Energy eigenvalue surfaces close to a degeneracy of unbound states: Crossings and anticrossings of energies and widths

E. Hernández,[1] A. Jáuregui,[2] and A. Mondragón[1]
[1]*Instituto de Física, UNAM, Apdo. Postal 20-364, 01000 México D.F., México*
[2]*Departamento de Física, Universidad de Sonora, Apdo. Postal 1626, Hermosillo, Sonora, México*
(Received 6 May 2005; published 25 August 2005)

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 sections of the energy eigenvalue surfaces in parameter space close to a degeneracy point.

DOI: 10.1103/PhysRevE.72.026221 PACS number(s): 05.45.Mt, 32.80.Bx, 03.65.Vf, 03.65.Nk

I. 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 nondissipative physics in a situation in which there are no particles incident [1]. This boundary condition makes the eigenvalue problem non-self-adjoint and the corresponding energy eigenvalues complex, $\mathcal{E}_n = E_n - i(1/2)\Gamma_n$, with $E_n > \Gamma_n > 0$ [1], even when the formal Hamiltonian, considered as an operator in the Hilbert space of square integrable functions is Hermitian (self-adjoint).

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, as will be shown below, unbound state physics differs radically from bound state physics in the presence of degeneracies, that is, coalescence of eigenvalues.

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], von Neumann and 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, 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 Yarkoni [5].

In the case of unbound energy states of the same Hamiltonian depending on parameters, the energy eigenvalues are complex, when a single parameter is varied, 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 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 a 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 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 δ-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 Vanroose [20].

The problem of the characterization of the singularities of the energy surfaces at a degeneracy of unbound states [7] 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 Heiss [24], and which was recently measured 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 δ-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], Bohm *et al.* [31], and Hernández, Jáuregui, and Mondragón [1].

II. REGULAR AND PHYSICAL SOLUTIONS OF THE RADIAL EQUATION

The nonrelativistic scattering of a spinless particle by a short ranged potential, $V(r;x_1,x_2)$, is described by the solution of a Schrödinger equation. When the potential is rotationally invariant, the wave function is expanded in partial waves and one is left with the radial equation

$$H_r^{(\ell)}(x_1,x_2)\,\phi_\ell(k,r)=k^2\phi_\ell(k,r), \tag{1}$$

where $H_r^{(\ell)}(x_1,x_2)$ is the formal differential expression

$$H_r^{(\ell)}(x_1,x_2)\equiv\frac{\hbar^2}{2\mu}\left[-\frac{d^2}{dr^2}+\frac{\ell(\ell+1)}{r^2}\right]+V(r;x_1,x_2), \tag{2}$$

and the potential $V(r;x_1,x_2)$ is a short ranged function of the radial distance, r, and depends on at least two external control parameters (x_1,x_2). In this case, 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). In this section, we will omit the control parameters in the arguments of the regular and physical solutions of Eq. (1), but 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.

As is usually done when discussing the analytic properties of the solutions of Eq. (1) as functions of k, rather than starting by defining the physical solutions $\psi_\ell^{(+)}(k,r)$, we define the regular and irregular solutions of Eq. (1) by boundary conditions which lead to simple properties as functions of k. The regular solution $\phi_\ell(k,r)$ is uniquely defined by the boundary condition [32]

$$\lim_{r\to 0}(2\ell+1)!!\,r^{-\ell-1}\phi_\ell(k,r)=1, \tag{3}$$

$\phi_\ell(k,r)$ may be expressed as a linear combination of two independent, irregular solutions of Eq. (1) which behave as outgoing and incoming waves at infinity,

$$\phi_\ell(k,r)=\tfrac{1}{2}ik^{-\ell-1}[f_\ell(-k)f_\ell(k,r)-(-1)^\ell f_\ell(k)f_\ell(-k,r)], \tag{4}$$

where $f_\ell(-k,r)$ is an outgoing wave at infinity defined by the boundary condition

$$\lim_{r\to\infty}\exp(-ikr)f_\ell(-k,r)=(+i)^\ell \tag{5}$$

and $f_\ell(k,r)$ is an incoming wave at infinity related to $f_\ell(-k,r)$ by

$$f_\ell(k,r)=(-1)^\ell f_\ell^*(-k,r) \tag{6}$$

for k real and nonvanishing.

The Jost function $f_\ell(-k)=f_\ell(-k,0)$ is given by

$$f_\ell(-k)=(-1)^\ell k^\ell W[f_\ell(-k,r),\phi_\ell(k,r)], \tag{7}$$

where $W[f,g]=fg'-f'g$ is the Wronskian. The Jost function $f_\ell(-k)$ has zeros (roots) on the imaginary axis and in the lower half of the complex k plane.

When the first and second absolute moments of the potential exist, and the potential decreases at infinity faster than any exponential [e.g., if $V(r)$ has a Gaussian tail or if it vanishes identically beyond a finite radius] the functions $f_\ell(-k)$, $\phi_\ell(k,r)$, and $k^\ell f_\ell(-k,r)$, for fixed $r>0$, are entire functions of k [32].

The scattering wave function $\psi_\ell^{(+)}(k,r)$ is the solution of Eq. (1) which vanishes at the origin and behaves at infinity as the sum of a free incoming spherical wave of unit flux plus a free outgoing spherical wave,

$$\psi_\ell^{(+)}(k,0)=0 \tag{8}$$

and

$$\lim_{r\to\infty}\{\psi_\ell^{(+)}(k,r)-[\hat{h}_\ell^{(-)}(k,r)-S_\ell(k)\hat{h}_\ell^{(+)}(k,r)]\}=0. \tag{9}$$

In this expression $\hat{h}_\ell^{(-)}(k,r)$ and $\hat{h}_\ell^{(+)}(k,r)$ are Ricatti-Hankel functions that describe incoming and outgoing waves, respectively, $S_\ell(k)$ is the scattering matrix.

