

Exceptional points and non-Hermitian degeneracy of resonances in a two-channel model

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We study the mixing and degeneracy of two unbound energy eigenstates (resonances) in a two coupled channel model of scattering and reactions. We derive the necessary and sufficient conditions for existence of an exceptional point in the extended spectrum of bound and resonance energy eigenvalues in this model and show that these are not the same as in the single channel case. When these conditions are satisfied, in the complex energy plane, the two simple resonance poles of the scattering matrix merge into one double pole at the exceptional point. In parameter space, the surface of the eigenenergies has a branch point of square root type and branch cuts in its real and imaginary parts that start at the exceptional point and extend in opposite directions. The rich phenomenology of crossings and anticrossings of energies and widths of the doublet of unbound states, as well as the changes of identity of the poles of the scattering matrix observed when one control parameter is varied while the other is kept constant, is fully explained in terms of sections of the eigenenergy surfaces.

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I. INTRODUCTION

In quantum scattering, an exceptional point occurs when two resonance energy eigenvalues coalesce and give rise to a double pole of the \mathbf{S} matrix [1–6]. More precisely, when the coalescing energy eigenvalues can be mathematically described as two branches of the same analytic function of two or more control parameters. In this picture, the exceptional point is a branch point of the multivalued function describing the complex resonance energy eigenvalues in parameter space [7–9]. Exceptional points have been found or observed in a wide variety of physical systems. Among them are acoustical systems [10], the spectra of the Hydrogen atom [11], and systems found in atoms in optical lattices [12,13], complex atoms in laser fields [14], and laser driven molecular photodissociation dynamics [15–18]. They have also been found in electron-molecule collisions [19], nuclear physics [4,20,21], chaotic optical microcavities [22], and the quantum phase transitions of superfluids and superconductors [23–25]. The experimental determination of an exceptional point in the resonance spectrum of a microwave cavity was described in terms of the eigenvalues and eigenvectors of a complex symmetric non-Hermitian 2×2 Hamiltonian matrix with its entries depending on the control parameters of the experimental setup [26–31]. Exceptional points also occur in optics [8,32] and in quantum mechanical systems such as the scattering of a beam of particles by a double barrier potential [33–36], periodic quasireactly soluble PT-symmetric potentials [37,38], and the mass spectrum of the heavy neutral Higgs bosons in the minimal supersymmetric extension of the standard model [39].

In this work we are concerned with some physical manifestations of the exceptional point phenomenon in the mixing and degeneracy of two unbound energy eigenstates in an isolated doublet of quantum resonances. The discussion is made in the framework of a two-coupled-channel model of quantum scattering and reactions in collisions of complex quantum systems [40].

In single channel scattering, a necessary and sufficient condition for the existence of an exceptional point at $E_{EP} = k_{EP}^2$,

with k_{EP} complex and $\text{Im}k_{EP} < 0$, is the vanishing of the Jost function and its first derivative with respect to k at that point. In the case of scattering in a two-coupled-channel system, the vanishing of the Jost determinant is a necessary but not a sufficient condition for the existence of an exceptional point. In this work, we derive the necessary and sufficient conditions for the existence of an exceptional point in the extended spectrum of resonance energy eigenvalues of a two-channel model of scattering and reactions. When these conditions are satisfied, the two degenerating complex energy eigenvalues coalesce, producing a double pole of the scattering matrix in the complex energy plane and a branch point singularity in the surface that represents the complex energy eigenvalues in parameter space. We will also show that, when the Jost determinant and its first derivative with respect to the wave number vanish at $k = k_n$, but the third condition for existence of an exceptional point in the coupled channel model is not satisfied, the scattering matrix has only a simple pole at $k = k_n$, which, of course, is not an exceptional point although the two zeros of the Jost determinant coincide at the same value $k = k_n$.

In the laboratory, when the control parameters are varied in a neighborhood of the critical values corresponding to the exceptional point, the branch point singularity of the eigenenergy surface manifests itself through a rich phenomenology of crossings and anticrossings of energies and widths [41], as well as the so called “change of identity” [42] of the poles of the \mathbf{S} matrix.

The characterization of the singularities of the energy surfaces at a degeneracy of unbound states in parameter space arises naturally also in connection with the Berry phase of unbound states predicted by Hernández *et al.* [43–45] and later and independently by Heiss [46]; see also the work by Mailybaev *et al.* [47]. The Berry phase of two resonant states was measured by Richter and the Darmstadt group [30,48].

The theoretical treatment of crossings, anticrossings, and changes of identity of resonance states presented in this paper is a generalization of a previous discussion on resonance degeneracy of unbound states in single channel scattering [9,35,44] to the case of mixing degeneracy and exceptional points in a multichannel model of scattering and reactions in

collisions of complex quantum systems. The plan of the paper is as follows: In Secs. II, III, and IV, we give a brief reminder of some relevant concepts on resonances in multichannel scattering. Sections V and VI are devoted to a discussion of doublets of resonances and degeneracy of resonances and exceptional points in a multichannel model of scattering and reactions. In Sec. VII, we show that the pole position function of the isolated doublet of unbound states has a branch point singularity at the exceptional point in parameter space. The singularity of the energy surface at the exceptional point is also characterized as a branch point in Sec. VIII, where we also introduce a contact equivalent approximant to the energy surface at the exceptional point. The numerical computation of the exceptional point is briefly described in Sec. IX. Section X is devoted to a discussion of crossings and anticrossings of resonance energies and widths, as well as the changes of identity of the poles of the \mathbf{S} matrix, in terms of sections of the energy surfaces. We end our paper with a short summary and some conclusions.

II. MULTICHANNEL SCATTERING

We start by defining our notation and briefly recalling some notions of scattering theory that are used below.

Let us consider the scattering of a spinless, structureless projectile on a spinless spherically symmetric target which has N bound states. The Hamiltonian of the system may be written as the sum of three terms,

$$H = H_0 + H_{\text{tar}} + H_{\text{int}}, \quad (1)$$

where H_0 is the Hamiltonian of the free relative motion of target and projectile, H_{tar} is the Hamiltonian of the target, and H_{int} is the interaction Hamiltonian between target and projectile.

By expanding the wave function $\Psi(\vec{x}_{\text{tar}}, \vec{r})$ of the total system in terms of the complete set of energy eigenfunctions of the target $\{\eta_{\mathcal{E}}(\vec{x}_{\text{tar}})\}$ we obtain

$$\Psi(\vec{x}_{\text{tar}}, \vec{r}) = \sum_{\alpha} \eta_{\mathcal{E}_{\alpha}}(\vec{x}_{\text{tar}}) \psi_{\alpha}(\vec{r}) + \int d\mathcal{E}' \eta_{\mathcal{E}'}(\vec{x}_{\text{tar}}) \psi_{\mathcal{E}'}(\vec{r}). \quad (2)$$

In this expression, the subindices \mathcal{E}_{α} and \mathcal{E}' are the energy eigenvalues in the discrete and continuum parts of the energy spectrum of the target, \vec{x}_{tar} is a shorthand for the coordinates of the constituent particles of the target, and \vec{r} is the relative distance between projectile and target. All position coordinates, \vec{x}_{tar} and \vec{r} , are measured from the center of mass of the total system.

Insertion of the expansion (2) of $\Psi(\vec{x}_{\text{tar}}, \vec{r})$ in the Schrödinger equation of the total system

$$H\Psi = E\Psi \quad (3)$$

gives us

$$\begin{aligned} & \sum_{\alpha'} \left[-\frac{\hbar^2}{2m} \nabla^2 + \mathcal{E}_{\alpha'} + H_{\text{int}}(\vec{x}_{\text{tar}}, \vec{r}) \right] \eta_{\mathcal{E}_{\alpha'}}(\vec{x}_{\text{tar}}) \psi_{\alpha'}(\vec{r}) \\ & + \int d\mathcal{E}' \left[-\frac{\hbar^2}{2m} \nabla^2 + \mathcal{E}' + H_{\text{int}}(\vec{x}_{\text{tar}}, \vec{r}) \right] \eta_{\mathcal{E}'}(\vec{x}_{\text{tar}}) \psi_{\mathcal{E}'}(\vec{r}) \\ & = E \left(\sum_{\alpha'} \eta_{\mathcal{E}_{\alpha'}}(\vec{x}_{\text{tar}}) \psi_{\alpha'}(\vec{r}) + \int d\mathcal{E}' \eta_{\mathcal{E}'}(\vec{x}_{\text{tar}}) \psi_{\mathcal{E}'}(\vec{r}) \right). \end{aligned} \quad (4)$$

We now multiply through by $\eta_{\mathcal{E}_{\alpha}}^*(\vec{x}_{\text{tar}})$ and integrate over the target coordinates. Because the functions $\eta_{\alpha}(\vec{x}_{\text{tar}})$ are orthogonal this gives the following infinite set of coupled equations

$$\begin{aligned} & -\frac{\hbar^2}{2m} \nabla^2 \psi_{\alpha}(\vec{r}) + \sum_{\alpha'} V_{\alpha, \alpha'}(\vec{r}) \psi_{\alpha'}(\vec{r}) \\ & + \int V_{\alpha, \mathcal{E}'}(\vec{r}) \psi_{\mathcal{E}'}(\vec{r}) d\mathcal{E}' = (E - \mathcal{E}_{\alpha}) \psi_{\alpha}(\vec{r}), \end{aligned} \quad (5)$$

where

$$V_{\alpha, \alpha'}(\vec{r}) = \int \eta_{\mathcal{E}, \alpha}^*(\vec{x}_{\text{tar}}) H_{\text{int}}(\vec{x}_{\text{tar}}, \vec{r}) \eta_{\mathcal{E}, \alpha'}(\vec{x}_{\text{tar}}) d\vec{\tau}_{\text{tar}}. \quad (6)$$

On the right-hand side of (6), integration is made over all coordinates of the constituent particles in the target.

