Crossings and Anticrossings of Energies and Widths and Changes of identity of the $S(E)$-matrix Poles.

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Contents

Background

The topological structure of the eigenenergy surface in parameter space at a degeneracy of unbound states arises naturally in connection with a number of subjects:

- Doublets and degeneracy of resonances in nuclear and particle physics and solid state physics
  P. von Brentano Phys. Rep. **264**, 57 (1996)
  E. Hernández and A. Mondragón Phys. Lett. **B326**,1 (1994);
  E. Hernández, A. Jáuregui and A. Mondragón, Phys. Rev. **A 67**, 022721-1, (2003); F. Keck, H.J. Korsch and S.Mossmann, J. Phys. A: Math. and Gen. **36** 2139 (2003); O.N. Kirillov, A.A. Mailybaev and A.P. Seyranian, J. Phys. A: Math. and Gen. **38**, 5531 (2005)
- Crossing and anticrossings of unbound levels
  P. von Brentano and M. Phillip Phys. Lett. **B 454**, 171 (1999); P. von Brentano, Rev. Mex. Fis. **48**, (S2), 1, (2002); A. Mondragón and E. Hernández J. Phys. A: Math. and Gen. **26**, 5595 (1993); Rev. Mex. Fis **49**, (S4), 60 (2003); Int. J. of Theor. Phys. (2005) in press; **W. Vanroose, Phys. Rev. A 64, 062708-1, (2001).**
- Topological Phase of resonant states
  A. Mondragón and E. Hernández J. Phys. A: Math. and Gen. **26**, 5595 (1993), Ibid **29**, 2567 (1996); C. Dembowski et al., Phys. Rev. Lett. **86**, (2001) 787; Phys. Rev. Lett. **90**, 034101-1, (2003); **W.D. Heiss Eur. Phys. D 7, 1, (1999)**
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- Resonance poles of higher rank in the scattering matrix;
  J.S. Bell and C.J. Goebel, Phys. Rev. **138 B**, 1198 (1995) E. Hernández, A. Jáuregui and A. Mondragón J. Phys. A: Math. and Gen. **33**, 4507, (2000)

Regular solutions of the radial equation

Consider a radial Hamiltonian depending on two real control parameters (X_1, X_2),

$$H_r^{(\ell)} \equiv \frac{\hbar^2}{2\mu}\Big[-\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2} + V(r; X_1, X_2)\Big].$$

The regular solution of the radial Schrödinger equation is the Jost solution

$$H_r^{(\ell)}(X_1, X_2)\phi_\ell(k, r; X_1, X_2) = k^2\phi_\ell(k, r; X_1, X_2)$$

$$\lim_{r\to 0}(2\ell+1)!!r^{-\ell-1}\phi_\ell(k, r; X_1, X_2) = 1.$$

The Jost solution, $\phi_\ell(k, r; X_1, X_2)$, is a linear combination of an incoming wave, $f(-k, r; X_1, X_2)$, and an outgoing wave $f(k, r; X_1, X_2)$

$$\phi_\ell(k, r) = \frac{1}{2}ik^{-\ell-1}\left[f_\ell(-k)f_\ell(k, r) - (-1)^\ell f_\ell(k)f_\ell(-k, r)\right]$$

The Jost function,

$$f_\ell(-k; X_1, X_2) \equiv f_\ell(-k, r = 0; X_1, X_2)$$

is a function of the complex wave number k and the real control parameters (X_1, X_2).

Physical solutions of the radial equation I

The scattering wave function, the scattering matrix and the Green's function have poles at the zeroes of the Jost function

Scattering wave function

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

Boundary conditions:

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

and

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

The scattering matrix is

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

The complete Green's function for outgoing particles or resolvent of the radial equation is

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

Physical solutions II

Bound and unbound or resonance state eigenfunctions

$$\frac{d^2 u_{n\ell}(r)}{dr^2} + \left[k_n^2 - \frac{\ell(\ell+1)}{r^2} - V(r; X_1, X_2, ...)\right] u_{n\ell}(r) = 0$$