Hence the scattering wave function $\psi_\ell^{(+)}(k,r)$ and the regular solution are related by

$$\psi_\ell^{(+)}(k,r)=\frac{k^{\ell+1}\phi_\ell(k,r)}{f_\ell(-k)}, \tag{10}$$

and the scattering matrix is given by

$$S_\ell(k)=\frac{f_\ell(k)}{f_\ell(-k)}. \tag{11}$$

The complete Green's function for outgoing particles or resolvent of the radial equation may also be written in terms of the regular solution $\phi_\ell(k,r)$ and the irregular solution $f_\ell(-k,r)$ which behaves as an outgoing wave at infinity

$$G_\ell^{(+)}(k;r,r')=(-1)^{\ell+1}k^\ell\frac{\phi_\ell(k,r_<)f_\ell(-k,r_>)}{f_\ell(-k)}. \tag{12}$$

III. BOUND AND RESONANT STATE EIGENFUNCTIONS

Bound and resonant state energy eigenfunctions are the solutions of Eq. (1) that vanish at the origin

$$u_{n\ell}(k_n,0)=0, \tag{13}$$

and at infinity satisfy the boundary condition

$$\lim_{r\to\infty}\left[\frac{1}{u_{n\ell}(k_n,r)}\frac{du_{n\ell}(k_n,r)}{dr}-ik_n\right]=0, \tag{14}$$

where k_n is a zero of the Jost function,

$$f_\ell(-k_n)=0. \tag{15}$$

From Eqs. (1) and (4) we verify that all roots (zeros) of the Jost function are associated with energy eigenfunctions of the Schrödinger equation. From Eqs. (10)–(12), we see that these same roots (zeros) of the Jost function give rise to poles in the scattering wave function, the scattering matrix, and the complete Green's function.

From Eqs. (4), (5), and (15), bound states and Gamow or resonance eigenfunctions take the form

$$u_{n\ell}(k_n,r)=N_{n\ell}^{-1}\frac{i}{2}\frac{(-1)^{\ell+1}}{k_n^{\ell+1}}f_\ell(k_n)f_\ell(-k_n,r), \tag{16}$$

where $N_{n\ell}$ is a normalization constant and $f(-k_n,r)$ is the outgoing wave solution of Eq. (1).

Bound state eigenfunctions are associated with the zeros of $f_\ell(-k)$ which are on the positive imaginary axis, while resonant or Gamow state eigenfunctions belong to the zeros of the Jost function which are in the fourth quadrant of the complex k-plane. Equation (16) shows, in a very explicit way, that the Gamow eigenfunctions $u_{n\ell}(k_n,r)$ with $k_n=\kappa_n-i\gamma_n$ and $\kappa_n>\gamma_n>0$, see [33], are solutions of Eq. (1) which vanish at the origin and asymptotically behave as purely outgoing waves which oscillate between envelopes that increase exponentially with r, the corresponding energy eigenvalues $\mathcal{E}_n$ are complex with $\mathrm{Re}\,\mathcal{E}_n>\mathrm{Im}\,\mathcal{E}_n$.

The bound state eigenfunctions $u_{s\ell}(k_s,r)$ are also solutions of Eq. (1) which vanish at the origin and satisfy the outgoing wave boundary condition (14), but, in this case the wave number is purely imaginary, with $k_s=i\kappa_s$ and $\kappa_s>0$. Hence the outgoing wave solution $f_\ell(-k_s,r)$ and the bound state eigenfunction $u_{s\ell}(k_s,r)$ as functions of r behave asymptotically as decreasing exponentials vanishing as r goes to infinity,

$$\lim_{r\to\infty}u_{s,\ell}(k_s,r)=0, \tag{17}$$

the corresponding energy eigenvalues $\mathcal{E}_s=-\hbar^2\kappa_s^2/2\mu$ are real and negative. Hence the bound state eigenfunctions are bounded for all values of r and, as functions of r, they are square integrable.

IV. ENERGY EIGENFUNCTIONS AS ELEMENTS OF A RIGGED HILBERT SPACE

Since bound state radial eigenfunctions vanish at the origin and are square integrable, they are elements of the Hilbert space $\mathcal{H}$ of square integrable functions of r,

$$\mathcal{H}=\mathcal{L}^2([0,\infty),dr). \tag{18}$$

Therefore we may refer to the formal Hamiltonian $H_r^{(\ell)}\times(x_1,x_2)$ occurring in the left-hand side of the radial Schödinger equation, Eq. (1), as an operator acting in a space of functions. When this space is the Hilbert space $\mathcal{H}$ of square integrable functions which vanish at the origin, the Hamiltonian $H_r^\ell(x_1,x_2)$ is bounded from below and essentially self-adjoint [31].

The self-adjointness (Hermiticity) of $H_r^{(\ell)}$ in $\mathcal{H}$ implies that $H_r^{(\ell)}$ as an operator in $\mathcal{H}$ has only real eigenvalues. Hence the Gamow state eigenfunctions cannot be elements of the Hilbert space $\mathcal{H}$.

Indeed, due to their nondecreasing oscillating behavior at large values of r, the scattering wave functions, $\psi_\ell^{(+)}(k,r)$, and the Gamow eigenfunctions, $u_{n,\ell}(k_n,r)$, are not square integrable functions of r, that is, they are not elements of the Hilbert space $\mathcal{H}$.

All the physical solutions of the radial Schrödinger equation (1) may be considered as elements of a space, but then, a space larger than the Hilbert space $\mathcal{H}$ is required. This larger space is a rigged Hilbert space [34] which is a triplet of spaces,

$$\Phi\subset\mathcal{H}\subset\Phi^\times, \tag{19}$$

where $\mathcal{H}$ is the Hilbert space $\mathcal{L}^2([0,\infty),dr)$, Φ is the space of very well-behaved functions in $\mathcal{H}$ (Schwarz space of test functions, i.e., the subspace of $\mathcal{H}$ of all functions admitting derivatives at all orders and such that they and their derivatives go to zero faster than any exponential at infinity) and $\Phi^\times$ is the space of antilinear functionals defined over the space Φ.

The action of the Hamiltonian $H_r^{(\ell)}$, which, as an operator, is, in principle, only defined on the elements of its domain in $\mathcal{H}$, can be extended to the elements of $\Phi^\times$ by defining the following extended operator $H_r^{(\ell)\times}$:

$$\langle\varphi|H_r^{(\ell)\times}F\rangle:=\langle H_r^{(\ell)}\varphi|F\rangle\ \forall\ \varphi\epsilon\Phi,\ F\epsilon\Phi^\times, \tag{20}$$

where the notation means, as usual,

$$\langle H_r^{(\ell)}\varphi|F\rangle=\int_0^\infty(H_r^{(\ell)}\varphi(r))^*F(r)dr. \tag{21}$$

We verify that Eq. (20) is satisfied as

$$\int_0^\infty\varphi^*(r)(H_r^{(\ell)\times}F(r))dr=\int_0^\infty(H_r^{(\ell)}\varphi(r))^*F(r)dr. \tag{22}$$