Under certain conditions, it may be a good approximation to retain in the summation over excited target states only a small number N of discrete terms and none of the continuum [40]. For example, many nuclei have a single strongly excitable low-lying collective state, such as the 2^+ state in ^{12}C or ^{24}Mg . This means that one can treat the scattering of α particles off such nuclei in a two state approximation, including just the ground state and this one collective state. In the case of a target which has only two bound states, $N = 2$, and separating the angular part, the set of coupled equations (5) reduces to the following set of coupled radial Schrödinger equations,

$$\mathbf{H}_{\ell} \Psi_{\ell}(k, r) = \mathbf{E} \Psi_{\ell}(k, r), \quad (7)$$

with

$$\mathbf{H}_{\ell} = -\frac{\hbar^2}{2m} \left(\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} \right) \mathbf{1} + \mathbf{V}, \quad (8)$$

where r is the radial coordinate, $\mathbf{1}$ is the 2×2 identity matrix, and \mathbf{V} is a 2×2 real symmetric matrix,

$$\mathbf{V} = \begin{pmatrix} V_{11}(r) & V_{12}(r) \\ V_{12}(r) & V_{22}(r) \end{pmatrix}, \quad (9)$$

and $\Psi_{\ell}(k, r)$ may be either a vector valued solution or a matrix valued solution. By \mathbf{E} we denote the diagonal matrix with the nonvanishing entries E_i , $\mathbf{E} = \text{diag}(E, E - \epsilon)$. The wave numbers k_i are related to the center of mass energy and the threshold of the inelastic channel Q by

$$k_1^2 = k^2 = \frac{2m}{\hbar^2} E, \quad k_2 = \sqrt{\frac{2m}{\hbar^2} (E - \epsilon)} = \sqrt{k^2 - Q}. \quad (10)$$

We assume that the potential terms, $V_{11}(r)$, $V_{22}(r)$, and $V_{12}(r)$, are short ranged and that the condition

$$\int_0^{\infty} \exp(\epsilon r) |V_{ij}(r)| dr < \infty, \quad (11)$$

is satisfied for any real $\epsilon > 0$. Under such assumptions, the Schrödinger equation (7) has two 2×2 matrix valued solutions $\mathbf{F}_{\ell}^{\pm}(k, r)$ such that

$$\lim_{r \rightarrow \infty} \mathbf{F}_{\ell}^{\pm}(k, r) = h_{\ell}^{\pm}(k, r) \approx \text{diag} \left(\exp \left[\pm i k_1 r - \frac{\ell \pi}{2} \right] \right), \quad (12)$$

where $h_{\ell}^{(\pm)}(kr)$ are the spherical Riccati-Hankel functions of first and second kind, respectively.

The columns of the $\mathbf{F}_\ell^\pm(k, r)$ matrices are the Jost solutions and, form a basis in a four-dimensional solution space of the Schrödinger equation with a given value of E . In general, these solutions are complex and satisfy the symmetry property

$$\mathbf{F}_\ell^\pm(k, r) = \mathbf{F}_\ell^{\pm*}(-k^*, r), \quad (13)$$

where asterisk denotes complex conjugation.

In the following we consider only the case of s -wave scattering, $\ell = 0$, and we will omit the subscript ℓ . We define the 2×2 matrix of the regular solutions $\Phi(k, r)$ by its behavior at the origin. For bounded s -wave potentials, these solutions satisfy

$$\Phi(k, 0) = 0, \quad \Phi'(k, 0) = \mathbf{1}, \quad (14)$$

where prime means derivative with respect to r and $\mathbf{1}$ denotes the 2×2 identity matrix. This definition shows that the columns, $\phi^{(1)}(k, r)$ and $\phi^{(2)}(k, r)$, of the matrix of the regular solution, $\Phi = [\phi^{(1)}, \phi^{(2)}]$, also form a basis in the solution space of the Schrödinger equation. In terms of the incoming and outgoing wave Jost solutions, the matrix of the regular solutions reads

$$\Phi(k, r) = \frac{i}{2} [\mathbf{F}^{(-)}(k, r) \mathbf{k}^{-1} \mathcal{F}^{(-)}(k) - \mathbf{F}^{(+)}(k, r) \mathbf{k}^{-1} \mathcal{F}^{(+)}(k)], \quad (15)$$

where $\mathcal{F}^{(-)}(k)$ and $\mathcal{F}^{(+)}(k)$ are the Jost matrices $\mathcal{F}^{(\pm)}(k) = \mathbf{F}^{(\mp)T}(k, 0)$ and \mathbf{k} is the diagonal matrix of the wave numbers, $\mathbf{k} = \text{diag}(k_1, k_2)$.

For real energies, the 2×2 matrix Φ of the regular solutions is purely real because they satisfy a system of coupled differential equations with real coefficients and real boundary conditions. Even more important for our discussion, since the boundary conditions (14) are independent of k and k_2 , and the potentials satisfy (11), the 2×2 matrix Φ of the regular solutions is an entire function of k and k_2 , for all finite values of these variables.

The 2×2 matrix of the physical solutions $\Psi = [\psi^{(1)}, \psi^{(2)}]$ is defined as the matrix of those solutions which are regular at the origin and have a unit incoming flux only in the i channel. Then the matrix $\Psi(k, r)$ of the physical solutions is obtained from the matrix of the regular solutions Eq. (15) as

$$\Psi(k, r) = \Phi(k, r) [\mathcal{F}^{(-)}(k)]^{-1}. \quad (16)$$

Therefore, the scattering matrix, which is symmetric, reads

$$\mathbf{S}(k) = \mathbf{k}^{-1/2} \mathcal{F}^{(+)}(k) [\mathcal{F}^{(-)}(k)]^{-1} \mathbf{k}^{+1/2}. \quad (17)$$

Bound and resonance energies correspond to zeros of the determinant of the Jost matrix,

$$\mathcal{J}^{(-)}(k_n) = \det[\mathcal{F}^{(-)}(k_n)] = 0. \quad (18)$$

III. TWO CHANNELS COUPLED BY SQUARE WELL POTENTIALS

Doublets of resonances and accidental degeneracy of unbound states may occur in the scattering of a projectile by a target when the interaction gives rise to two regions of wave trapping. In the two-coupled-channel model we are discussing, the two regions of trapping are determined by the

diagonal terms $V_{11}(r)$ and $V_{22}(r)$ in the interaction matrix \mathbf{V} . The coupling term $V_{12}(r)$ allows the mixing and interaction of the resonances in the doublet.

In this section we consider the simple but illustrative case of two $\ell = 0$ channels with constant attractive channel potentials V_{ii} of range a

$$V_{ii}(r) = -|V_{ii}|, \quad i = 1, 2, \quad 0 \leq r \leq a, \quad (19)$$

$$V_{ii}(r) = 0, \quad r > a,$$

coupled by a constant potential barrier of height V_{12}

$$V_{12}(r) = |V_{12}|, \quad 0 \leq r \leq a, \quad (20)$$

$$V_{12}(r) = 0, \quad r > a.$$

In this case, the set of coupled equations (7) and (8) may be written as

$$\frac{d^2 \Psi(k, r)}{dr^2} + \frac{2m}{\hbar^2} (\mathbf{E} - \mathbf{V}) \Psi(k, r) = 0, \quad (21)$$

with \mathbf{V} nonvanishing and independent of r for $0 \leq r \leq a$ and $\mathbf{V} = 0$ for $r > a$.

The Jost regular solutions may be readily computed by diagonalizing the 2×2 matrix $(\mathbf{E} - \mathbf{V})$ by means of the orthogonal transformation \mathbf{O} ,

$$\mathbf{O}(\mathbf{E} - \mathbf{V})\mathbf{O}^T = \mathbf{K} = \frac{\hbar^2}{2m} \text{diag}[K_1^2, K_2^2], \quad (22)$$

where the matrix \mathbf{O} is a function of the wave number k and the potential parameters V_{11} , V_{22} , and V_{12} ,

$$\mathbf{O} = \frac{1}{\sqrt{(K_1^2 - K_2^2)(\mathcal{K}_1^2 - \mathcal{K}_2^2)}} \begin{pmatrix} \mathcal{K}_1^2 - K_2^2 & U_{12} \\ -U_{12} & \mathcal{K}_1^2 - K_2^2 \end{pmatrix}, \quad (23)$$

in this expression

$$\mathcal{K}_1^2 = k^2 - U_{11}, \quad U_{ij} = \frac{2m}{\hbar^2} V_{ij}, \quad i, j = 1, 2. \quad (24)$$

The diagonalization of $(\mathbf{E} - \mathbf{V})$ decouples the system of differential Eq. (21). Therefore, in the internal region, the 2×2 matrix of the Jost regular solutions takes the form

$$\Phi(k, r) = \mathbf{O}(\sin \mathbf{K}r) \mathbf{K}^{-1} \mathbf{O}^T, \quad 0 \leq r \leq a, \quad (25)$$

where

$$\sin \mathbf{K}r = \text{diag}(\sin K_1 r, \sin K_2 r), \quad (26)$$

is the diagonal matrix of the solutions of the decoupled system in the internal region. It may be easily verified that the expression (25) for $\Phi(k, r)$ satisfies the boundary conditions at the origin Eq. (14).

The squares of the internal wave numbers, K_1^2 and K_2^2 , are the solutions of the quadratic equation

$$(K^2 - k^2 + U_{11})(K^2 - k^2 + U_{22} + Q) - U_{12}^2 = 0, \quad (27)$$

obtained by substitution of expression (25) for Φ in Eq. (21). Hence,

$$K_{1,2}^2 = k^2 - \frac{1}{2}(U_{11} + U_{22} + Q) \pm \frac{1}{2} \sqrt{(U_{11} - U_{22} - Q)^2 + 4U_{12}^2}. \quad (28)$$

In the external region, $r > a$, the 2×2 matrix of the regular solutions takes the form

$$\Phi(k, r) = \frac{i}{2} [\exp(-i\mathbf{k}r) \mathbf{k}^{-1} \mathcal{F}^{(-)}(k) - \exp(i\mathbf{k}r) \mathbf{k}^{-1} \mathcal{F}^{(+)}(k)], \quad r > a. \quad (29)$$

The Jost matrices $\mathcal{F}^{(-)}(k)$ and $\mathcal{F}^{(+)}(k)$ are determined by the requirement of continuity of $\Phi(k, r)$ and its first derivative $\Phi'(k, r)$ at $r = a$. From Eqs. (25) and (29), one finds

$$\mathcal{F}^{(-)}(k) = \exp(ika) [\mathbf{O}\mathbf{K} \cos \mathbf{K}a - i\mathbf{k}\mathbf{O} \sin \mathbf{K}a] \mathbf{K}^{-1} \mathbf{O}^T, \quad (30)$$

and $\mathcal{F}^{(+)}(k) = \mathcal{F}^{(-)}(-k)$.