Boundary conditions

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

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

This condition is satisfied when k_n is a zero (root) of the Jost function,

$$f_\ell(-k_n) = 0$$

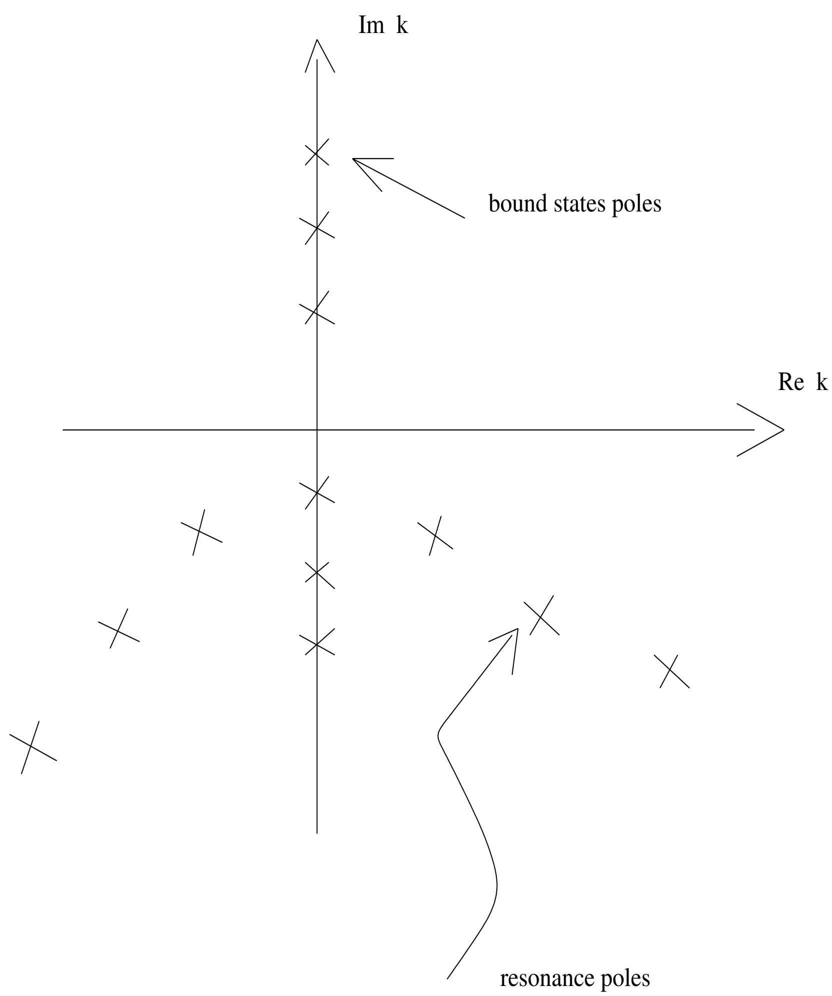
The zeroes of the Jost function define:

- the real (bound states) and complex (unbound states) energy eigenvalues
- the real (bound state) and complex (resonance states) poles of the scattering wave function, $\phi(k, r)$, the scattering matrix, $S(k)$, and the Green's function $G^{(+)}(k; r, r')$.

