;\; m = n, n+1 \tag{34}$$

and

$$Im[\hat{C}_m(\pi_i)] = Im\hat{\mathcal{E}}_m(\xi_1, \bar{\xi}_2^{(i)}) \;\; m = n, n+1 \tag{35}$$

respectively.

From Eqs. (18)-(20), and keeping $\xi_2 = \bar{\xi}_2^{(i)}$, we obtain

$$\Delta E = E_n - E_{n+1} = \left(Re\hat{\mathcal{E}}_n - Re\hat{\mathcal{E}}_{n+1}\right)\Big|_{\xi_2=\bar{\xi}_2^{(i)}}$$

$$= \frac{\sigma_R^{(n)}\sqrt{2}}{2}\left[\sqrt[+]{(\vec{R}\cdot\vec{\xi})^2 + (\vec{I}\cdot\vec{\xi})^2} + (\vec{R}\cdot\vec{\xi})\right]^{1/2}\Bigg|_{\xi_2=\bar{\xi}_2^{(i)}} \tag{36}$$

and

$$\Delta\Gamma = (\Gamma_n - \Gamma_{n+1}) = 2\left[Im\mathcal{E}_{n+1} - Im\mathcal{E}_n\right]$$

$$= - \, \sigma_I^{(n)}\sqrt{2}\left[\sqrt[+]{(\vec{R}\cdot\vec{\xi})^2 + (\vec{I}\cdot\vec{\xi})^2} - (\vec{R}\cdot\vec{\xi})\right]^{1/2}\Bigg|_{\xi_2=\bar{\xi}_2^{(i)}} \tag{37}$$

These expressions allow us to relate the terms $(\vec{R}\cdot\vec{\xi})$ and $(\vec{I}\cdot\vec{\xi})$ directly with observables of the isolated doublet of resonances. Taking the product of $\Delta E \Delta\Gamma$, and recalling eq.(16), we get

$$\Delta E \Delta\Gamma = -\left(\vec{I}\cdot\vec{\xi}\right)\Big|_{\xi_2=\bar{\xi}_2^{(i)}} \tag{38}$$

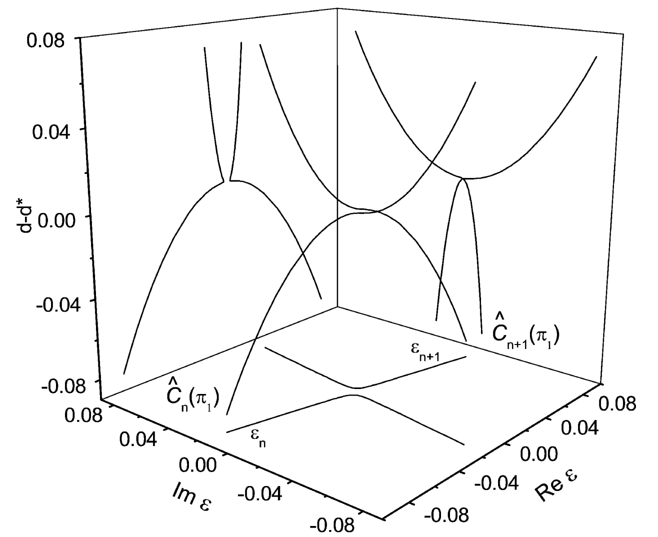

FIGURE 1. The curves $\hat{C}_n(\pi_1)$ and $\hat{C}_{n+1}(\pi_1)$ are the trajectories traced by the points $\hat{\mathcal{E}}_n(\xi_1, \bar{\xi}_2^{(1)})$ and $\hat{\mathcal{E}}_{n+1}(\xi_1, \bar{\xi}_2^{(1)})$ on the hypersurface $\hat{\mathcal{E}}_{n,n+1}(\xi_1, \bar{\xi}_2^{(1)})$ when the point $(\xi_1, \bar{\xi}_2^{(1)})$ moves along the straight line path π_1 in parameter space. In the figure, the path π_1 runs parallel to the vertical axis and crosses the line $\mathcal{L}_I$ at a point $(\xi_{1,c}, \bar{\xi}_2^{(1)})$ with $\xi_{1,c} < \xi_1^*$ and $\bar{\xi}_2^{(1)} < \xi_2^*$. The projections of $\hat{C}_n(\pi_1)$ and $\hat{C}_{n+1}(\pi_1)$ on the plane $(Im\mathcal{E}, \xi_1)$ are sections of the surface S_I; the projections of $\hat{C}_n(\pi_1)$ and $\hat{C}_{n+1}(\pi_1)$ on the plane $(Re\mathcal{E}, \xi_1)$ are sections of the surface S_R. The projections of $\hat{C}_n(\pi_1)$ and $\hat{C}_{n+1}(\pi_1)$ on the plane $(Re\mathcal{E}, Im\mathcal{E})$ are the trajectories of the $S-$matrix poles in the complex energy plane. In the figure, $d - d^* = \xi_1$.