Finally, using the definition (20) and Eq. (22), and integrating by parts in the right-hand side of Eq. (22), when $F(r)$ is the Gamow eigenfunction $u_{n\ell}(k_n,r)$, we get

$$\int_0^\infty\varphi^*(r)(H_r^{(\ell)}u_n(k_n,r))dr=k_n^2\int_0^\infty\varphi^*(r)u_n(k_n,r)dr. \tag{23}$$

If the arbitrary test function $\varphi\epsilon\Phi$ is omitted in this last equation, we recover the differential equation

$$H_r^{(\ell)}u_{n\ell}(k_n,r)=k_n^2u_{n\ell}(k_n,r), \tag{24}$$

where $H_r^{(\ell)}$ is the "formal Hamiltonian" given in Eq. (2). This last result shows that we may consider (define) the same formal Hamiltonian $H_r^{(\ell)}$ as an extended operator $H^{(\ell)\times}$ acting in the larger space $\Phi^\times$ which contains the Hilbert space $\mathcal{H}$ of square integrable eigenfunctions, the scattering wave functions, and the Gamow eigenfunctions. In such a space, the "formal Hamiltonian" $H_r^{(\ell)}$ can have eigenfunctions which are not square integrable and have complex energy eigenvalues. We also notice that when $H_r^{(\ell)\times}$ is expressed as a formal differential operator acting on the elements of $\Phi^\times$, it has exactly the same form as $H_r^{(\ell)}$ given in Eq. (2) which is essentially self-adjoint, that is Hermitian, in the Hilbert space $\mathcal{H}$.

Considered as elements of a rigged Hilbert space, bound state eigenfunctions, Gamow eigenfunctions, and scattering wave functions may be characterized as energy eigenkets. But whereas Dirac kets describing scattering states are associated with a real value of the energy in the continuous Hilbert space spectrum of the self-adjoint Hamiltonian $H_r^{(\ell)}$, the Gamow eigenkets are not, but have complex eigenvalues. The existence of these Gamow eigenfunctions (or eigenkets) allows us to interpret resonances as well-defined quantum states of physical systems labeled with a complete set of quantum numbers.

V. RESONANCE ENERGY EIGENVALUE SURFACES CLOSE TO DEGENERACY

In this section, we will be concerned with the degeneracy of two complex resonance energy eigenvalues of the radial Schrödinger Hamiltonian, $H_r^{(\ell)}(x_1,x_2)$, defined in Eq. (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].

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

$$f(-k_n;x_1,x_2)=0. \tag{25}$$

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

The condition (25) 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.

A. 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 $(x_1,x_2)\epsilon\mathcal{M}$, the Jost function has two and only two zeros, k_n and k_{n+1}, in the finite domain $\mathcal{D}\epsilon\mathbf{C}$, all other zeros 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

$$f(-k;x_1,x_2)=[k-k_n(x_1,x_2)][k-k_{n+1}(x_1,x_2)]\times g_{n,n+1}(k;x_1,x_2) \tag{26}$$

which may be conveniently rearranged as

$$f(-k;x_1,x_2)=\left(\left\{k-\frac{1}{2}[k_n(x_1,x_2)+k_{n+1}(x_1,x_2)]\right\}^2-\frac{1}{4}[k_n(x_1,x_2)-k_{n+1}(x_1,x_2)]^2\right)g_{n,n+1}(k;x_1,x_2). \tag{27}$$

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 zeros, $k_n(x_1,x_2)$ 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 neighborhood of the exceptional point $(x_1^*,x_2^*)\epsilon\mathcal{M}$ and $k\epsilon\mathcal{D}$, we may write

$$g_{n,n+1}(k;x_1,x_2)\approx g_{n,n+1}(k_d;x_1^*,x_2^*)\neq 0. \tag{28}$$

Then

$$\left\{k-\frac{1}{2}[k_n(x_1,x_2)+k_{n+1}(x_1,x_2)]\right\}^2-\frac{1}{4}[k_n(x_1,x_2)-k_{n+1}(x_1,x_2)]^2\approx\frac{f(-k;x_1,x_2)}{g_{n,n+1}(k_d;x_1^*,x_2^*)}, \tag{29}$$

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, nonvanishing, 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. (27) for $k_{n,n+1}$, we get

$$k_{n,n+1}(x_1,x_2)=\frac{1}{2}[k_n(x_1,x_2)+k_{n+1}(x_1,x_2)]+\sqrt{\frac{1}{4}[k_n(x_1,x_2)-k_{n+1}(x_1,x_2)]^2} \tag{30}$$

with $(x_1,x_2)\epsilon\mathcal{M}$. 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

$$\sqrt{F}=|\sqrt{F}|\exp\left(i\frac{1}{2}\arg F\right),\quad 0\leqslant\arg F\leqslant 2\pi \tag{31}$$

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

Equation (30) 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.

B. The analytical behavior of the pole-position function at the exceptional point

According to the preparation theorem of Weierstrass [35] the functions $1/2[k_n(x_1,x_2)+k_{n+1}(x_1,x_2)]$ and $1/4[k_n(x_1,x_2)-k_{n+1}(x_1,x_2)]^2$ are regular at the exceptional point and admit a Taylor series expansion about this point. The required derivatives of these functions may be readily computed from the Jost function with the help of the implicit function theorem [35],

$$\left[\left(\frac{\partial[k_n(x_1,x_2)-k_{n+1}(x_1,x_2)]^2}{\partial x_1}\right)_{x_2}\right]_{k=k_d} = \frac{-8}{\left[\left(\frac{\partial^2 f(-k;x_1,x_2)}{\partial k^2}\right)_{x_1^*,x_2^*}\right]_{k=k_d}}\left[\left(\frac{\partial f(-k;x_1,x_2)}{\partial x_1}\right)_{x_2}\right]_{k=k_d}, \tag{32}$$

$$\begin{aligned}\frac{1}{2}\left[\left(\frac{\partial[k_n(x_1,x_2)+k_{n+1}(x_1,x_2)]}{\partial x_1}\right)_{x_2}\right]_{k=k_d} &= \frac{-1}{\left[\left(\frac{\partial^2 f(-k;x_1,x_2)}{\partial k^2}\right)_{x_1^*,x_2^*}\right]_{k=d_d}}\Bigg\{\left[\left(\frac{\partial^2 f(-k;x_1,x_2)}{\partial x_1\partial k}\right)_{x_2}\right]_{k=k_d} \\ &\quad - \frac{1}{\left[\left(\frac{\partial^2 f(-k;x_1,x_2)}{\partial k^2}\right)_{x_1^*,x_2^*}\right]_{k=k_d}} \\ &\quad \times\frac{1}{3}\left[\left(\frac{\partial^3 f(-k;x_1,x_2)}{\partial k^3}\right)_{x_1^*,x_2^*}\right]_{k=k_d} \\ &\quad \times\left[\left(\frac{\partial f(-k;x_1,x_2)}{\partial x_1}\right)_{x_2}\right]_{k=k_d}\Bigg\}.\end{aligned} \tag{33}$$