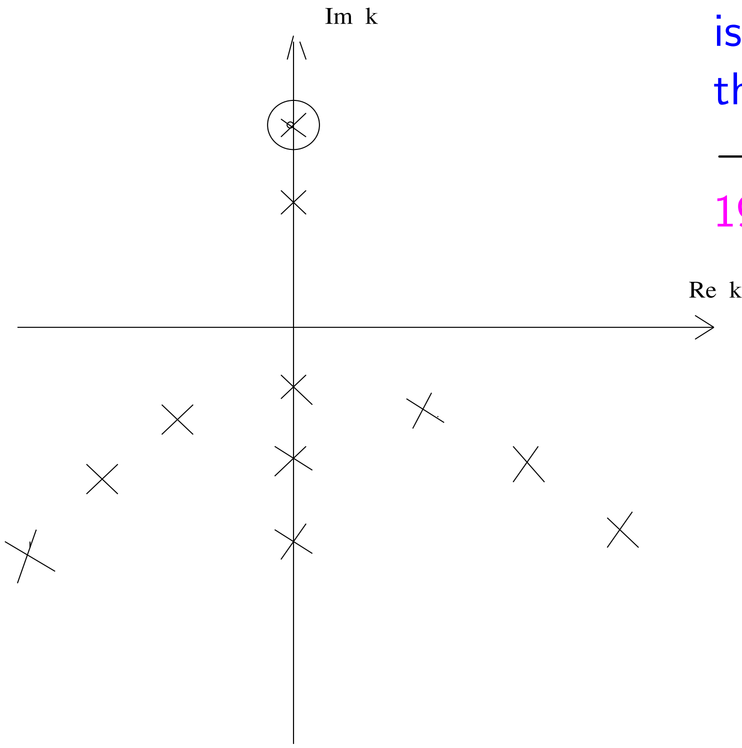
Zeroes of the Jost function

- When the first and second absolute moments of the potential exist and the potential decreases at infinity faster than any exponential, the functions $\phi_\ell(k,r)$, $k^\ell f_\ell(-k,r)$ and $f_\ell(-k)$, for fixed $r > 0$, are entire functions of k.

- The Jost function $f_\ell(-k)$ has zeroes (roots) on the imaginary axis and in the lower half of the complex k-plane



The no-crossing rule for bound states



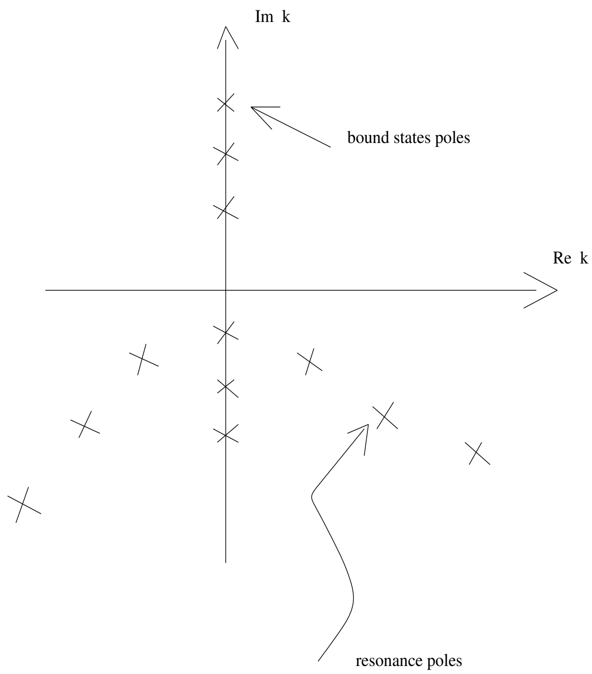
when $k_n = i\kappa_n$, $v_{n\ell}(\kappa_n, r)$ is the eigenfunction belonging to the real energy eigenvalue $\mathcal{E}_n = -\frac{\hbar^2}{2m}\kappa_n^2 < 0$ (R.G. Newton 1960).

$$N_{n\ell}^2 = \frac{1}{i4k_n^{2(\ell+1)}} f_\ell(k_n) \left(\frac{df_\ell(-k)}{dk}\right)_{k_n} = \int_o^\infty |u_{n\ell}(k_n, r)|^2 dr > 0$$

Hence $\left(\frac{df_\ell(-k)}{dk}\right)_{k_n} \neq 0$

- The zero of $f_\ell(-k_n)$ must be simple. The corresponding pole $G_\ell^{(+)}(k; r, r')$ and $S_\ell(k)$ must be simple
- In the absence of symmetry, the real negative energy eigenvalues of the radial Schrödinger equation can not be degenerate
- An accidental degeneracy is not possible between bound state eigenfunctions with the same ℓ values.

Accidental Degeneracy of Resonances I



Resonant States: When $k_n = \kappa_n - i\lambda_n$ and $u_{n\ell}(k_n, r)$ is the Gamow eigenfunction belonging to the complex energy eigenvalue $\mathcal{E}_n = \frac{2m}{\hbar}[(\kappa_n^2 - \lambda_n^2) - i2\kappa_n\lambda_n]$. Then, T. Berggreen (1968)

$$\frac{1}{i4k_n^{2(\ell+1)}} f_\ell(k_n) \left(\frac{df_\ell(-k)}{dk}\right)_{k_n} = \lim_{\mu\to 0} \int_o^\infty e^{-\mu r^2} u_{n\ell}^2(k_n, r) dr$$

The integral is a complex number and may vanish

$$\lim_{\mu\to 0} \int_o^\infty e^{-\mu r^2} u_{n\ell}^2(k_n, r) dr = 0 \quad \Leftrightarrow \quad \left(\frac{df_\ell(-k)}{dk}\right)_{k_n} = 0$$

- Whereas bound state poles of $S_\ell(k)$, $G_\ell^{(+)}(k; r, r')$ and $\psi_\ell^{(+)}(k, r)$ must be s imple, there is no general prohibition of multiple resonance poles in the complex k-plane.