From Eqs. (17) and (30), the scattering matrix is

$$\mathbf{S}(k) = \mathbf{k}^{-1/2} \mathbf{M}(-k) \mathbf{M}^{-1}(k) \mathbf{k}^{1/2}, \quad (31)$$

where

$$\mathbf{M}(k) = \exp(ika) [\mathbf{O}\mathbf{K} \cos \mathbf{K}a - i\mathbf{k}\mathbf{O} \sin \mathbf{K}a]. \quad (32)$$

The matrix $\mathbf{M}(k)$ satisfies the symmetry property

$$\mathbf{M}(k) = \mathbf{M}^*(-k^*), \quad (33)$$

which it inherits from the Jost matrix $\mathcal{F}^{(-)}(k)$ and the defining equations (23), (25), and (27). Then it may readily be shown that the scattering matrix $\mathbf{S}(k)$ is symmetric,

$$\mathbf{S}(k) = \mathbf{S}^T(k), \quad (34)$$

and unitary,

$$\mathbf{S}^\dagger(k) = \mathbf{S}^{-1}(k). \quad (35)$$

A short proof of the unitarity of $\mathbf{S}(k)$ is given in the Appendix.

Finally, the determinant of the Jost matrix is

$$\begin{aligned} \mathcal{J}^{(-)}(k) &= \det[\mathcal{F}^{(-)}(k)] \\ &= \frac{1}{K_1 K_2} \exp(ika) \exp(ik_2 a) \sin K_1 a \sin K_2 a \\ &\quad \times \left[(K_1 \cot K_1 a - ik)(K_2 \cot K_2 a - ik_2) \right. \\ &\quad \left. - i \frac{U_{12}^2}{(K_2^2 - K_1^2)(K_1^2 - \mathcal{K}_2^2)} (K_2 \cot K_2 a \right. \\ &\quad \left. - K_1 \cot K_1 a)(k - k_2) \right], \end{aligned} \quad (36)$$

where $\mathcal{K}_2^2 = k^2 - U_{22} - Q$.

IV. RESONANCES

In the two-coupled-channel system we are considering here, bound and resonant energies are obtained as zeros of the determinant of the Jost matrix.

The scattering matrix,

$$\mathbf{S}(k) = \mathbf{k}^{-1/2} \mathbf{M}(-k) \mathbf{M}^{-1}(k) \mathbf{k}^{1/2}, \quad (37)$$

has poles at the zeros of $\det \mathbf{M}(k)$.

When $\det \mathbf{M}(k)$ is not vanishing, the matrices $\mathbf{M}(k)$ and $\mathbf{M}^{-1}(k)$ may always be written in the biorthonormal basis of their own right and left eigenvectors as

$$\mathbf{M}(k) = \sum_{i=1}^2 |u_i(k)\rangle m_i(k) \langle v_i(k)| \quad (38)$$

and

$$\mathbf{M}^{-1}(k) = \sum_{i=1}^2 |u_i(k)\rangle m_i^{-1}(k) \langle v_i(k)|, \quad (39)$$

where $m_{1,2}(k)$ are the eigenvalues of $\mathbf{M}(k)$ and $|u_{1,2}(k)\rangle$ and $\langle v_{1,2}(k)|$ are the corresponding right and left eigenvectors of $\mathbf{M}(k)$, respectively.

If $\det \mathbf{M}(k)$ has a simple zero at $k = k_n$, one of the two eigenvalues of $\mathbf{M}(k)$ vanishes at $k = k_n$, say $m_2(k_n) = 0$. Then

$$\det \mathbf{M}(k) \approx (k - k_n) m_1(k_n) m_2'(k_n) + O[(k - k_n)^2], \quad (40)$$

where $m_2'(k_n)$ is the derivative of $m_2(k)$ with respect to k at $k = k_n$. In this case, the rank of $\mathbf{M}(k)$ is one and

$$\mathbf{M}(k_n) = |u_1(k_n)\rangle m_1(k_n) \langle v_1(k_n)|, \quad (41)$$

and $\mathbf{S}(k)$ takes the following form:

$$\begin{aligned} \lim_{k \rightarrow k_n} (k - k_n) \mathbf{S}(k) \\ = \frac{1}{m_2'(k_n)} \mathbf{k}_n^{-1/2} \mathbf{M}(-k_n) |u_1(k_n)\rangle \langle v_1(k_n)| \mathbf{k}_n^{1/2}. \end{aligned} \quad (42)$$

The symmetry of the $\mathbf{S}(k)$ matrix implies that its residue at $k = k_n$ is also symmetric. Therefore, the following relation holds:

$$\mathbf{k}_n^{-1/2} \mathbf{M}(-k_n) |u_1(k_n)\rangle = \mathbf{k}_n^{1/2} |v_1(k_n)\rangle. \quad (43)$$

Now let us introduce the notation

$$\frac{1}{[m_2'(k_n)]^{1/2}} \mathbf{k}_n^{1/2} |v_2(k_n)\rangle = \begin{pmatrix} \gamma_1(k_n) \\ \gamma_2(k_n) \end{pmatrix}, \quad (44)$$

where $\gamma_{1,2}(k_n)$ are the partial half-widths at the resonance. In this notation (42) is written as

$$\lim_{k \rightarrow k_n} (k - k_n) \mathbf{S}(k) = \begin{pmatrix} \gamma_1(k_n) \gamma_1(k_n) & \gamma_1(k_n) \gamma_2(k_n) \\ \gamma_2(k_n) \gamma_1(k_n) & \gamma_2(k_n) \gamma_2(k_n) \end{pmatrix} \quad (45)$$

Therefore, close to a simple pole at $k = k_n$, the scattering matrix $\mathbf{S}(k)$ takes the following form:

$$\mathbf{S}(k) \approx \frac{\hbar^2}{m} \frac{k_n}{E - \mathcal{E}_n} \begin{pmatrix} \gamma_1(k_n) \gamma_1(k_n) & \gamma_1(k_n) \gamma_2(k_n) \\ \gamma_2(k_n) \gamma_1(k_n) & \gamma_2(k_n) \gamma_2(k_n) \end{pmatrix}. \quad (46)$$

Each complex zero of $\det \mathbf{M}(k)$ will give rise to a resonant term in $\mathbf{S}(k)$:

$$\mathbf{S}(k) = \sum_n \frac{\hbar^2}{m} \frac{k_n}{E - \mathcal{E}_n} \begin{pmatrix} \gamma_1(k_n) \gamma_1(k_n) & \gamma_1(k_n) \gamma_2(k_n) \\ \gamma_2(k_n) \gamma_1(k_n) & \gamma_2(k_n) \gamma_2(k_n) \end{pmatrix} + \mathbf{S}_B(k), \quad (47)$$

$$\mathbf{S}(k) = \mathbf{S}^{\text{res}}(k) + \mathbf{S}_B(k). \quad (48)$$

$\mathbf{S}_B(k)$ is the background term.

V. DOUBLETS OF RESONANCES AND DOUBLE RESONANCES

In a system of two coupled channels with short ranged, square well attractive potentials with constant depths V_{11} and V_{22} and the same common range a , there are two regions of wave trapping that may resonate together when coupled by a square potential barrier of height V_{12} and the same common range a . As will be seen in the numerical example in Sec. IX, it may happen that, when the control parameters (V_{11} , V_{22} , and V_{12}) take values in some region \mathcal{R} of parameter space, the Jost determinant has an isolated pair of resonance zeros in some domain \mathcal{D} of the same Riemann sheet of the complex k plane, all other resonance zeros lying outside \mathcal{D} . In this case, the scattering matrix $\mathbf{S}(k)$ has an isolated doublet of closely spaced resonances. In this section, it is shown that the condition of two simple zeros of the Jost determinant coinciding at the same complex value, $k_n = k_{n+1} = k_d$, is a necessary but not a sufficient condition for the scattering matrix $\mathbf{S}(k)$ having a double pole at $k = k_d$. We find under what conditions the merging of two simple zeros into one double zero of the Jost determinant gives rise to one double pole (double resonance) of the scattering matrix $\mathbf{S}(k)$ and we derive explicit expressions for the analytical structure of the scattering matrix $\mathbf{S}(k)$ for k close to a double pole (double resonance) at $k = k_n$.

Let us consider the case when the Jost determinant has two simple zeros which for some special values of the control parameters of the system, say $(V_{11}^*, V_{22}^*, V_{12}^*)$, may exactly coincide.

At the point of coincidence, the two simple zeros give rise to one double zero of the Jost determinant at $k = k_n$. This possibility may be realized in two ways.

(1) First, when both eigenvalues of the matrix $\mathbf{M}(k)$ have one simple zero at $k = k_n$. In this case, $\text{Tr}\mathbf{M}(k_n) = 0$ and $\det\mathbf{M}(k_n) = 0$, the matrix $\mathbf{M}(k)$ itself is proportional to $(k - k_n)$, and the scattering matrix takes the factorized form

$$\mathbf{S}(k) = \left(\frac{k - k_n^*}{k - k_n} \right) \mathbf{S}'(k). \quad (49)$$

In this case, although the two simple zeros of the Jost determinant coincide at the same value k_n the scattering matrix $\mathbf{S}(k)$ has only one simple pole at $k = k_n$, and the reduced scattering matrix $\mathbf{S}'(k)$ is regular at $k = k_n$.