From these expressions, we obtain the first terms in a Taylor series expansion of the functions $1/2[k_n(x_1,x_2)+k_{n+1}(x_1,x_2)]$ and $1/4[k_n(x_1,x_2)-k_{n+1}(x_1,x_2)]^2$ about the exceptional point (x_1^*,x_2^*). When these results are substituted in Eq. (30), we get

$$\hat{k}_{n,n+1}(x_1,x_2) = k_d(x_1^*,x_2^*) + \Delta k_d(x_1,x_2) + \sqrt{\frac{1}{4}[c_1^{(1)}(x_1-x_1^*)+c_2^{(1)}(x_2-x_2^*)]} \tag{34}$$

for (x_1,x_2) in a neighborhood 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.

C. Energy-pole position function

Let us take the square of both sides of Eq. (30), multiplying them by $(\hbar^2/2\mu)$ and recalling $\mathcal{E}_n=(\hbar^2/2\mu)k_n^2$, in the approximation of Eq. (34), we get

$$\hat{\mathcal{E}}_{n,n+1}(x_1,x_2) = \mathcal{E}_d(x_1^*,x_2^*) + \Delta\mathcal{E}_d(x_1,x_2) + \hat{\epsilon}_{n,n+1}(x_1,x_2), \tag{35}$$

where

$$\hat{\epsilon}_{n,n+1}(x_1,x_2) = \sqrt{\frac{1}{4}[(\vec{R}\cdot\vec{\xi})+i(\vec{I}\cdot\vec{\xi})]}. \tag{36}$$

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,

$$\vec{\xi} = \begin{pmatrix}\xi_1\\ \xi_2\end{pmatrix} = \begin{pmatrix}x_1-x_1^*\\ x_2-x_2^*\end{pmatrix}, \tag{37}$$

$$\vec{R} = \begin{pmatrix}\mathrm{Re}\, C_1^{(1)}\\ \mathrm{Re}\, C_2^{(1)}\end{pmatrix}, \quad \vec{I} = \begin{pmatrix}\mathrm{Im}\, C_1^{(1)}\\ \mathrm{Im}\, C_2^{(1)}\end{pmatrix}. \tag{38}$$

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

$$\mathrm{Re}\,\hat{\epsilon}_{n,n+1}(x_1,x_2) = \pm\frac{1}{2\sqrt{2}}\left[{}_+\sqrt{(\vec{R}\cdot\vec{\xi})^2+(\vec{I}\cdot\vec{\xi})^2}+\vec{R}\cdot\vec{\xi}\right]^{1/2}, \tag{39}$$

$$\mathrm{Im}\,\hat{\epsilon}_{n,n+1}(x_1,x_2) = \pm\frac{1}{2\sqrt{2}}\left[{}_+\sqrt{(\vec{R}\cdot\vec{\xi})^2+(\vec{I}\cdot\vec{\xi})^2}-\vec{R}\cdot\vec{\xi}\right]^{1/2}, \tag{40}$$

and

$$\mathrm{sgn}(\mathrm{Re}\,\hat{\epsilon}_{n,n+1})\mathrm{sgn}(\mathrm{Im}\,\hat{\epsilon}_{n,n+1}) = \mathrm{sgn}(\vec{I}\cdot\vec{\xi}). \tag{41}$$

It follows from Eq. (39) that $\mathrm{Re}\,\hat{\epsilon}_{n,n+1}(x_1,x_2)$ 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 $(\mathrm{Re}\,\hat{\epsilon}_{n,n+1},\xi_1,\xi_2)$. The two branches of $\mathrm{Re}\,\hat{\epsilon}_{n,n+1}(\xi_1,\xi_2)$ 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 Eq. (39) 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

$$\vec{I} \cdot \hat{\xi}_c = 0 \quad \text{and} \quad \vec{R} \cdot \hat{\xi}_c = -|\vec{R} \cdot \hat{\xi}_c|. \tag{42}$$

A similar analysis shows that the imaginary part of the energy-pole position function, $\text{Im}\, \mathcal{E}_{n,n+1}(x_1, x_2)$, 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. (42).

The branch cut lines, $\mathcal{L}_R$ and $\mathcal{L}_I$, are in orthogonal subspaces of a four-dimensional Euclidean space with coordinates $(\text{Re}\, \epsilon_{n,n+1}, \text{Im}\, \epsilon_{n,n+1}, \xi_1, \xi_2)$, 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

$$\begin{aligned}\hat{\mathcal{E}}_m(\xi_1, \xi_2) = {} & \mathcal{E}_d(0,0) + \Delta\mathcal{E}_{n,n+1}(\xi_1, \xi_2) \\ & + \sigma_R^{(m)} \frac{1}{2\sqrt{2}} [{}_{+}\sqrt{(\vec{R}\cdot\vec{\xi})^2 + (\vec{I}\cdot\vec{\xi})^2} + (\vec{R}\cdot\vec{\xi})]^{1/2} \\ & + i\sigma_I^{(m)} \frac{1}{2\sqrt{2}} [{}_{+}\sqrt{(\vec{R}\cdot\vec{\xi})^2 + (\vec{I}\cdot\vec{\xi})^2} - (\vec{R}\cdot\vec{\xi})]^{1/2},\end{aligned} \tag{43}$$

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

$$\sigma_R^{(n)} = -\sigma_R^{n+1} = \frac{\text{Re}\, \mathcal{E}_n - \text{Re}\, \mathcal{E}_{n+1}}{|\text{Re}\, \mathcal{E}_n - \text{Re}\, \mathcal{E}_{n+1}|}, \tag{44}$$

$$\sigma_I^{(n)} = -\sigma_I^{n+1} = \frac{\text{Im}\, \mathcal{E}_n - \text{Im}\, \mathcal{E}_{n+1}}{|\text{Im}\, \mathcal{E}_n - \text{Im}\, \mathcal{E}_{n+1}|}. \tag{45}$$