  THE NO CROSSING RULE DOES NOT HOLD FOR RESONANT STATES

- Accidental degeneracy of complex energy eigenvalues may occur between resonant states with the same ℓ value.

Pole Position Function and Energy Hypersurfaces

The condition

$$f(-k; X_1, X_2) = 0$$

defines implicitly the Pole Position Functions

$$k_n = k_n(X_1, X_2)$$

as branches of a multivalued function

$$k_n = f^{-1}(0; X_1, X_2).$$

Each branch, $k_n(X_1, X_2)$, is a continuous single-valued function of the control parameters (X_1, X_2)

The energy eigenvalues are obtained from the zeros of the Jost function (Pole Position Function):

$$\mathcal{E}_n = \frac{\hbar^2}{2m} k_n^2(X_1, X_2)$$

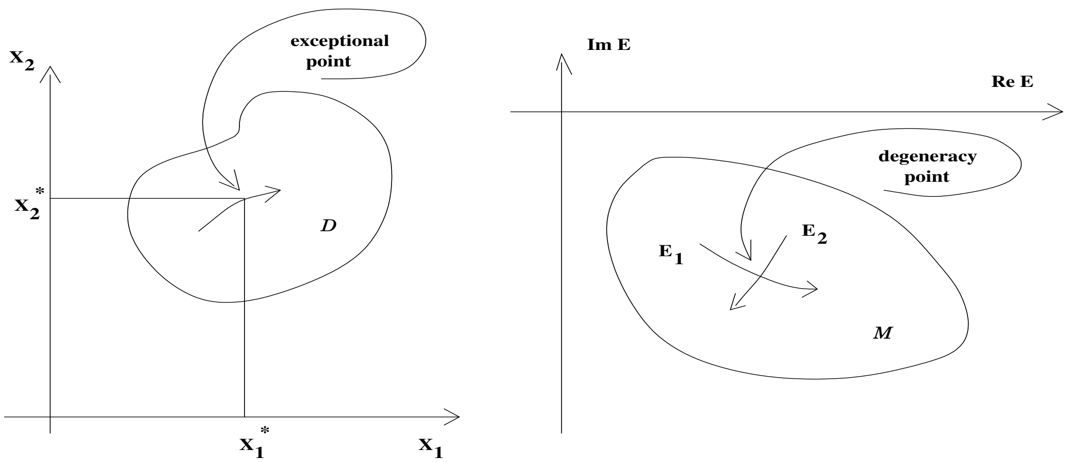
Each energy eigenvalue is represented as an energy hypersurface

$$\mathcal{E}_n = \mathcal{E}_n(X_1, X_2)$$

in a space with coordinates $(Re\mathcal{E}_n, Im\mathcal{E}_n, X_1, X_2)$

Isolated Doublet of Unbound States (IDUS)

A potential $V(r; X_1, X_2)$ with two regions of trapping may have isolated doublets of resonances



$$f(-k; X_1, X_2) = \Big(k - k_n(X_1, X_2)\Big)\Big(k - k_{n+1}(X_1, X_2)\Big) g(k)$$

$$\left.\begin{array}{c} g(k) \neq 0 \\ \frac{dg(k)}{dk} \neq 0 \end{array}\right\} \quad \text{when} \quad \begin{array}{c} (X_1, X_2) \,\epsilon\, \mathcal{D} \\ k \,\epsilon\, \mathcal{M} \end{array}$$

no other zeroes of $f(-k)$ in $\mathcal{M}$.