(2) Second, when one of the eigenvalues of the matrix $\mathbf{M}(k)$, say $m_2(k)$, has one double zero at $k = k_n$ and the other eigenvalue is nonvanishing at $k = k_n$, then $\text{Tr}\mathbf{M}(k_n) \neq 0$ but $\det\mathbf{M}(k_n) = 0$.

Let us consider this second case in more detail, the matrix $\mathbf{M}^{-1}(k)$ may be written, in the biorthonormal basis of the left

and right eigenvectors of $\mathbf{M}(k)$ as

$$\mathbf{M}^{-1}(k) = |u_1(k)\rangle \frac{1}{m_1(k)} \langle v_1(k)| + |u_2(k)\rangle \frac{1}{m_2(k)} \langle v_2(k)|, \quad (50)$$

and

$$m_1(k_n) \neq 0, \quad m_2(k) = \frac{1}{2}(k - k_n)^2 m_2''(k), \quad m_2''(k_n) \neq 0. \quad (51)$$

From this expression and Eq. (37),

$$\begin{aligned} & \lim_{k \rightarrow k_n} (k - k_n)^2 \mathbf{S}(k) \\ &= \frac{2}{m_2''(k_n)} \mathbf{k}_n^{-1/2} \mathbf{M}(-k_n) |u_2(k_n)\rangle \langle v_2(k_n)| \mathbf{k}_n^{1/2}. \end{aligned} \quad (52)$$

As before, the symmetry of $\mathbf{S}(k)$ implies that its residue at the double pole at k_n is also symmetric. Therefore,

$$\frac{2}{m_2''(k_n)} \mathbf{k}_n^{-1/2} \mathbf{M}(-k_n) |u_2(k_n)\rangle = \mathbf{k}_n^{1/2} |v_2(k_n)\rangle. \quad (53)$$

Then the residue of $\mathbf{S}(k)$ at the double pole may be written as

$$\lim_{k \rightarrow k_n} (k - k_n)^2 \mathbf{S}(k) = \begin{pmatrix} \gamma_1(k_n) \gamma_1(k_n) & \gamma_1(k_n) \gamma_2(k_n) \\ \gamma_2(k_n) \gamma_1(k_n) & \gamma_2(k_n) \gamma_2(k_n) \end{pmatrix}, \quad (54)$$

where

$$\begin{pmatrix} \gamma_1(k_n) \\ \gamma_2(k_n) \end{pmatrix} = \sqrt{\frac{\langle v_2(k_n) | \mathbf{M}^T(-k_n) \mathbf{k}_n^{-1} | v_2(k_n) \rangle}{\frac{1}{2} m_2''(k_n)}} \mathbf{k}_n^{1/2} |u_2(k_n)\rangle. \quad (55)$$

These results allow us to write the $\mathbf{S}(k)$ matrix for k in a neighborhood of k_n as

$$\mathbf{S}(k) \approx \frac{1}{(k - k_n)^2} \mathbf{N}(k), \quad (56)$$

where

$$\mathbf{N}(k) = \begin{pmatrix} \gamma_1(k) \gamma_1(k) & \gamma_1(k) \gamma_2(k) \\ \gamma_2(k) \gamma_1(k) & \gamma_2(k) \gamma_2(k) \end{pmatrix}. \quad (57)$$

The analytical structure of the matrix $\mathbf{S}(k)$ for k close to k_n is obtained expanding the matrix $\mathbf{N}(k)$ in a Taylor series in k about $k = k_n$,

$$\mathbf{S}(k) \approx \frac{\mathbf{N}(k_n)}{(k - k_n)^2} + \frac{\mathbf{N}'(k_n)}{(k - k_n)} + \dots; \quad (58)$$

that is,

$$\mathbf{S}(k) = \frac{1}{(k - k_n)^2} \begin{pmatrix} \gamma_1(k_n) \gamma_1(k_n) & \gamma_1(k_n) \gamma_2(k_n) \\ \gamma_2(k_n) \gamma_1(k_n) & \gamma_2(k_n) \gamma_2(k_n) \end{pmatrix} + \frac{1}{k - k_n} \begin{pmatrix} 2\gamma_1(k_n) \bar{\gamma}_1(k_n) & \gamma_1(k_n) \bar{\gamma}_2(k_n) + \bar{\gamma}_1(k_n) \gamma_2(k_n) \\ \gamma_2(k_n) \bar{\gamma}_1(k_n) + \bar{\gamma}_2(k_n) \gamma_1(k_n) & 2\gamma_2(k_n) \bar{\gamma}_2(k_n) \end{pmatrix} + \mathbf{S}_B(k), \quad (59)$$

where

$$\bar{\gamma}_i(k_n) = \left(\frac{d\gamma_i(k)}{dk} \right)_{k_n}. \quad (60)$$

Therefore, when one of the eigenvalues of the matrix $\mathbf{M}(k)$ has one double zero and the other is nonvanishing at $k = k_n$, the scattering matrix $\mathbf{S}(k)$ has one double pole and one simple pole at $k = k_n$, as shown in Eq. (59).

VI. UNIFORMIZATION

In the foregoing discussion, the channel wave numbers, k and k_2 , were considered as independent variables. Expressing each channel wave number in terms of the energy, as in Eq. (10), the scattering matrix and the Jost determinant, as functions of the wave number, have a branch point at the threshold of the inelastic channel. Therefore, in order to discuss the analytic properties of the zeros of the Jost determinant as functions of the control parameters (V_{11}, V_{22}, V_{12}), it is convenient to define a new independent variable t , as

$$t^2 = \frac{k - \sqrt{Q}}{k + \sqrt{Q}}, \quad k = \sqrt{Q} \frac{1 + t^2}{1 - t^2}, \quad k_2 = 2\sqrt{Q} \frac{t}{1 - t^2}. \quad (61)$$

In terms of t , the scattering matrix $\mathbf{S}(t)$ and the Jost determinant $\mathcal{J}^{(-)}(t; V_{11}, V_{22}, V_{12})$ are analytic, single valued functions of t complex [40]. Furthermore, $\mathcal{J}^{(-)}(t)$ is an entire function of t complex. Then, all zeros of $\mathcal{J}^{(-)}(t; V_{11}, V_{22}, V_{12})$ are points on the complex t plane which has only one single Riemann sheet.

Pole position function. The position of the poles of the scattering matrix $\mathbf{S}(k)$ in the complex t plane is determined by the zeros of the Jost determinant

$$\mathcal{J}^{(-)}(t_n; V_{11}, V_{22}, V_{12}) = 0. \quad (62)$$

According to the implicit function theorem of Weierstrass, this condition defines, implicitly, the pole position function

$$t_n = t_n(V_{11}, V_{22}, V_{12}), \quad (63)$$

as branches of a multivalued function of the control parameters (V_{11}, V_{22}, V_{12}),

$$t_n(V_{11}, V_{22}, V_{12}) = \mathcal{J}^{-1}(0; V_{11}, V_{22}, V_{12}). \quad (64)$$

Each branch of the pole position function t_n is a continuous single valued function of the control parameters (V_{11}, V_{22}, V_{12}).

The energy eigenvalues are obtained from the pole position function as

$$\mathcal{E}_{n,i}(V_{11}, V_{22}, V_{12}) = \frac{\hbar^2}{2m} k_n^2(V_{11}, V_{22}, V_{12}) + Q\delta_{i,2}, \quad i = 1, 2, \quad (65)$$

where

$$k_n^2(V_{11}, V_{22}, V_{12}) = Q \left(\frac{1 + t_n^2(V_{11}, V_{22}, V_{12})}{1 - t_n^2(V_{11}, V_{22}, V_{12})} \right)^2. \quad (66)$$

Each energy eigenvalue, $\mathcal{E}_n(V_{11}, V_{22}, V_{12})$, may be represented as a surface in a parameter space with coordinates $(\text{Re}\mathcal{E}, \text{Im}\mathcal{E}, V_{11}, V_{22}, V_{12})$.

VII. SINGULARITY OF THE DOUBLET'S POLE POSITION FUNCTION AT THE EXCEPTIONAL POINT

In this section, we discuss the analytical structure and properties of the singularity of the pole position function of

the isolated doublet of unbound states at the exceptional point (degeneracy of resonance eigenenergies) in parameter space.

Let us start by recalling that the codimension of a resonance degeneracy is two [49]; hence, it will be enough to consider the Jost determinant as a function of only two control parameters, say $V_{11} = V_{22} = v$ and $V_{12} = u$, all other control parameters of the problem will be kept fixed. When the system has an isolated doublet of resonances which may become degenerate, the corresponding branches of the pole position function, say $t_1(v, u)$ and $t_2(v, u)$, may be equal (cross or coincide) at an exceptional point. In this case, it is not possible to solve the implicit Eq. (62) for the pole position function of the two individual members of the doublet and one must solve (62) for the pole position function of the isolated doublet of resonances.

The physical system has a degeneracy of unbound states (resonances), at $t = t_d$, if two simple resonance zeros of the Jost determinant merge into one double resonance zero at t_d , $t_1(v^*, u^*) = t_2(v^*, u^*) = t_d \neq 0$,

$$\begin{aligned} \mathcal{J}^{(-)}(t_d; v^*, u^*) = 0, \quad \left(\frac{\partial \mathcal{J}^{(-)}(t; v, u)}{\partial t} \right)_{t_d} = 0, \\ \left(\frac{\partial^2 \mathcal{J}^{(-)}(t; v, u)}{\partial t^2} \right)_{t_d} \neq 0, \end{aligned} \quad (67)$$

and the conditions for a double pole in $\mathbf{S}(k)$ are satisfied,

$$\det \mathbf{M}(t_d) = 0, \quad \text{Tr} \mathbf{M}(t_d) \neq 0. \quad (68)$$

The pole position function $t_{1,2}(v, u)$ of the isolated doublet of resonances is implicitly defined by the equation

$$\mathcal{J}^{(-)}(t_{1,2}; v, u) = 0, \quad (69)$$

and the conditions (68) for (v, u) in a neighborhood of the exceptional point (v^*, u^*) .