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

$$\text{Re}\, \mathcal{E}_n(x_1, x_2) = \text{Re}\, \mathcal{E}_{n+1}(x_1, x_2) \tag{46}$$

but

$$\text{Im}\, \mathcal{E}_n(x_1, x_2) \neq \text{Im}\, \mathcal{E}_{n+1}(x_1, x_2). \tag{47}$$

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

$$\text{Im}\, \mathcal{E}_n(x_1, x_2) = \text{Im}\, \mathcal{E}_{n+1}(x_1, x_2), \tag{48}$$

but

$$\text{Re}\, \mathcal{E}_n(x_1, x_2) \neq \text{Re}\, \mathcal{E}_{n+1}(x_1, x_2). \tag{49}$$

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, a variation of the vector of parameters splits the degenerate eigenvalue $\mathcal{E}_d$ in two non-degenerate eigenvalues $\mathcal{E}_n$ and $\mathcal{E}_{n+1}$. In this case, perturbation series expansion of the eigenvalues $\mathcal{E}_n, \mathcal{E}_{n+1}$ about $\mathcal{E}_d$ takes the form of a Puiseux series

$$\begin{aligned}\mathcal{E}_{n,n+1}(x_1, x_2) = {} & \mathcal{E}_d(x_1^*, x_2^*) + |\xi|^{1/2} \sqrt{\frac{1}{4}[(\vec{R}\cdot\hat{\xi}) + i(\vec{I}\cdot\hat{\xi})]} \\ & + \Delta\mathcal{E}_d(x_1, x_2) + O(|\xi|^{3/2})\end{aligned} \tag{50}$$

with fractional powers $|\xi|^{j/2}$, $j = 0, 1, 2, \ldots$ of the small parameter $|\xi|$ [35,37].

VI. UNFOLDING OF THE DEGENERACY POINT

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

$$\begin{aligned}\hat{f}_{doub}(-k; \xi_1, \xi_2) = {} & \{k - [k_d(0,0) + \Delta^{(1)} k_d(\xi_1, \xi_2)]\}^2 \\ & - \tfrac{1}{4}[(\vec{\mathcal{R}}\cdot\vec{\xi}) + i(\vec{\mathcal{I}}\cdot\vec{\xi})],\end{aligned} \tag{51}$$

and

$$\Delta^{(1)} k_d(x_1, x_2) = \sum_{i=1}^{2} d_i^{(1)} \xi_i. \tag{52}$$

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

$$f(-k; \xi_1, \xi_2) \approx \frac{1}{g_{n,n+1}(k_d; 0,0)} \hat{f}_{doub}(-k; \xi_1, \xi_2), \tag{53}$$

the term $[g_{n,n+1}(k_d, 0, 0)]^{-1}$ may be understood as a nonvanishing 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 [36,38] of $f(-k; \xi_1, \xi_2)$ with the following features.

(1) It includes all possible small perturbations of the degeneracy conditions

$$f(-k_d; \xi_1, \xi_2) = 0, \quad \left(\frac{\partial f(-k; \xi_1, \xi_2)}{\partial k}\right)_{k_d} = 0, \tag{54}$$

$$\left(\frac{\partial^2 f(-k; \xi_1, \xi_2)}{\partial k^2}\right)_{k_d} \neq 0 \tag{55}$$

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 [36] 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

$$\hat{k}_{n,n+1}(\xi_1,\xi_2) = k_d + \Delta^{(1)}_{n,n+1}k_d(\xi_1,\xi_2) \pm \left[\tfrac{1}{4}(\vec{\mathcal{R}}\cdot\vec{\xi} + i\vec{\mathcal{I}}\cdot\vec{\xi})\right]^{1/2} \tag{56}$$

and the corresponding energy-pole position function $\hat{\mathcal{E}}_{n,n+1}(\xi_1,\xi_2)$ given in Eq. (35).

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. (43)–(45), 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.

VII. 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 $\mathcal{E}_n(\xi_1,\bar{\xi}_2)-\mathcal{E}_{n+1}(\xi_1,\bar{\xi}_2)=\Delta E-i(1/2)\Delta\Gamma$ is measured as a 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,

$$\hat{\mathcal{E}}_n(\xi_1,\bar{\xi}_2^{(i)}) - \hat{\mathcal{E}}_{n+1}(\xi_1,\bar{\xi}_2^{(i)}) = \hat{\epsilon}_{n,n+1}(\xi_1,\bar{\xi}_2^{(i)}) \tag{57}$$

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 nondegenerate 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,

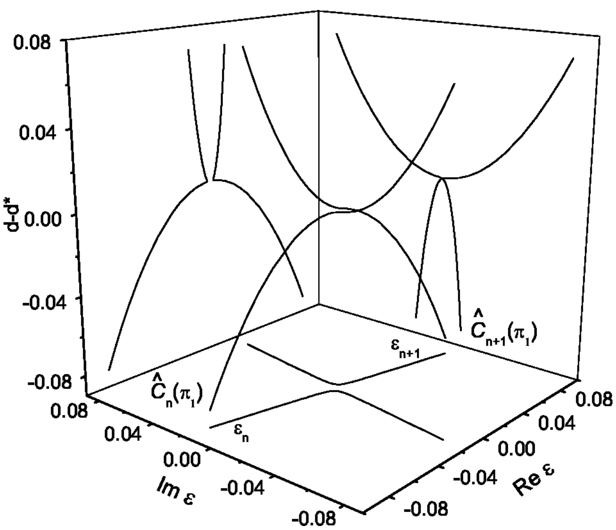

FIG. 1. The curves $\hat{C}_n(\pi_1)$ and $\hat{C}_{n+1}(\pi_1)$ are the trajectories traced by the points $\hat{\mathcal{E}}_n(\xi_1,\bar{\xi}_2^{(1)})$ and $\hat{\mathcal{E}}_{n+1}(\xi_1,\bar{\xi}_2^{(1)})$ on the hypersurface $\hat{\mathcal{E}}_{n,n+1}(\xi_1,\bar{\xi}_2^{(1)})$ when the point $(\xi_1,\bar{\xi}_2^{(1)})$ 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 $\xi_{1,c}<\xi_1^*=0$ and $\bar{\xi}_2^{(1)}<\xi_2^*=0$. The projections of $\hat{C}_n(\pi_1)$ and $\hat{C}_{n+1}(\pi_1)$ on the plane $(\mathrm{Im}\,\mathcal{E},\xi_1)$ 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 $(\mathrm{Re}\,\mathcal{E},\xi_1)$ 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 $(\mathrm{Re}\,\mathcal{E},\mathrm{Im}\,\mathcal{E})$ are the trajectories of the S-matrix poles in the complex energy plane. In the figure, $\xi_1=d-d^*$.