Degeneracy conditions: If for some value $(X_1^*, X_2^*) \,\epsilon\, \mathcal{D}$

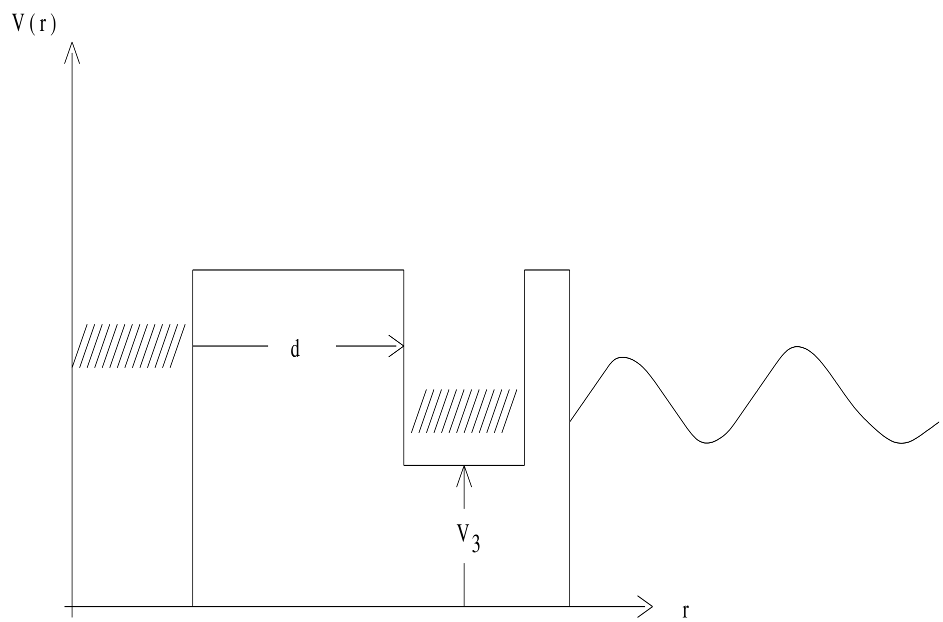
$$\left.\begin{array}{c} f(-k; X_1^*, X_2^*) = 0 \\ \frac{df(-k)}{dk} = 0 \end{array}\right\} \implies \left\{\begin{array}{c} (k - k_n^*)(k - k_{n+1}^*) = 0 \\ (k - k_n^*) + (k - k_{n+1}^*) = 0 \end{array}\right.$$

$$k_n(X_1^*, X_2^*) = k_{n+1}(X_1^*, X_2^*) = k_d$$

Scattering by a double barrier potential

E. Hernández, A. Jáuregui and A. Mondragón, Rev. Mex. Fis. **49**, (S4), 60 (2003). Doublets of resonances and accidental degeneracy of resonances may occur in the scattering of a beam of particles by a potential well with two regions of trapping. A simple example is provided by two concentric spherical potential barriers which divide space in three regions.

The system has seven parameters, we choose (d and V_3) as the external control parameters all other parameters are kept constant.