We may solve formally this equation for $t_{1,2}(v, u)$ by first recalling that the Jost determinant $\mathcal{J}^{(-)}(t; v, u)$ is an entire function of t and may be written in the form of an infinite product, according to Hadamard's form of the Weierstrass factorization theorem [50] and by using a theorem of Pfluger [51], we may write

$$\mathcal{J}^{(-)}(t; v, u) = \left[\left(t - \frac{1}{2}(t_1 + t_2) \right)^2 - \frac{1}{4}(t_1 - t_2)^2 \right] \mathcal{G}_{1,2}(t; v, u), \quad (70)$$

where

$$\mathcal{G}_{1,2}(t; v, u) = \exp[G(t)] \frac{1}{t_1(v, u)t_2(v, u)} \prod_3^{\infty} \left(1 - \frac{t}{t_n(v, u)} \right). \quad (71)$$

In this expression $G(t)$ is an entire function of t and $\{t_n(v, u)\}$ is the set of zeros of $\mathcal{J}^{(-)}(t; v, u)$.

The first factor on the right-hand side of (70) may be written as

$$\begin{aligned} \left(t - \frac{1}{2}[t_1(v, u) + t_2(v, u)] \right)^2 - \frac{1}{4}(t_1(v, u) - t_2(v, u))^2 \\ = (t - t_{1,2}^{(+)}(v, u))(t - t_{1,2}^{(-)}(v, u)). \end{aligned} \quad (72)$$

This equation relates the pole position function, $t_{1,2}(v, u)$, of the doublet to the pole position functions of the individual unbound (resonance) states.

Solving (72) for $t_{1,2}(v,u)$ when $\mathcal{J}^{(-)}(t;v,u)$ vanishes and $\mathcal{G}_{1,2}(t,v,u)$ is nonvanishing, we get

$$t_{1,2}(v,u) = \Sigma_{1,2}(v,u) \pm \sqrt{\Delta_{1,2}(v,u)}, \quad (73)$$

where

$$\Sigma_{1,2}(v,u) = \frac{1}{2}[t_1(v,u) + t_2(v,u)] \quad (74)$$

and

$$\Delta_{1,2}(v,u) = \frac{1}{4}[t_1(v,u) - t_2(v,u)]^2, \quad (75)$$

with (v,u) in a neighborhood of the exceptional point (v^*,u^*) .

According to the preparation theorem of Weierstrass [50], the functions $\Sigma_{1,2}(v,u)$ and $\Delta_{1,2}(v,u)$ appearing in the right-hand side of Eq. (73), are regular functions of (v,u) at the exceptional point, and admit a Taylor series expansion about that point. Then, from Eqs. (73), (74), and (75), it follows

that the pole position function of the degenerating doublet of resonances $t_{1,2}(v,u)$ has a branch point of square root type at the exceptional point, when $\Delta_{1,2}(v^*,u^*)$ vanishes.

VIII. SINGULARITY OF THE ENERGY SURFACES AT THE EXCEPTIONAL POINT

The resonance energy eigenvalues $\mathcal{E}_1(v,u)$ and $\mathcal{E}_2(v,u)$ of the isolated doublet of resonances may be obtained from the corresponding zeros $t_1(v,u)$ and $t_2(v,u)$ of the Jost determinant through

$$\mathcal{E}_i(v,u) = \frac{\hbar^2 Q}{2m} \left(\frac{1 + t_i^2(v,u)}{1 - t_i^2(v,u)} \right)^2, \quad i = 1, 2. \quad (76)$$

From this expression, and (74) and (75), we find that the sum and the difference of the energy eigenvalues may be expressed in terms of the regular functions $\Sigma_{1,2}(v,u)$ and $\Delta_{1,2}(v,u)$ as

$$\frac{1}{2}(\mathcal{E}_1 + \mathcal{E}_2) = \left(\frac{\hbar^2 Q}{2m} \right) \frac{(1 - [\Sigma_{1,2}^2(v,u) - \Delta_{1,2}(v,u)]^2)^2 + 16\Sigma_{1,2}^2(v,u)\Delta_{1,2}(v,u)}{\{[1 - \{\Sigma_{1,2}^2(v,u) - \Delta_{1,2}(v,u)\}]^2 - 4\Delta_{1,2}(v,u)\}^2}, \quad (77)$$

$$\frac{1}{4}(\mathcal{E}_1 - \mathcal{E}_2)^2 = \left(\frac{4\hbar^2 Q}{m} \right)^2 \frac{\Sigma_{1,2}^2(v,u)\Delta_{1,2}(v,u)[1 - \{\Sigma_{1,2}^2(v,u) - \Delta_{1,2}(v,u)\}]^2}{\{[1 - \{\Sigma_{1,2}^2(v,u) - \Delta_{1,2}(v,u)\}]^2 - 4\Delta_{1,2}(v,u)\}^4}. \quad (78)$$

Therefore, the functions $1/2[\mathcal{E}_1(v,u) + \mathcal{E}_2(v,u)]$ and $1/4[\mathcal{E}_1(v,u) - \mathcal{E}_2(v,u)]^2$ are regular at the exceptional point and admit a Taylor series expansion about that point.

The two energy eigenvalues, \mathcal{E}_1 and \mathcal{E}_2 , in the isolated doublet of unbound states may be expressed in terms of the two regular functions of the control parameters of the system in Eqs. (77) and (78) as

$$\mathcal{E}_{1,2}(v,u) = \frac{1}{2}(\mathcal{E}_1(v,u) + \mathcal{E}_2(v,u)) \pm \sqrt{\frac{1}{4}[\mathcal{E}_1(v,u) - \mathcal{E}_2(v,u)]^2}. \quad (79)$$

This expression shows that the two degenerating energy eigenvalues in an isolated doublet of unbound states are two branches of a multivalued function of the control parameters. If we represent the real and imaginary parts of the energy eigenvalues of the system as surfaces in parameter space, these surfaces have four sheets, which are connected in pairs at the degeneracy point.

A contact equivalent approximant, $\hat{\mathcal{E}}_{1,2}$, to the doublet eigenenergy surface at the crossing point is readily obtained when the expressions (77) and (78) are substituted for $1/2[\mathcal{E}_1(v,u) + \mathcal{E}_2(v,u)]$ and $1/4[\mathcal{E}_1(v,u) - \mathcal{E}_2(v,u)]^2$ in Eq. (79) and the functions $\Sigma_{1,2}^2(v,u)$ and $\Delta_{1,2}^2(v,u)$, are expanded in a Taylor series and we keep only the first-order terms,

$$\mathcal{E}_{1,2}(v,u) \approx \mathcal{E}_d(v^*,u^*) + \Delta\mathcal{E}_d(v,u) + \hat{\mathcal{E}}_{1,2}(v,u), \quad (80)$$

where

$$\hat{\mathcal{E}}_{1,2}(v,u) = \pm \sqrt{\frac{1}{4}[C_1^{(1)}(v - v^*) + C_2^{(1)}(u - u^*)]}. \quad (81)$$

The complex coefficients $C_i^{(1)}$ may readily be computed from the Jost determinant with the help of the implicit function theorem [50].

In order to simplify the notation, let us call $\vec{\eta}$ the real position vector of the point (v,u) relative to the exceptional point (v^*,u^*) in parameter space, $\eta_1 = v - v^*$ and $\eta_2 = u - u^*$ and let the components of the real constant vectors \vec{R} and \vec{I} be the real and imaginary parts of the complex coefficients $C_i^{(1)}$,

$$\vec{\eta} = \begin{pmatrix} v - v^* \\ u - u^* \end{pmatrix}, \quad \vec{R} = \begin{pmatrix} \text{Re}C_1^{(1)} \\ \text{Re}C_2^{(1)} \end{pmatrix}, \quad \vec{I} = \begin{pmatrix} \text{Im}C_1^{(1)} \\ \text{Im}C_2^{(1)} \end{pmatrix}. \quad (82)$$

In this notation

$$\hat{\mathcal{E}}_{1,2} = \frac{1}{2}[\vec{R} \cdot \vec{\eta} + i\vec{I} \cdot \vec{\eta}]^{1/2}. \quad (83)$$

Solving for the real and imaginary parts of the function $\hat{\mathcal{E}}_{1,2}(v,u)$, we obtain

$$\text{Re}\hat{\mathcal{E}}_{1,2}(v,u) = \pm \frac{1}{2\sqrt{2}}[+\sqrt{(\vec{R} \cdot \vec{\eta})^2 + (\vec{I} \cdot \vec{\eta})^2} + \vec{R} \cdot \vec{\eta}]^{1/2}, \quad (84)$$

$$\text{Im}\hat{\mathcal{E}}_{1,2}(v,u) = \pm \frac{1}{2\sqrt{2}}[+\sqrt{(\vec{R} \cdot \vec{\eta})^2 + (\vec{I} \cdot \vec{\eta})^2} - \vec{R} \cdot \vec{\eta}]^{1/2}, \quad (85)$$

and

$$\text{sgn}(\text{Re}\hat{\mathcal{E}}_{1,2})\text{sgn}(\text{Im}\hat{\mathcal{E}}_{1,2}) = \text{sgn}(\vec{I} \cdot \vec{\eta}), \quad (86)$$

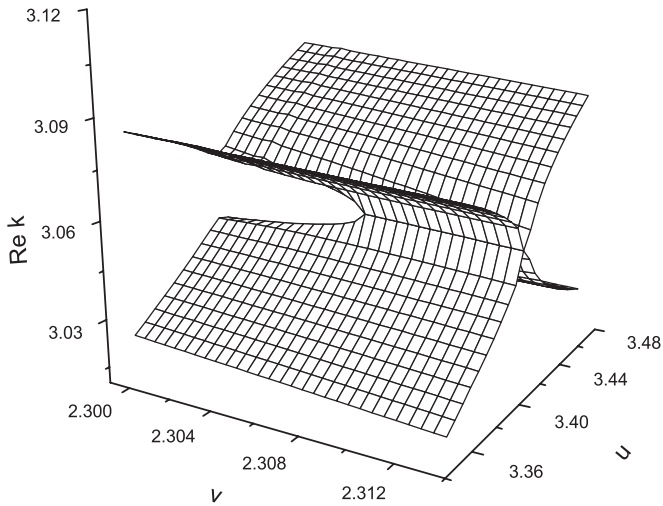


FIG. 1. The real part of the degenerating energy eigenvalues of the doublet as function of the control parameters is represented as a two-sheeted surface. This surface has a branch point of square root type at the exceptional point where the two energy eigenvalues coincide and a branch cut along a line that starts at the exceptional point and extends in the *positive* direction of the Ov axis.

where

$$\vec{I} \cdot \hat{\eta}_o = 0 \quad \text{and} \quad \vec{R} \cdot \hat{\eta}_o = -|\vec{R} \cdot \hat{\eta}_o|. \quad (87)$$

$\hat{\eta}_o$ is the unit vector parallel to $\vec{\eta}$.