$$\pi_i{:}\xi_{1,i}\leqslant\xi_1\leqslant\xi_{1,f},\quad \xi_2=\bar{\xi}_2^{(i)} \tag{58}$$

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 E_3 with Cartesian coordinates $(\mathrm{Re}\,\epsilon,\mathrm{Im}\,\epsilon,\xi_1)$, see Figs. 1–3. The projections of the curves $\hat{C}_n(\pi_i)$ and $\hat{C}_{n+1}(\pi_i)$ on the planes $(\mathrm{Re}\,\epsilon,\xi_1)$ and $(\mathrm{Im}\,\epsilon,\xi_1)$ are

$$\mathrm{Re}[\hat{C}_m(\pi_i)] = \mathrm{Re}\,\hat{\mathcal{E}}_m(\xi_1,\bar{\xi}_2^{(i)}),\quad m=n,n+1 \tag{59}$$

and

$$\mathrm{Im}[\hat{C}_m(\pi_i)] = \mathrm{Im}\,\hat{\mathcal{E}}_m(\xi_1,\bar{\xi}_2^{(i)}),\quad m=n,n+1, \tag{60}$$

respectively.

From Eqs. (43)–(45), and keeping $\xi_2=\bar{\xi}_2^{(i)}$, we obtain

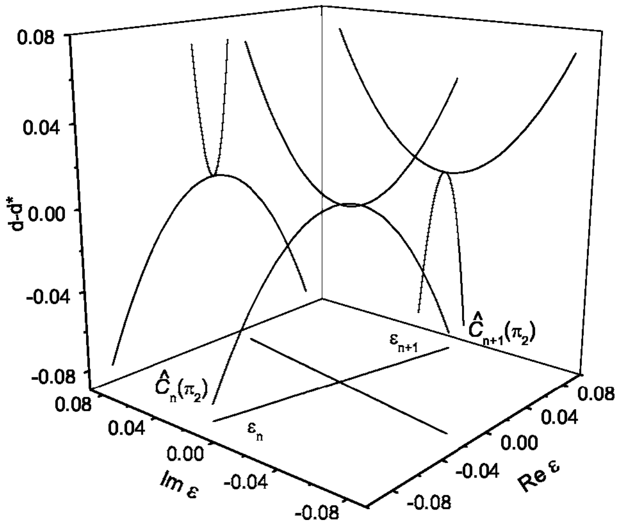

FIG. 2. The curves $\hat{C}_n(\pi_2)$ and $\hat{C}_{n+1}(\pi_2)$ are the trajectories of the points $\hat{\mathcal{E}}_n(\xi_1,\xi_2^*)$ and $\hat{\mathcal{E}}_{n+1}(\xi_1,\xi_2^*)$ on the hypersurface $\hat{\mathcal{E}}_{n,n+1}(\xi_1,\xi_2)$ when the point (ξ_1,ξ_2^*) moves along a straight line path 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 $(\mathrm{Re}\,\mathcal{E},\xi_1)$ and $(\mathrm{Im}\,\mathcal{E},\xi_1)$ 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 $(\mathrm{Re}\,\mathcal{E},\mathrm{Im}\,\mathcal{E})$ 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 $S(E)$.

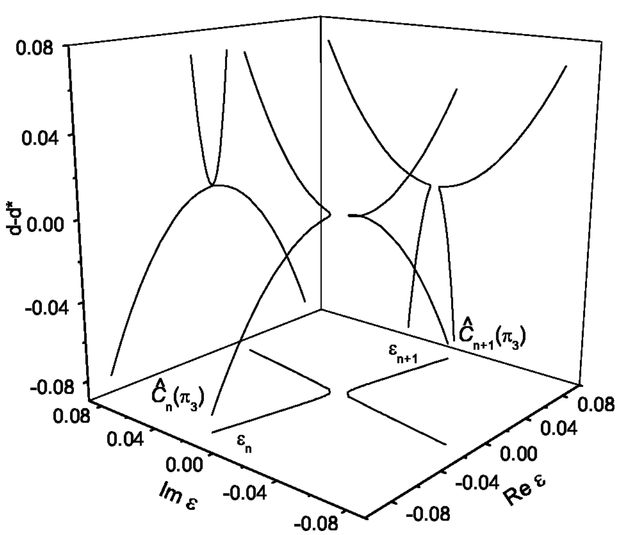

FIG. 3. The curves $\hat{C}_n(\pi_3)$ and $\hat{C}_{n+1}(\pi_3)$ are the trajectories traced by the points $\hat{\mathcal{E}}_n(\xi_1,\bar{\xi}_2^{(3)})$ and $\hat{\mathcal{E}}_{n+1}(\xi_1,\bar{\xi}_2^{(3)})$ on the hypersurface $\mathcal{E}_{n,n+1}(\xi_1,\bar{\xi}_2^{(3)})$ when the point $(\xi_1,\bar{\xi}_2^{(3)})$ moves along a straight line path π_3 going through the point $(\xi_{1,c},\bar{\xi}_2^{(3)})$ with $\xi_{1,c}>\xi_1^*=0$. 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 $(\mathrm{Re}\,\mathcal{E},\xi_1)$ show a crossing, but the projections on the planes $(\mathrm{Im}\,\mathcal{E},\xi_1)$ and $(\mathrm{Re}\,\mathcal{E},\mathrm{Im}\,\mathcal{E})$ do not cross. In the figure, $\xi_1=d-d^*$.

$$\Delta E = E_n - E_{n+1} = (\mathrm{Re}\,\hat{\mathcal{E}}_n - \mathrm{Re}\,\hat{\mathcal{E}}_{n+1})\big|_{\xi_2=\bar{\xi}_2^{(i)}}$$
$$= \frac{\sigma_R^{(n)}\sqrt{2}}{2}\Big[{}_+\sqrt{(\vec{R}\cdot\vec{\xi})^2+(\vec{I}\cdot\vec{\xi})^2}+(\vec{R}\cdot\vec{\xi})\Big]^{1/2}\Bigg|_{\xi_2=\bar{\xi}_2^{(i)}} \qquad (61)$$

and

$$\Delta\Gamma = (\Gamma_n - \Gamma_{n+1})$$
$$= 2[\mathrm{Im}\,\mathcal{E}_{n+1} - \mathrm{Im}\,\mathcal{E}_n]$$
$$= -\sigma_I^{(n)}\sqrt{2}\Big[{}_+\sqrt{(\vec{R}\cdot\vec{\xi})^2+(\vec{I}\cdot\vec{\xi})^2}-(\vec{R}\cdot\vec{\xi})\Big]^{1/2}\Big|_{\xi_2=\bar{\xi}_2^{(i)}}. \qquad (62)$$