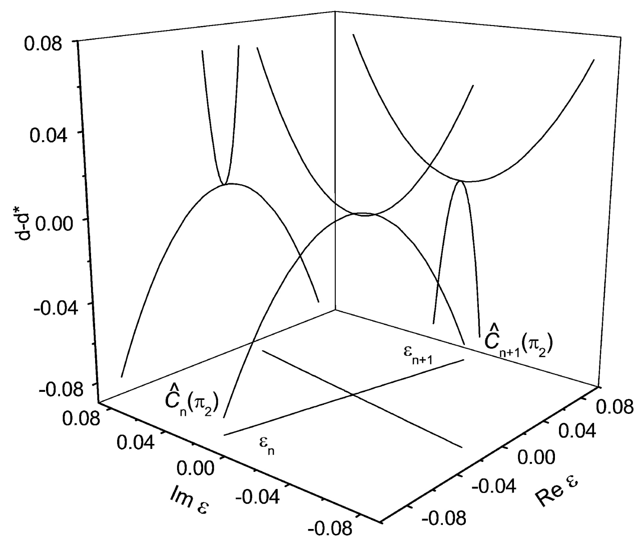

FIGURE 2. The curves $\hat{C}_n(\pi_2)$ and $\hat{C}_{n+1}(\pi_2)$ are the trajectories of the points $\hat{\mathcal{E}}_n(\xi_1, \xi_2^*)$ and $\hat{\mathcal{E}}_{n+1}(\xi_1, \xi_2^*)$ on the hypersurface $\hat{\mathcal{E}}_{n,n+1}(\xi_1, \xi_2)$ when the point (ξ_1, ξ_2^*) moves along a straight line path π_2 that goes through the exceptional point (ξ_1^*, ξ_2^*) in parameter space. The projections of $\hat{C}_n(\pi_2)$ and $\hat{C}_{n+1}(\pi_2)$ on the planes $(Re\mathcal{E}, \xi_1)$ and $(Im\mathcal{E}, \xi_1)$ are sections of the surfaces S_R and S_I respectively, and show a joint crossing of energies and widths. The projections of $\hat{C}_n(\pi_2)$ and $\hat{C}_{n+1}(\pi_2)$ on the plane $(Re\mathcal{E}, Im\mathcal{E})$ are two straight line trajectories of the $S-$matrix poles crossing at 90° in the complex energy plane. At the crossing point, the two simple poles coalesce into one double pole of $S(E)$.