The real and imaginary parts of the pole position function $\text{Re}\mathcal{E}_{1,2}(v,u)$ and $\text{Im}\mathcal{E}_{1,2}(v,u)$, as functions of the real parameters (v,u) , both have an algebraic branch point of square root type at the exceptional point. The functions $\text{Re}\mathcal{E}_{1,2}(v,u)$ and $\text{Im}\mathcal{E}_{1,2}(v,u)$ both have branch cuts that start at the same exceptional point but extend in opposite directions in parameter space (see Figs. 1 and 2).

Equality of the complex resonance energy eigenvalues (degeneracy of resonances), $\mathcal{E}_1(v^*,u^*) = \mathcal{E}_2(v^*,u^*) = \mathcal{E}_d(v^*,u^*)$, occurs only at the exceptional point with coordinates (v^*,u^*) and only at that point.

IX. NUMERICAL COMPUTATION OF THE EXCEPTIONAL POINT

In order to locate the exceptional point in the energy spectrum of the two-coupled-channel system, the coupled equations (67) and (68) were solved numerically. The zeros of the Jost determinant are found by an algebraic computer package that searches for the minima of $|\mathcal{J}^-(t_n; v, u)|$ in the complex t plane. In the computation, the parameters $Q = 0.6$, $a = 1$ were kept fixed and only the parameters $V_{12} = V_{21} = u$ and $V_{11} = V_{22} = v$ were allowed to vary. Starting with the values $v = 2.30653$ and $u = 3.400891$, we find the first isolated doublet of resonances at $t_1 = 0.633873 - i0.118476$, and $t_2 = 0.633905 - i0.118439$, corresponding to the following values of the wave number $k_1 = 3.055631794 - i1.239436172$ and $k_2 = 3.056124704 - i1.239315385$.

Then the numerical values of the control parameters v and u are adjusted until t_1 and t_2 become equal to some common value t_d . We also computed $|\partial \mathcal{J}^-(t; v, u) / \partial t|_{t=t_d}$ to verify that the second equation (67) was also satisfied to some previously

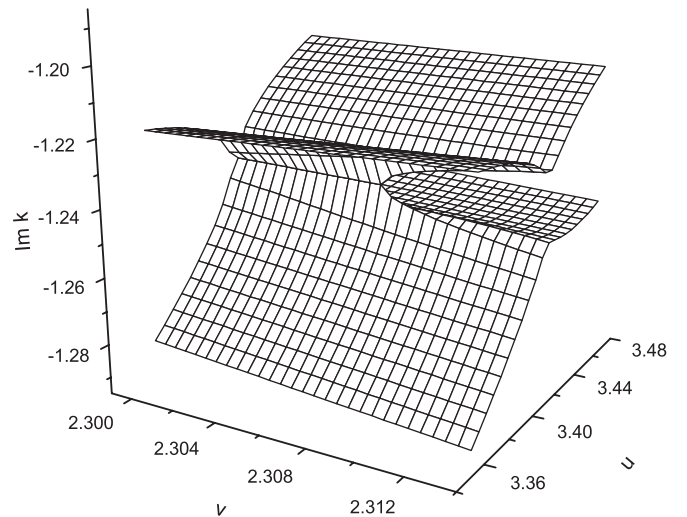


FIG. 2. The imaginary part of the degenerating energy eigenvalues of the doublet as function of the control parameters is shown as a two-sheeted surface. This surface has a branch point at the exceptional point and a branch cut that starts at the exceptional point and extends in the *negative* direction of the Ov axis.

prescribed accuracy. In this way, by fine tuning the control parameters to the values $v = 2.3065339869$ and $u = 3.4008932173$, we found that the first doublet of resonances becomes degenerate at the value $t_d = 0.633889 - i0.118458$ corresponding to the following value of the wave number $k_d = 3.0558764 - i1.23937571$.

We numerically solved the implicit transcendental equations (67) and (68) that define the eigenenergy surface of the degenerating isolated doublet of unbound states. The results of this numerical computation of the real and imaginary parts of the pole position function of the degenerating doublet of unbound state are represented as surfaces in Euclidean spaces with coordinates $(\text{Re}k, v, u)$ and $(\text{Im}k, v, u)$ (see Figs. 1 and 2).

X. PHENOMENOLOGY OF THE EXCEPTIONAL POINT

For the sake of completeness, in this section we discuss briefly some of the rich phenomenology observed when the complex energy eigenvalues of the doublet are measured as functions of the control parameters of the system. This phenomenology gives a direct evidence on the topology of the energy surfaces at the exceptional point. A more detailed discussion of this topic in the case of resonances in a single channel elastic scattering in a physical system with a double barrier potential may be found in Hernández *et al.* [35].

The topological and geometrical properties of the singularity of the energy surfaces at an exceptional point are accessible to experimental determination. When one control parameter is slowly varied while keeping the other constant, crossings and anticrossings of energies and widths are experimentally observed [26,27,41]. When the system is slowly transported in a double circuit around the exceptional point in parameter space, it is observed that the wave function of the system acquires a geometric or Berry phase [30,43,45–48,52,53]. Additional information on the topology of the singularity of

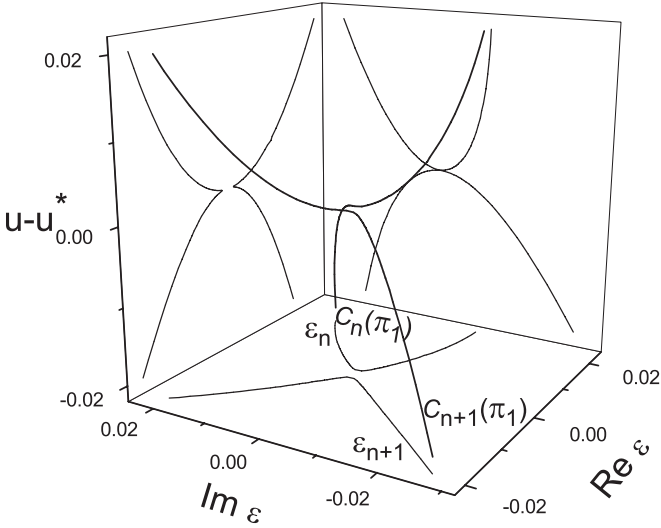


FIG. 3. The curves $\hat{C}_n(\pi_1)$ and $\hat{C}_{n+1}(\pi_1)$ are the intersection of the hyperplane $\pi_1 : \eta_1 = \bar{\eta}_1 > 0$ and the two-sheeted surface $\hat{\varepsilon}_{n,n+1}$. The projections of $\hat{C}_n(\pi_1)$ and $\hat{C}_{n+1}(\pi_1)$ on the planes $(\text{Im}\mathcal{E}, \eta_2)$ and $(\text{Re}\mathcal{E}, \eta_2)$ show a crossing of widths and anticrossing of energies, respectively. The projections on the plane $(\text{Re}\mathcal{E}, \text{Im}\mathcal{E})$ are the trajectories of the S-matrix poles in the complex energy plane. In the figure, $\eta_2 = u - u^*$.

the energy surface at an exceptional point is obtained from the so called changes of identity of the poles of the scattering matrix [42,54].

Sections of the energy surfaces. The adiabatic measurement of the difference of complex energy eigenvalues of the doublet as one of the control parameters, say η_2 , is varied, while the other parameter is kept constant allows the experimental determination of the intersection of this eigenenergy surface with the plane defined by the condition $\eta_1 = \bar{\eta}_1$, with $\bar{\eta}_1$ constant,

$$\hat{\mathcal{E}}_n(\bar{\eta}_1, \eta_2) - \hat{\mathcal{E}}_{n+1}(\bar{\eta}_1, \eta_2) = \hat{\varepsilon}_{n,n+1}(\bar{\eta}_1, \eta_2). \quad (88)$$

This intersection defines two three-dimensional curves for each value of $\bar{\eta}_1$

$$\hat{\varepsilon}_{n,n+1}(\bar{\eta}_1, \eta_2) \cap \pi_i = \begin{cases} \hat{C}_n(\pi_i) & i = 1, 2, 3. \\ \hat{C}_{n+1}(\pi_i) \end{cases} \quad (89)$$

The projections of the sections $\hat{C}_n(\pi_i)$ and $\hat{C}_{n+1}(\pi_i)$ on the planes $(\text{Re}\hat{\mathcal{E}}_{n,n+1}, \text{Im}\hat{\mathcal{E}}_{n,n+1})$ are the trajectories of the S-matrix poles in the complex energy plane. The projections of the sections $C_n(\pi_i)$ and $C_{n+1}(\pi_i)$ on the planes $(\text{Re}\hat{\mathcal{E}}_{n,n+1}, \eta_2)$ and $(\text{Im}\hat{\mathcal{E}}, \eta_2)$ show the crossings and anticrossings of energies and widths, respectively. In Figs. 3, 4, and 5 we show these sections and their projections for three fixed values of the parameter η_1 : $\bar{\eta}_1(1) < 0$, $\bar{\eta}_1(2) = 0$, and $\bar{\eta}_1(3) > 0$. The condition $\bar{\eta}_1 = \text{constant}$ with $\bar{\eta}_1(1) < 0$ defines a plane π_1 which intersects $\hat{\mathcal{E}}_{n,n+1}$ in the region where the two sheets of $\text{Re}\hat{\mathcal{E}}_{n,n+1}$ are well separated but the two sheets of $\text{Im}\hat{\mathcal{E}}_{n,n+1}$ cross at the branch cut; $\bar{\eta}_1(2) = 0$ defines a plane π_2 that intersects $\hat{\mathcal{E}}_{n,n+1}$ at the exceptional point where both $\text{Re}\hat{\mathcal{E}}_{n,n+1}$ and $\text{Im}\hat{\mathcal{E}}_{n,n+1}$ cross; $\bar{\eta}_1(3) > 0$ defines a plane π_3 that intersects $\hat{\mathcal{E}}_{n,n+1}$ in the region where the two sheets of $\text{Re}\hat{\mathcal{E}}_{n,n+1}$ cross at the branch cut but the two sheets of $\text{Im}\hat{\mathcal{E}}_{n,n+1}$ are well separated and do not cross.