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. (41), we get

$$\Delta E\Delta\Gamma = -(\vec{I}\cdot\vec{\xi})\big|_{\xi_2=\bar{\xi}_2^{(i)}} \qquad (63)$$

and taking the differences of the squares of the left-hand sides of Eqs. (61) and (62), we get

$$(\Delta E)^2 - \tfrac{1}{4}(\Delta\Gamma)^2 = (\vec{R}\cdot\vec{\xi})\big|_{\xi_2=\bar{\xi}_2^{(i)}}. \qquad (64)$$

At a crossing of energies ΔE vanishes, and at a crossing of widths $\Delta\Gamma$ vanishes. Hence the relation found in Eq. (63) 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. (61) and (62),

(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 von Brentano and his collaborators in a series of beautiful experiments [15–17].

VIII. 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

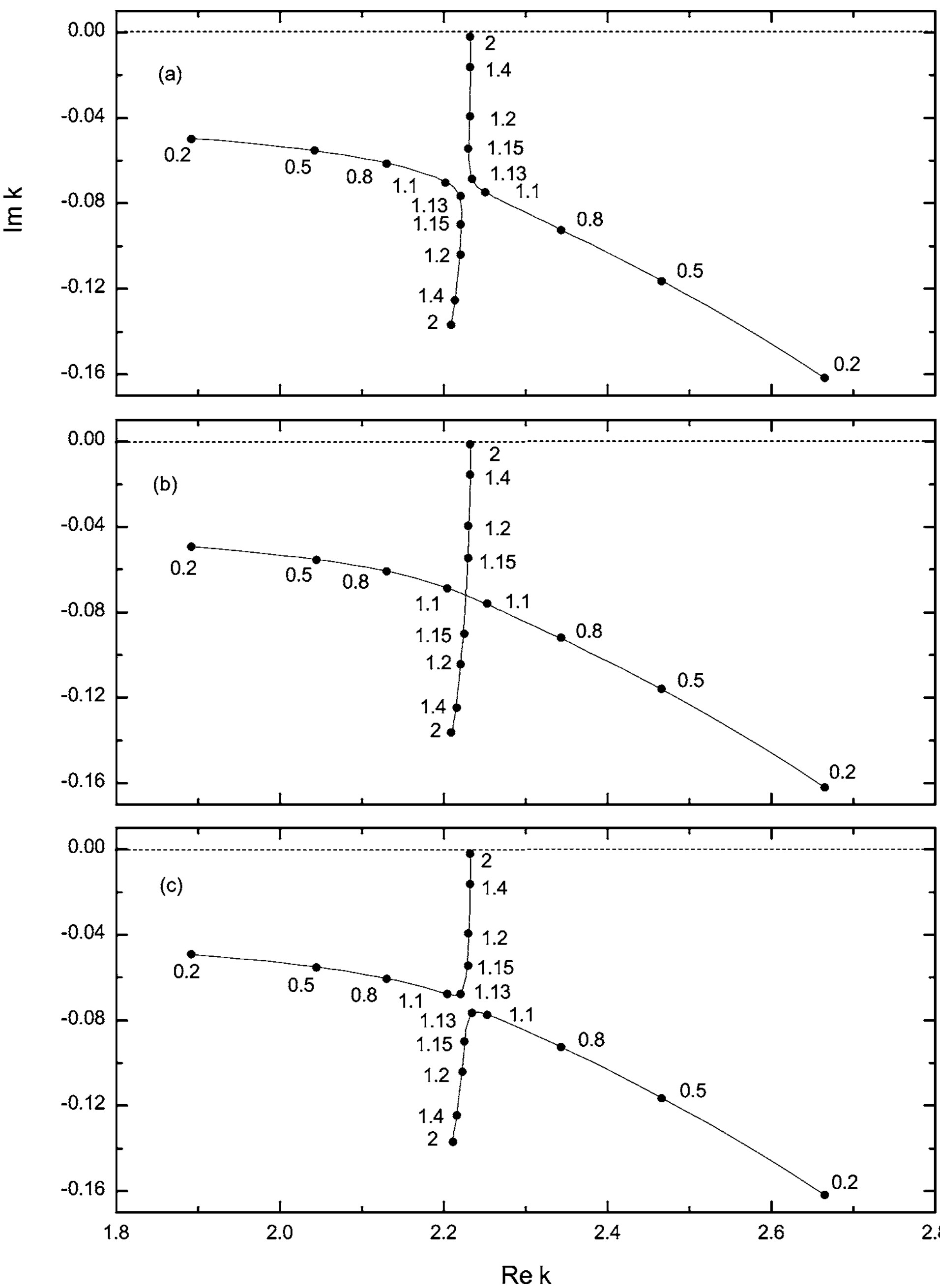

FIG. 4. Trajectories of the poles of the scattering matrix, $S(k)$ of an isolated doublet of resonances in a double barrier potential [27], close to a degeneracy of unbound states. The control parameters are the width d of the inner barrier and the depth, V_3, of the outer well. The trajectories are 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 $(\xi_1,\xi_2)=(d-d^*,V_3-V_3^*)$.

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 $(\mathrm{Re}\,\epsilon,\mathrm{Im}\,\epsilon)$, see Figs. 1–3.

An equation for the trajectories of the S-matrix poles in the complex energy plane is obtained by eliminating ξ_1 between $\mathrm{Re}\,\hat{\mathcal{E}}_n(\xi_1,\bar{\xi}_2^{(i)})$ and $\mathrm{Im}\,\hat{\mathcal{E}}_n(\xi_1,\bar{\xi}_2^{(i)})$, Eqs. (43)–(45).

A straightforward calculation gives

$$(\mathrm{Re}\,\hat{\mathcal{E}}_n)^2 - 2\cot\phi_1(\mathrm{Re}\,\hat{\mathcal{E}}_n)(\mathrm{Im}\,\hat{\mathcal{E}}_n) - (\mathrm{Im}\,\hat{\mathcal{E}}_n)^2 - \tfrac{1}{4}(\vec{R}\cdot\vec{\xi}_c^{(i)}) = 0, \tag{65}$$

where

$$\cot\phi_1 = \frac{R_1}{I_1} \tag{66}$$

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

$$(\vec{I}\cdot\vec{\xi}_c)\big|_{\xi_2=\bar{\xi}_2^{(i)}} = 0, \tag{67}$$

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

The discriminant of Eq. (65), $4(\cot^2\phi_1+1)$, is positive. Therefore, close to the crossing point, the trajectories of the S-matrix poles are the branches of a hyperbola defined by Eq. (65).