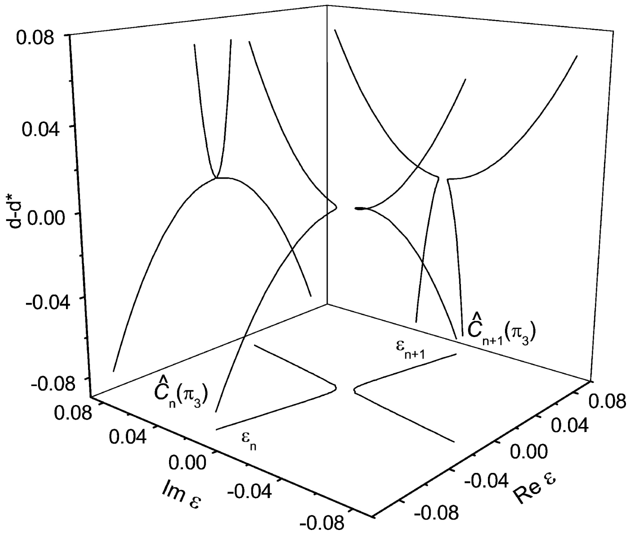

FIGURE 3. The curves $\hat{C}_n(\pi_3)$ and $\hat{C}_{n+1}(\pi_3)$ are the trajectories traced by the points $\hat{\mathcal{E}}_n(\xi_1,\bar{\xi}_2^{(3)})$ and $\hat{\mathcal{E}}_{n+1}(\xi_1,\bar{\xi}_2^{(3)})$ on the hypersurface $\mathcal{E}_{n,n+1}(\xi_1,\bar{\xi}_2^{(3)})$ when the point $(\xi_1,\bar{\xi}_2^{(3)})$ moves along a straight line path π_3 going trough the point $(\xi_{1,c},\bar{\xi}_2^{(3)})$ with $\xi_{1,c} > \xi_1^*$. The path π_3 crosses the line $\mathcal{L}_R$. The projections of $\hat{C}_n(\pi_3)$ and $\hat{C}_{n+1}(\pi_3)$ on the plane $(Re\mathcal{E},\xi_1)$ show a crossing, but the projections on the planes $(Im\mathcal{E},\xi_1)$ and $(Re\mathcal{E},Im\mathcal{E})$ do not cross. In the figure, $\xi_1 = d - d^*$.

and taking the differences of the squares of the left hand sides of (36) and (37), we get

$$(\Delta E)^2 - \frac{1}{4}(\Delta\Gamma)^2 = \left(\vec{R}\cdot\vec{\xi}\right)\Big|_{\xi_2=\bar{\xi}_2^{(i)}} \tag{39}$$

At a crossing of energies ΔE vanishes, and at a crossing of widths $\Delta\Gamma$ vanishes. Hence, the relation found in eq.(38) means that *a crossing of energies or widths can occur if and only if* $(\vec{I}\cdot\vec{\xi})_{\bar{\xi}_2^{(i)}}$ *vanishes*

For a vanishing $(\vec{I}\cdot\vec{\xi}_c)_{\bar{\xi}_2^{(i)}} = 0 = \Delta E\Delta\Gamma$, we find three cases, which are distinguished by the sign of $(\vec{R}\cdot\vec{\xi}_c)_{\bar{\xi}_2^{(i)}}$. From eqs. (36) and (37),

1. $(\vec{R}\cdot\vec{\xi}_c)_{\bar{\xi}_2^{(i)}} > 0$ *implies* $\Delta E \neq 0$ *and* $\Delta\Gamma = 0$, *i.e. energy anticrossing and width crossing*.
2. $(\vec{R}\cdot\vec{\xi}_c)_{\bar{\xi}_2^{(i)}} = 0$ *implies* $\Delta E = 0$ *and* $\Delta\Gamma = 0$, *that is, joint energy and width crossings, which is also degeneracy of the two complex resonance energy eigenvalues*.
3. $(\vec{R}\cdot\vec{\xi}_c)_{\bar{\xi}_2^{(i)}} < 0$ *implies* $\Delta E = 0$ *and* $\Delta\Gamma \neq 0$, *i.e. energy crossing and width anticrossing*.

This rich physical scenario of crossings and anticrossings for the energies and widths of the complex resonance energy eigenvalues, extends a theorem of von Neumann and Wigner [2] for bound states to the case of unbound states.

The general character of the crossing-anticrossing relations of the energies and widths of a mixing isolated doublet of resonances, discussed above, has been experimentally established by P. von Brentano and his collaborators in a series of beautiful experiments [15–17].

5. Trajectories of the S-matrix poles and changes of identity

The trajectories of the $S-$matrix poles (complex resonances energy eigenvalues), $\hat{\mathcal{E}}_n(\xi_1,\xi_2)$ and $\hat{\mathcal{E}}_{n+1}(\xi_1,\xi_2)$, in the complex energy plane are the projections of the three-dimensional trajectories (sections) $\hat{C}_n(\pi_i)$ and $\hat{C}_{n+1}(\pi_i)$ on the plane $(Re\epsilon, Im\epsilon)$, see Figs. 1, 2 and 3.

An equation for the trajectories of the $S-$matrix poles in the complex energy plane is obtained by eliminating ξ_1 between $Re\hat{\mathcal{E}}_n(\xi_1,\bar{\xi}_2^{(i)})$ and $Im\hat{\mathcal{E}}_n(\xi_1,\bar{\xi}_2^{(i)})$, Eqs. (18), (19) and (20).