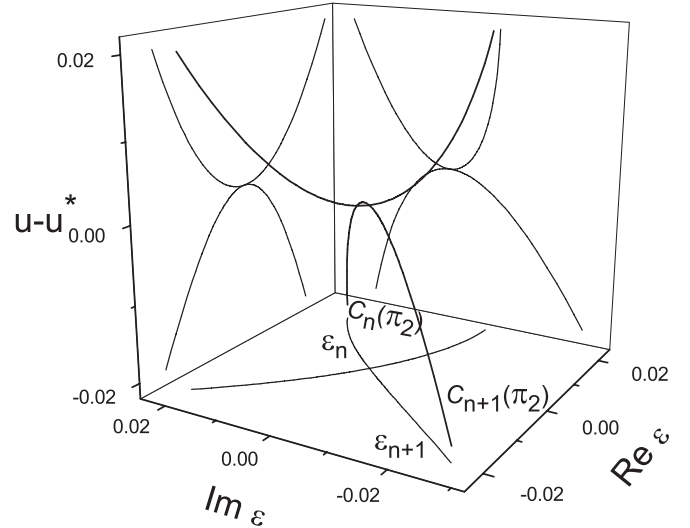


FIG. 4. The curves $\hat{C}_n(\pi_2)$ and $\hat{C}_{n+1}(\pi_2)$ are the intersections of the hyperplane π_2 that goes through the exceptional point (η_1^*, η_2^*) in parameter space and the two-sheeted surface $\hat{\varepsilon}_{n,n+1}(\eta_1, \eta_2)$. The projections of $\hat{C}_n(\pi_2)$ and $\hat{C}_{n+1}(\pi_2)$ on the planes $(\text{Re}\mathcal{E}, \eta_2)$ and $(\text{Im}\mathcal{E}, \eta_2)$ show a joint crossing of energies and widths. The projections on the plane $(\text{Re}\mathcal{E}, \text{Im}\mathcal{E})$ are the critical trajectories of the S-matrix poles in the complex energy plane. At the crossing point, the two simple poles coalesce into one double pole of $S(E)$.

[In Eq. (88) and the following, the subindices $(n, n+1)$ have been substituted for $(1, 2)$ to stress the fact that our analysis applies to any isolated pair of coherent resonant states.]

Crossings and anticrossings of energies and widths. When the difference of complex resonance energy eigenvalues, $\hat{\mathcal{E}}_n(\eta_1, \bar{\eta}_2) - \hat{\mathcal{E}}_{n+1}(\eta_1, \bar{\eta}_2) = \Delta E - i/2\Delta\Gamma$, is measured as a function of the slowly varying parameter η_1 , keeping the other parameter constant, $\eta_2 = \bar{\eta}_2$, crossings or anticrossings of energies and widths are experimentally observed.

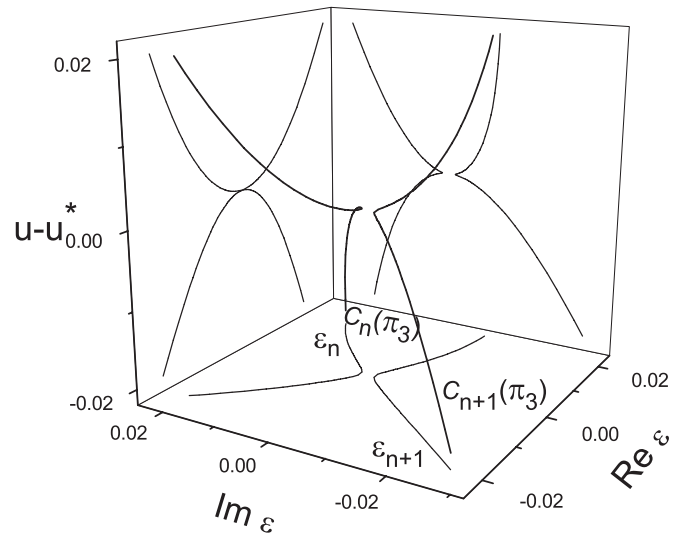


FIG. 5. The curves $\hat{C}_n(\pi_3)$ and $\hat{C}_{n+1}(\pi_3)$ are the intersection of the hyperplane $\pi_3 : \eta_1 = \bar{\eta}_1 < 0$ and the two-sheeted surface $\hat{\varepsilon}_{n,n+1}$. The projections of $\hat{C}_n(\pi_3)$ and $\hat{C}_{n+1}(\pi_3)$ on the planes $(\text{Re}\mathcal{E}, \eta_2)$ and $(\text{Im}\mathcal{E}, \eta_2)$ show a crossing of energies and an anticrossing of widths, respectively. The projections of on the plane $(\text{Re}\mathcal{E}, \text{Im}\mathcal{E})$ do not cross.

From Eqs. (84)–(86), we obtain

$$\Delta E = \frac{\sqrt{2}}{2} [+\sqrt{(\vec{R} \cdot \vec{\eta})^2 + (\vec{I} \cdot \vec{\eta})^2} + (\vec{R} \cdot \vec{\eta})]^{1/2} |_{\eta_1 = \bar{\eta}_1}, \quad (90)$$

and

$$\Delta \Gamma = -\sqrt{2} [+\sqrt{(\vec{R} \cdot \vec{\eta})^2 + (\vec{I} \cdot \vec{\eta})^2} - (\vec{R} \cdot \vec{\eta})]^{1/2} |_{\eta_1 = \bar{\eta}_1}. \quad (91)$$

Hence,

$$\begin{aligned} \Delta E \Delta \Gamma &= -(\vec{I} \cdot \vec{\eta}) |_{\eta_1 = \bar{\eta}_1}, \\ (\Delta E)^2 - \frac{1}{4}(\Delta \Gamma)^2 &= (\vec{R} \cdot \vec{\eta}) |_{\eta_1 = \bar{\eta}_1}. \end{aligned} \quad (92)$$

Therefore,

(1) $(\vec{R} \cdot \vec{\eta}) |_{\eta_1 = \bar{\eta}_1} > 0$ implies $\Delta E \neq 0$ and $\Delta \Gamma = 0$, that is, energy anticrossing and width crossing;

(2) $(\vec{R} \cdot \vec{\eta}) |_{\eta_1 = \bar{\eta}_1} = 0$ 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) $(\vec{R} \cdot \vec{\eta}) |_{\eta_1 = \bar{\eta}_1} < 0$ implies $\Delta E = 0$ and $\Delta \Gamma \neq 0$, that is, energy crossing and width anticrossing.

These three possibilities are graphically shown in Figs. 3, 4, and 5.

These results generalize the well known level repulsion theorem of von Neumann and Wigner [55] from the case of bound states in a single channel potential model to the case of resonant states in a two-coupled-channel model of scattering and reactions.

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 *et al.* [26,27,41].

Trajectories of the S matrix poles and changes of identity. Close to the crossing point, the trajectories of the S matrix poles in the complex energy plane are the branches of a hyperbola whose equation is obtained by eliminating η_2 between $\text{Re} \hat{\mathcal{E}}_m(\bar{\eta}_1, \eta_2)$ and $\text{Im} \hat{\mathcal{E}}_m(\bar{\eta}_1, \eta_2)$, $m = 1, 2$ [Eqs. (84)–(86)],

$$\begin{aligned} (\text{Re} \hat{\mathcal{E}}_m)^2 - 2 \cot \phi_1 (\text{Re} \hat{\mathcal{E}}_m)(\text{Im} \hat{\mathcal{E}}_m) - (\text{Im} \hat{\mathcal{E}}_m)^2 \\ - \frac{1}{4} (\vec{R} \cdot \vec{\eta}_c)_{\bar{\eta}_1} = 0, \end{aligned} \quad (93)$$

where $\cot \phi_1 = \frac{R_1}{I_1}$ and the constant vector $\vec{\eta}_c$ is such that $(\vec{I} \cdot \vec{\eta}_c)_{\bar{\eta}_1} = 0$. We find three types of trajectories, which are distinguished by the sign of $(\vec{R} \cdot \vec{\eta}_c)_{\bar{\eta}_1}$, as shown in Figs. 3, 4, and 5.

A small change in the control parameter $\bar{\eta}_1$ may change the sign of $(\vec{R} \cdot \vec{\eta}_c)_{\bar{\eta}_1}$. When this happens, it produces a small change in the initial position of the poles, but the trajectories may change from the type shown in Fig. 3 to the type shown in Fig. 5. This sudden change of the trajectories' type exchanges almost exactly the final position of the poles, as can be appreciated from Figs. 3 and 5. This dramatic change was called a “change of identity” [42], and it is due to the topology of the energy hypersurface in the neighborhood of the exceptional point.