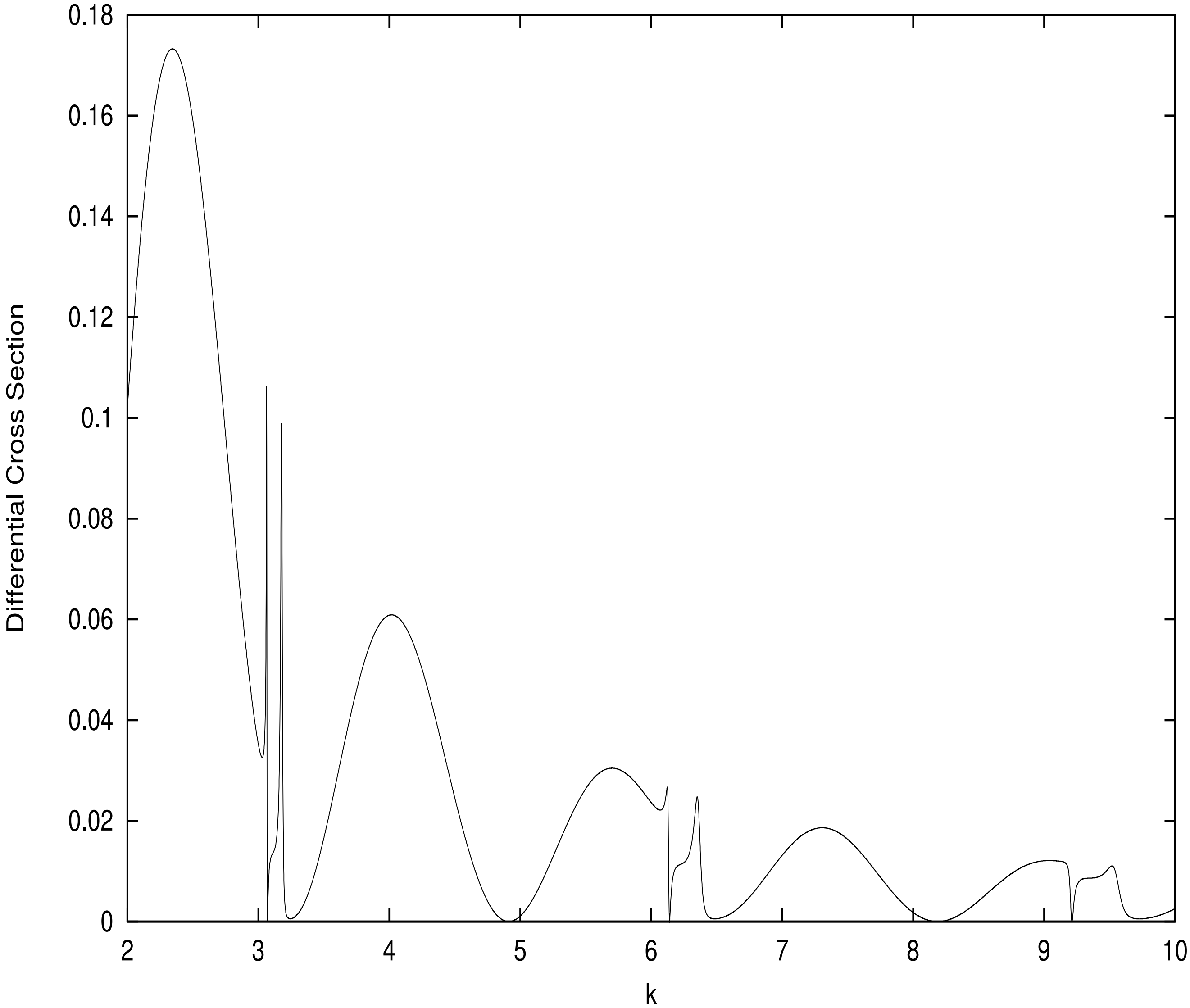
The s-wave radial Schrödinger equation is:

$$\frac{d^2\psi(k,r)}{dr^2} + \left(k^2 - V(r)\right)\psi(k,r) = 0$$

The scattering wavefunction, $\psi(k,r)$, is related to the regular Jost solution $\phi(k,r)$ and the Jost function $f(-k)$ by

$$\psi(k,r) = -\frac{2ik}{f(-k)}\phi(k,r)$$

Isolated doublet of unbound states in a double barrier potential



Pole Position Function of an IDUS

When the Jost function has an isolated doublet of zeros

$$f(-k;X_1,X_2) = \Big(k - k_n(X_1,X_2)\Big)\Big(k - k_{n+1}(X_1,X_2)\Big)g_{n,n+1}(k)$$

$$g_{n,n+1}(k;X_1,X_2) \neq 0 \qquad \frac{dg_{n,n+1}(k;X_1,X_2)}{dk} \neq 0$$

The vanishing of the Jost function defines the Pole Position Function $k_{n,n+1}(X_1,X_2)$ of the Isolated Doublet of Unbound States (IDUS)

$$\Big[k_{n,n+1} - \frac{1}{2}(k_n(X_1,X_2) + k_{n+1}(X_1,X_2)\Big]^2 - \frac{1}{4}\Big(k_n(X_1,X_2) - k_{n+1}(X_1,X_2)\Big)^2 = \frac{f(-k;X_1,X_2)}{g_{n,n+1}(k;X_1,X_2)}$$

Hence,

$$\begin{aligned} k_{n,n+1}(X_1,X_2) &= \frac{1}{2}\Big(k_n(X_1,X_2) + k_{n+1}(X_1,X_2)\Big) \\ &\pm \sqrt{\frac{1}{4}\Big(k_n(X_1,X_2) - k_{n+1}(X_1,X_2)\Big)^2} \end{aligned}$$

this expression relates the Pole Position Function of IDUS to the Pole Position Functions of the individual unbound states in the doublet

The Pole Position Function of an IDUS at an exceptional point

From the preparation theorem (Weierstrass)

$$f(-k; X_1, X_2) = \Big[\Big(k - \frac{1}{2}\big(k_n(X_1, X_2) + k_{n+1}(X_1, X_2)\big)\Big)^2 - \frac{1}{4}\Big(k_n(X_1, X_2) - k_{n+1}(X_1, X_2)\Big)^2\Big] g_{n,n+1}(k; X_1, X_2)$$