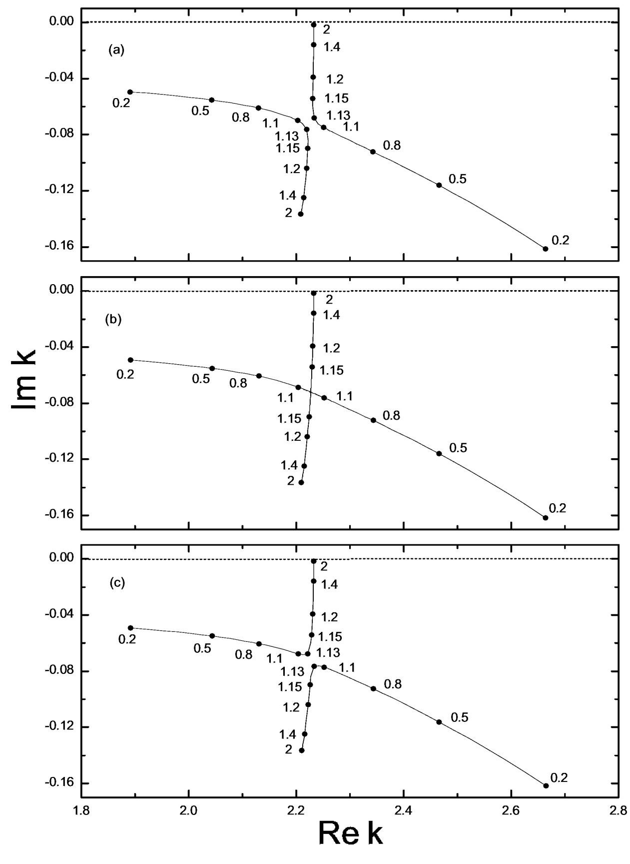

FIGURE 4. Trajectories of the poles of the scattering matrix, $S(k)$ of an isolated doublet of resonances in a double barrier potential [27], close to a degeneracy of unbound states. The control parameters are the width d of the inner barrier and the depth, V_3, of the outer well. The trajectories are traced by the poles $k_n(d,\bar{V}_3^{(i)})$ and $k_{n+1}(d,\bar{V}_3^{(i)})$ on the complex $k-$plane when the point $(d,\bar{V}_3^{(i)})$ moves on the straight line path π_i; $V_3 = \bar{V}_3^{(i)}$. The top, middle and bottom figures show the trajectories corresponding to $(\vec{R}\cdot\vec{\xi}_c)_{\bar{\xi}_2^{(i)}} < 0$, $(\vec{R}\cdot\vec{\xi}_c)_{\bar{\xi}_2^{(i)}} = 0$, and $(\vec{R}\cdot\vec{\xi}_c)_{\bar{\xi}_2^{(i)}} > 0$, respectively, with $(\xi_1,\xi_2) = (d-d^*, V_3-V_3^*)$.

A straightforward calculation gives

$$Re(\hat{\mathcal{E}}_n)^2 - 2\cot\phi_1(Re\hat{\mathcal{E}}_n)(Im\hat{\mathcal{E}}_n) - (Im\hat{\mathcal{E}}_n)^2 + (\vec{R}\cdot\bar{\xi}_c^{(i)}) = 0 \tag{40}$$

where

$$\cot\phi_1 = \frac{R_1}{I_1} \tag{41}$$

and the constant vector $\bar{\xi}_c^{(i)}$ is such that,

$$\left(\vec{I}\cdot\vec{\xi}_c\right)\Big|_{\xi_2=\bar{\xi}_2^{(i)}} = 0 \tag{42}$$

which is the previously found condition for the occurrence of a crossing of ΔE or $\Delta\Gamma$.

The discriminant of eq.(40), $4(\cot^2\phi_1 + 1)$, is positive. Therefore, *close to the crossing point, the trajectories of the $S-$matrix poles are the branches of a hyperbola* defined by Eq. (40).

The asymptotes of the hyperbola are the two straight lines defined by

$$Im\mathcal{E}^{(I)} = \tan\frac{\phi_1}{2}Re\mathcal{E}^{(I)} \tag{43}$$

and

$$Im\mathcal{E}^{(II)} = -\cot\frac{\phi_1}{2}Re\mathcal{E}^{(II)} \tag{44}$$

The two asymptotes divide the complex energy plane in four quadrants. The two branches of the hyperbola are in opposite, that is, not adjacent, quadrants of the complex energy plane.

We verify that, if $\mathcal{E}_n$ satisfies Eq. (40), so does $-\mathcal{E}_n=\mathcal{E}_{n+1}$. Therefore, if the trajectory followed by the pole $\mathcal{E}_n$ is one branch of the hyperbola, the trajectory followed by the pole $\mathcal{E}_{n+1}$ is the other branch of the hyperbola. Initially, the poles move towards each other from opposite ends of the two branches of the hyperbola until they come close to the crossing point, then they move away from each other, each pole on its own branch of the hyperbola.