Changes of identity when going around the exceptional point. The double valued nature of the eigenenergy surface in the neighborhood of the exceptional point is made evident by the motion of the resonance poles in the complex k plane

when the system is transported in a closed path around the exceptional point in parameter space. When the physical system is transported once around the exceptional point in parameter space, the two poles of the isolated doublet of unbound states trace the two halves of a starlike trajectory until the positions of the poles are exactly exchanged (see Fig. 6). When the physical system is transported twice around the exceptional point in parameter space, each one of the two poles traces a complete closed starlike trajectory and

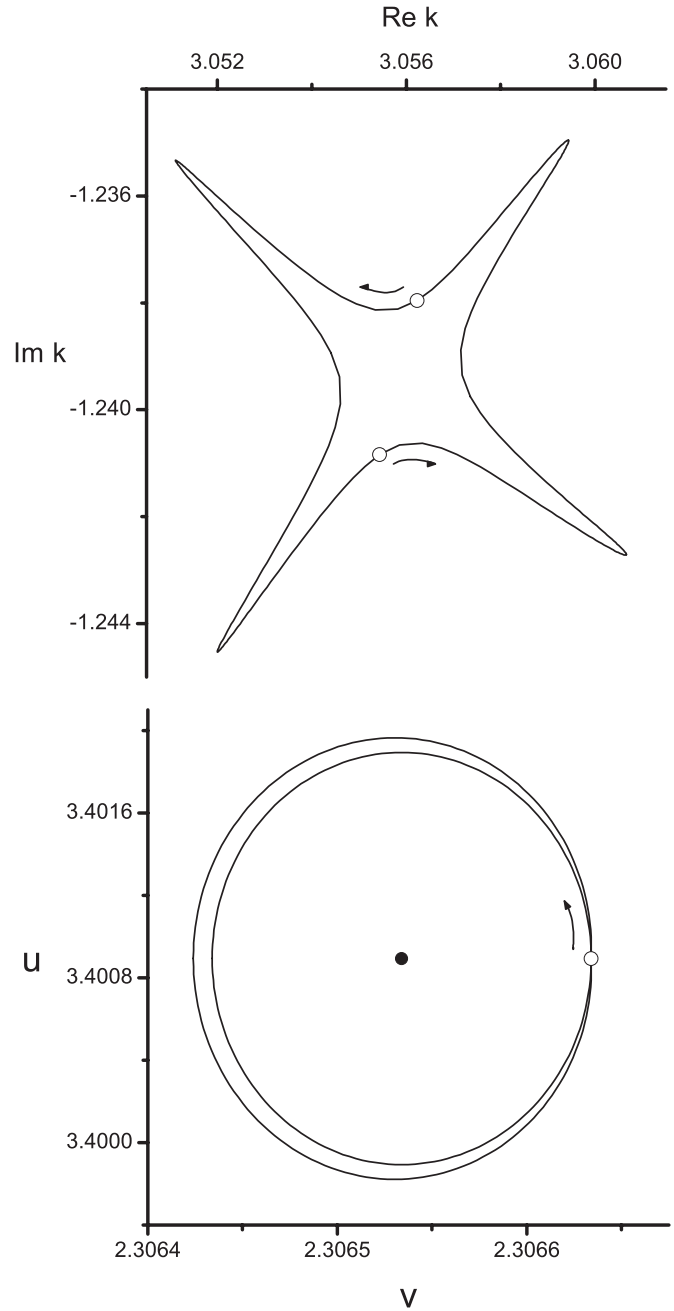


FIG. 6. The two poles of the isolated doublet of unbound states trace a starlike trajectory in the complex k plane, shown on the upper part of the figure, when the physical system is transported in parameter space twice around the exceptional point in the circular path shown at the lower part of the figure. The two loops in the circular path are shown in the figure slightly displaced for easy viewing.

returns to its initial position in the complex k plane (see Fig. 6). The corresponding eigenfunctions of the system also return to their initial values but they acquire a geometric phase [30,43,45–48,52,53].

XI. SUMMARY AND CONCLUSION

In this paper, we have been concerned with some mathematical and physical aspects of the mixing and degeneracy of two unbound energy eigenstates of a two-coupled-channel model of scattering and reactions in collisions of complex quantum systems. The physical system is described in terms of a two-channel Hermitian Hamiltonian matrix with a short ranged 2×2 potential matrix \mathbf{V} . We find that the vanishing of the Jost determinant and its first derivative with respect to t at some value of t , say $t = t_n$, is a necessary but not a sufficient condition for the existence of an exceptional point at t_n . The necessary and sufficient condition for the existence of an exceptional point at $t = t_n$ may be expressed in terms of the matrix $\mathbf{M}(k)$ [Eq. (32)] as

$$\begin{aligned} \mathcal{J}^{(-)}(t_d; v^*, u^*) &= 0, & (94) \\ \left(\frac{\partial \mathcal{J}^{(-)}(t)}{\partial t} \right)_{t_d} &= 0 \quad \text{and} \quad \left(\frac{\partial^2 \mathcal{J}^{(-)}(t)}{\partial t^2} \right)_{t_d} \neq 0, & (95) \end{aligned}$$

and

$$\det \mathbf{M}(t_d) = 0, \quad \text{tr} \mathbf{M}(t_d) \neq 0, \quad (96)$$

where

$$\mathbf{M}(t) = \mathcal{F}^{(-)}(t) \mathbf{O} \mathbf{K}, \quad (97)$$

in these expressions $\mathcal{J}^{(-)}(t)$ is the Jost determinant and $\mathcal{F}^{(-)}(t)$ is the Jost matrix, \mathbf{K} is the diagonal matrix of the wave numbers in the inner region and \mathbf{O} is the orthogonal matrix that diagonalizes the potential matrix \mathbf{V} in the inner region.

The coupled equations (94)–(96) were solved numerically to locate the exceptional point in the extended energy spectrum of the two-coupled-channel system. We also solved numerically the implicit transcendental equations (69) and (94)–(96) that define the eigenenergy surface of the degenerating isolated doublet of unbound states in the two-coupled-channel system in the simple but illustrative case of two square well confining potentials coupled by square potential barrier. From the explicit knowledge of the Jost determinant and the $\mathbf{M}(k)$ matrix as functions of the control parameters it is possible to obtain a two parameter function which is contact equivalent to the exact energy-pole position function at the degeneracy point in parameter space. This function is an unfolding of the exceptional point in parameter space and gives a very precise and accurate representation of the eigenenergy hypersurface in the neighborhood of the exceptional point. The hypersurface that represent the complex energy eigenvalues in parameter space has a branch point of rank 1 (square root type) at the exceptional point, it also has branch cuts in its real and imaginary parts that start at the same exceptional point but extend in opposite directions in parameter space. The properties of plane sections of the energy hypersurfaces with this interesting topology allow us to explain the rich phenomenology of crossings and anticrossings of energies and widths of the resonances in an isolated doublet and the

sudden change of shape of the \mathbf{S} -matrix pole trajectories in the complex energy plane observed when one control parameter is varied while the other is kept constant at a value close to the exceptional value.

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APPENDIX: PROPERTIES OF THE $\mathbf{S}(k)$ MATRIX

From Eq. (17), the scattering matrix is

$$\mathbf{S}(k) = \mathbf{k}^{-1/2} \mathcal{F}^{(+)}(k) [\mathcal{F}^{(-)}(k)]^{-1} \mathbf{k}^{+1/2}, \quad (A1)$$

and from Eq. (30) the Jost matrix $\mathcal{F}^{(-)}(k)$ is

$$\mathcal{F}^{(-)}(k) = \exp(ika) [\mathbf{O} \mathbf{K} \cos \mathbf{K}a - ik \mathbf{O} \sin \mathbf{K}a] \mathbf{K}^{-1} \mathbf{O}^T. \quad (A2)$$

From (A1) and (A2), the scattering matrix may be written as

$$\mathbf{S}(k) = \mathbf{k}^{-1/2} \mathbf{M}(-k) \mathbf{M}^{-1}(k) \mathbf{k}^{1/2}, \quad (A3)$$

where

$$\mathbf{M}(k) = \exp(ika) [\mathbf{O} \mathbf{K} \cos \mathbf{K}a - ik \mathbf{O} \sin \mathbf{K}a]. \quad (A4)$$

The matrix $\mathbf{M}(k)$ satisfies the symmetry property

$$\mathbf{M}(k) = \mathbf{M}^*(-k^*), \quad (A5)$$

which it inherits from the Jost matrix $\mathcal{F}^{(-)}(k)$ and the defining equations (28), (A2), and (A4).

The time reversal invariance of the system of coupled equations (10) implies that the scattering matrix $\mathbf{S}(k)$ is symmetric as may readily be verified from the expression (A3) and (A4).

First, from (A4)

$$\begin{aligned} \mathbf{M}^T(-k) \mathbf{k}^{-1} \mathbf{M}(k) &= \mathbf{K} \cos \mathbf{K}a (\mathbf{O}^T \mathbf{k}^{-1} \mathbf{O}) \mathbf{K} \cos \mathbf{K}a \\ &\quad + \sin \mathbf{K}a (\mathbf{O}^T \mathbf{k} \mathbf{O}) \sin \mathbf{K}a. \end{aligned} \quad (A6)$$

Since \mathbf{K} and \mathbf{k} are diagonal, the matrix on the right hand side of this equation is obviously symmetric.

Therefore,

$$\mathbf{M}^T(k) \mathbf{k}^{-1} \mathbf{M}(-k) = \mathbf{M}^T(-k) \mathbf{k}^{-1} \mathbf{M}(k). \quad (A7)$$

From this relation, it follows that

$$\mathbf{M}^T(-k) \mathbf{k}^{-1} = \mathbf{M}^T(k) \mathbf{k}^{-1} \mathbf{M}(-k) \mathbf{M}^{-1}(k), \quad (A8)$$

and

$$\mathbf{k}^{1/2} [\mathbf{M}(-k) \mathbf{M}^{-1}(k)]^T \mathbf{k}^{-1/2} = \mathbf{k}^{-1/2} \mathbf{M}(-k) \mathbf{M}^{-1}(k) \mathbf{k}^{1/2}. \quad (A9)$$

Comparing this last expression with Eq. (A3), we get

$$\mathbf{S}(k) = \mathbf{S}^T(k). \quad (A10)$$

Hence, the scattering matrix $\mathbf{S}(k)$ is symmetric.

Then, from (A3), (A5), and (A10), it follows that the scattering matrix is unitary:

$$\mathbf{S}^\dagger(k) = \mathbf{S}^{-1}(k). \quad (A11)$$

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