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

$$\mathrm{Im}\,\mathcal{E}^{(I)} = \tan\frac{\phi_1}{2}\,\mathrm{Re}\,\mathcal{E}^{(I)} \tag{68}$$

and

$$\mathrm{Im}\,\mathcal{E}^{(II)} = -\cot\frac{\phi_1}{2}\,\mathrm{Re}\,\mathcal{E}^{(II)}. \tag{69}$$

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. (65), 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 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. 4(a).

(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. 4(b).

(3) Trajectories of type III, 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. 4(c).

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 vice versa, 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 Vanroose, Van Leuven Arickx and Broeckhove [18] who discussed an example of this phenomenon in the *S*-matrix poles in a two-channel model, Vanroose [20] and Hernández, Jáuregui, and 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.

IX. 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 a function of the control parameters of the system, we derived a two-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, at the exceptional point, and branch cuts in its real and imaginary parts extending from the exceptional point in opposite directions in parameter space. 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. 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 vicinity of the crossing point.

ACKNOWLEDGMENTS

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

[1] E. Hernández, A. Jáuregui, and A. Mondragón, Phys. Rev. A **67**, 022721 (2003).
[2] J. von Neumann and E. P. Wigner, Phys. Z. **30**, 467 (1929).
[3] E. Teller, J. Phys. Chem. **41**, 109 (1937).
[4] M. V. Berry, in *Chaotic Behaviour in Quantum Systems*, Vol. 120 of *NATO ASI Series B*, edited by G. Casati (Plenum, New York, 1985), p. 123.
[5] D. R. Yarkoni, Rev. Mod. Phys. **68**, 985 (1996).
[6] H. Friedrich and D. Wintgen, Phys. Rev. A **32**, 3231 (1985).
[7] A. Mondragón and E. Hernández, J. Phys. A **26**, 5595 (1993).
[8] E. Hernández and A. Mondragón, Phys. Lett. B **326**, 1 (1994).
[9] P. von Brentano, Phys. Lett. B **238**, 1 (1990).
[10] P. von Brentano, Phys. Rep. **264**, 57 (1996).
[11] K. E. Lassila and V. Ruuskanen, Phys. Rev. Lett. **17**, 490 (1966).
[12] P. L. Knight, Phys. Lett. A **72**, 309 (1979).
[13] N. J. Kylstra and C. J. Joachain, Europhys. Lett. **36**, 657 (1996).
[14] N. J. Kylstra and C. J. Joachain, Phys. Rev. A **57**, 412 (1998).
[15] P. von Brentano and M. Philipp, Phys. Lett. B **454**, 171 (1999).
[16] M. Philipp, P. von Brentano, G. Pascovici, and A. Richter, Phys. Rev. E **62**, 1922 (2000).
[17] P. von Brentano, Rev. Mex. Fis. **48**, Suppl 2, 1 (2000).
[18] W. Vanroose, P. Van Leuven, F. Arickx, and J. Broeckhove, J. Phys. A **30**, 5543 (1997).
[19] E. Hernández, A. Jáuregui, and A. Mondragón, J. Phys. A **33**, 4507 (2000).
[20] W. Vanroose, Phys. Rev. A **64**, 062708 (2001).
[21] E. Hernández, A. Jáuregui, and A. Mondragón, Rev. Mex. Fis. **38**, Suppl 2, 128 (1992).
[22] A. Mondragón and E. Hernández, J. Phys. A **29**, 2567 (1996).
[23] A. Mondragón and E. Hernández, in *Irreversibility and Causality: Semigroup and Rigged Hilbert Space*, Vol. 504 of *Lecture Notes in Physics*, edited by A. Bohm, D.-H. Doebner, and P. Kielanowski (Springer-Verlag, Berlin, 1998), p. 257.
[24] W. D. Heiss, Eur. Phys. J. D **7**, 1 (1999).
[25] C. Dembowski, H.-D. Gräf, H. L. Harney, A. Heine, W. D. Heiss, H. Rehfeld, and A. Richter, Phys. Rev. Lett. **86**, 787 (2001).
[26] C. Dembowski, B. Dietz, H.-D. Gräf, H. L. Harney, A. Heine, W. D. Heiss, and A. Richter, Phys. Rev. Lett. **90**, 034101 (2003).
[27] E. Hernández, A. Jáuregui, and A. Mondragón, Rev. Mex. Fis. **49**, Suppl. 4 60 (2003).
[28] H. J. Korsch and S. Mossmann, J. Phys. A **36**, 2139 (2003).
[29] F. Keck, H. J. Korsch, and S. Mossmann, J. Phys. A **36**, 2125 (2003).
[30] I. Antoniou, M. Gadella, and G. Pronko, J. Math. Phys. **39**, 2429 (1998).
[31] A. Bohm, M. Loewe, S. Maxson, P. Patuleanu, C. Püntmann, and M. Gadella, J. Math. Phys. **38**, 6072 (1997).
[32] R. G. Newton, *Scattering Theory of Waves and Particles*, 2nd ed. (Springer-Verlag, New York, 1982), Chap. 12.
[33] A. Bohm, *Quantum Mechanics: Foundations and Applications*, 3rd ed., *Texts and Monographs in Physics* (Springer-Verlag, New York, 1993), Chap. XXI.
[34] A. Bohm and M. Gadella, *Dirac Kets, Gamow Vectors and Gel'fand Triplets. The Rigged Hilbert Space Formulation of Quantum Mechanics*, Vol. 348 of *Lecture Notes in Physics* (Springer-Verlag, Berlin, 1989).
[35] S. G. Krantz and H. R. Parks, *The Implicit Function Theorem* (Birkhäuser, Boston, 2002), Chap. 5.
[36] R. Seydel, *Practical Bifurcation and Stability Analysis. IAM5*, 2nd ed. (Springer-Verlag, New York, 1991), Chap. 8.
[37] T. Kato, *Perturbation Theory for Linear Operators*, 2nd ed. (Springer-Verlag, Berlin, 1980), p. 65.
[38] T. Poston and I. Stewart, *Catastrophe Theory and its Applications* (Pitman, Boston, 1978), Chap. 8.