We find three types of trajectories, which are distinguished by the sign of $(\vec{R}\cdot\vec{\xi}_c)|_{\xi_2=\bar{\xi}_2^{(i)}}$.

1. Trajectories of type I, when $(\vec{R}\cdot\vec{\xi}_c)|_{\xi_2=\bar{\xi}_2^{(i)}} > 0$.

   In this case there is a crossing of energies and an anticrossing of widths.

   Hence, one branch of the hyperbola, say, the trajectory followed by the pole $\mathcal{E}_n$, lies above a horizontal straight line, parallel to the real axis, and going through the crossing point $\mathcal{E}_d$. The other branch of the hyperbola, the trajectory followed by the pole $\mathcal{E}_{n+1}$, lies below the horizontal line, parallel to the real axis, going through the crossing point $\mathcal{E}_d$, see Fig. 4c.

2. Critical trajectories (type II), when $(\vec{R}\cdot\vec{\xi}_c)|_{\xi_2=\bar{\xi}_2^{(i)}} = 0$.

   There is a joint crossing of energies and widths.

   The trajectories are the asymptotes of the hyperbola.

   The two poles, $\mathcal{E}_n$ and $\mathcal{E}_{n+1}$, start from opposite ends of the same straight line, and move towards each other until they meet at the crossing point, where they coalesce to form a double pole of the $S-$matrix. From here, they separate moving away from each other on a straight line at 90° with respect to the first asymptote, see Fig. 4b.

3. Trajectories of type III, when $(\vec{R}\cdot\vec{\xi}_c)|_{\xi_2=\bar{\xi}_2^{(i)}} < 0$.

   In this case, there is an anticrossing of energies and a crossing of widths.

   Therefore, one branch of the hyperbola, say, the trajectory followed by the pole $\mathcal{E}_n$, lies to the left of a vertical straight line, parallel to the imaginary axis and going through the crossing point $\mathcal{E}_d$. The other branch of the hyperbola, the trajectory followed by the pole $\mathcal{E}_{n+1}$, lies to the right of the line parallel to the imaginary axis that goes through the crossing point $\mathcal{E}_d$, see Fig. 4a.

It is interesting to notice that, a small change in the external control parameter $\bar{\xi}_2^{(i)}$ produces a small change in the initial position of the poles, $\mathcal{E}_n$ and $\mathcal{E}_{n+1}$, but when the small change in $\bar{\xi}_2^{(i)}$ changes the sign of $(\vec{R}\cdot\vec{\xi}_c)|_{\xi_2=\bar{\xi}_2^{(i)}}$, the trajectories change suddenly from type I to type III and viceversa, this very large and sudden change of the trajectories exchanges almost exactly the final positions of the poles $\mathcal{E}_n$ and $\mathcal{E}_{n+1}$, see Fig. 4. This dramatic change has been termed a “change of identity” by W. Vanroose, P. Van Leuven F. Arickx and J. Broeckhove [18] who discussed an example of this phenomenon in the $S-$matrix poles in a two-channel model, W. Vanroose [20] and E. Hernández, A. Jáuregui and A. Mondragón [19, 27] have also discussed these properties in the case of the scattering of a beam of particles by a double barrier potential with two regions of trapping.

6. Summary and conclusions

We developed the theory of the unfolding of the energy eigenvalue surfaces close to a degeneracy point (exceptional point) of two unbound states of a Hamiltonian depending on control parameters. From the knowledge of the Jost function, as function of the control parameters of the system, we derived a 2-parameter family of functions which is contact equivalent to the exact energy-pole position function at the exceptional point and includes all small perturbations of the degeneracy conditions. A simple and explicit, but very accurate, representation of the eigenenergy surfaces close to the exceptional point is obtained. In parameter space, the hypersurface representing the complex resonance energy eigenvalues has an algebraic branch point of rank one, and branch cuts in its real and imaginary parts extending in opposite directions in parameter space. The rich phenomenology of crossings and anticrossings of the energies and widths of the resonances of an isolated doublet of unbound states of a quantum system, as well as, the sudden change in the shape of the $S-$matrix pole trajectories, observed when one control parameter is varied and the other is kept constant close to an exceptional point, is fully explained in terms of the local topology of the eigenenergy hypersurface in the vecinity of the crossing point.

A detailed account of these and other results will be published elsewhere [37, 38].

Acknowledgments

This work was partially supported by CONACyT México under contract number 40162-F and by DGAPA-UNAM contract No. PAPIIT:IN116202

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