The functions, $\frac{1}{2}\big(k_n(X_1, X_2)+k_{n+1}(X_1, X_2)\big)$ and $\frac{1}{2}\big(k_n(X_1, X_2)-k_{n+1}(X_1, X_2)\big)^2$, are regular at the exceptional point (X_1^*, X_2^*), and admit a Taylor series expansion about that point

$$\frac{1}{4}\Big(k_n(X_1, X_2) - k_{n+1}(X_1, X_2)\Big)^2 = c_1^{(1)}(X_1 - X_1^*) + c_2^{(1)}(X_2 - X_2^*) + \ldots.$$

$$\frac{1}{2}\Big(k_n(X_1, X_2) + k_{n+1}(X_1, X_2)\Big) = d_1^{(1)}(X_1 - X_1^*) + d_2^{(2)}(X_2 - X_2^*) + \ldots$$

where,

$$c_{1,2}^{(1)} = \frac{-2}{\Big[\Big(\frac{\partial^2 f(-k;x_1,x_2)}{\partial k^2}\Big)_{x_1^*,x_2^*}\Big]_{k=k_d}} \Big[\Big(\frac{\partial f(-k; x_1, x_2)}{\partial x_{1,2}}\Big)_{x_{2,1}}\Big]_{k_d},$$

$$d_{1,2}^{(1)} = \frac{-1}{\Big[\Big(\frac{\partial^2 f(-k;x_1,x_2)}{\partial k^2}\Big)_{x_1^*,x_2^*}\Big]_{k=d_d}} \Big\{\Big[\Big(\frac{\partial^2 f(-k; x_1, x_2)}{\partial x_1 \partial k}\Big)_{x_2}\Big]_{k=k_d} - \frac{1}{\Big[\Big(\frac{\partial^2 f(-k;x_1,x_2)}{\partial k^2}\Big)_{x_1^*,x_2^*}\Big]_{k=k_d}} \frac{1}{3}\Big[\Big(\frac{\partial^3 f(-k; x_1, x_2)}{\partial k^3}\Big)_{x_1^*,x_2^*}\Big]_{k=k_d} \times \Big[\Big(\frac{\partial f(-k; x_1, x_2)}{\partial x_1}\Big)_{x_2}\Big]_{k=k_d}\Big\}.$$

The contact equivalent normal form

The two families of functions

$$\begin{aligned} k_{n,n+1}(X_1, X_2) &= \frac{1}{2}\Big(k_n(X_1, X_2) + k_{n+1}(X_1, X_2)\Big) \\ &\pm \sqrt{\frac{1}{4}\Big(k_n(X_1, X_2) - k_{n+1}(X_1, X_2)\Big)^2} \end{aligned}$$

and

$$\begin{aligned} \hat{k}_{n,n+1}(X_1, X_2) &= k_d + \Delta^{(1)}k(X_1, X_2) \\ &\pm \sqrt{c_1^{(1)}(X_1 - X_1^*) + c_2^{(2)}(X_2 - X_2^*)} \end{aligned}$$

are contact equivalent at the exceptional point (X_1^*, X_2^*)

Theorem

At the exceptional point (X_1^*, X_2^*), the multivalued Pole Position Function of the Isolated Doublet of Unbound States, $k_{n,n+1}(X_1, X_2)$ has an algebraic branch point of square root type (rank one).

Unfolding of a Rank one Degeneracy Point

The two parameter family of functions:

$$\hat{f}_{doub}(-k;\xi_1,\xi_2) = \Big[k - \Big(k_d + \Delta^{(1)}k_d(\xi_1,\xi_2)\Big)\Big]^2 - \frac{1}{4}\Big((\vec{\mathcal{R}}\cdot\vec{\xi}) + i(\vec{\mathcal{I}}\cdot\vec{\xi})\Big),$$

is conctact equivalent to the Jost function $f(-k;\xi_1,\xi_2)$, at the exceptional point. It is also an unfolding of $f(-k;\xi_1,\xi_2)$ with the following features:

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

   $$\hat{f}_{doub}(-k;\xi_1,\xi_2) = 0$$

   and

   $$\Big(\frac{\partial \hat{f}_{doub}(-k;\xi_1,\xi_2)}{\partial k}\Big)_{k_d} = 0, \qquad \Big(\frac{\partial^2 \hat{f}_{doub}(-k;\xi_1,\xi_2)}{\partial k^2}\Big)_{k_d} \neq 0$$

   up to contact equivalence, and gives

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

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

Therefore, $\hat{f}_{doub}(-k;\xi_1,\xi_2)$ is a universal unfolding of the Jost function $f(-k;\xi_1,\xi_2)$ at the degeneracy of unbound states $\big(k = k_d$, $\xi_1 = (X_1 - X_1^*) = 0,\ \xi_2 = (X_2 - X_2^*) = 0\big)$

Contact equivalent approximant to the energy hypersurface

From

$$\left(\mathcal{E}_n - \mathcal{E}_{n+1}\right)^2 = \frac{\hbar^2}{2m}\left(k_n + k_{n+1}\right)^2\left(k_n - k_{n+1}\right)^2$$

and our previous results:

- The energy hypersurface $\mathcal{E}_{n,n+1}(X_1, X_2)$ is contact equivalent to the function

$$\begin{aligned}\hat{\mathcal{E}}_{n,n+1}(X_1, X_2) &= \frac{1}{2}\Big(\mathcal{E}_n(X_1, X_2) + \mathcal{E}_{n+1}(X_1, X_2)\Big) \\ &\pm \sqrt{\mathcal{C}_1^{(1)}(X_1 - X_1^*) + \mathcal{C}_2^{(2)}(X_2 - X_2^*)}\end{aligned}$$

  at the exceptional point (X_1^*, X_2^*) in parameter space

- The hypersurfaces representing the complex resonance energy eigenvalues, as functions of the external control parameters, have an algebraic branch point of square root type (rank one) at the exceptional point (X_1^*, X_2^*) in parameter space.

Branch point and branch cuts in parameter space I

Notation

$$\vec{\xi} = \begin{pmatrix} \xi_1 \\ \xi_2 \end{pmatrix} = \begin{pmatrix} X_1 - X_1^* \\ X_2 - X_2^* \end{pmatrix}, \quad \vec{R} = \begin{pmatrix} Re\ C_1^{(1)} \\ Re\ C_2^{(1)} \end{pmatrix}, \quad \vec{I} = \begin{pmatrix} Im\ C_1^{(1)} \\ Im\ C_2^{(1)} \end{pmatrix}.$$

Then, the energy-pole position function is

$$\hat{\mathcal{E}}_{n,n+1}(\xi_1, \xi_2) = \mathcal{E}_d + \Delta^{(1)}\mathcal{E}_d(\xi_1, \xi_2) + \hat{\epsilon}_{n,n+1}(\xi_1, \xi_2),$$

where

$$\hat{\epsilon}_{n,n+1}(\xi_1, \xi_2) = \sqrt{\frac{1}{4}\left[(\vec{R} \cdot \vec{\xi}) + i(\vec{I} \cdot \vec{\xi})\right]}$$

A little algebra gives,

$$Re\hat{\epsilon}_{n,n+1}(\xi_1, \xi_2) = \pm\frac{1}{2\sqrt{2}}\left[+\sqrt{\left(\vec{R} \cdot \vec{\xi}\right)^2 + \left(\vec{I} \cdot \vec{\xi}\right)^2} + \vec{R} \cdot \vec{\xi}\right]^{1/2}$$

and

$$Im\ \hat{\epsilon}_{n,n+1}(\xi_1, \xi_2) = \pm\frac{1}{2\sqrt{2}}\left[+\sqrt{\left(\vec{R} \cdot \vec{\xi}\right)^2 + \left(\vec{I} \cdot \vec{\xi}\right)^2} - \vec{R} \cdot \vec{\xi}\right]^{1/2}$$

Branch point and branch cuts in parameter space II

From our previous results, $(\xi_i = X_i - X_i^*) \quad i = 1, 2$

$$Re\hat{\epsilon}_{n,n+1}(\xi_1, \xi_2) = \pm\frac{1}{2\sqrt{2}}\left[+\sqrt{\left(\vec{R}\cdot\vec{\xi}\right)^2 + \left(\vec{I}\cdot\vec{\xi}\right)^2} + \vec{R}\cdot\vec{\xi}\right]^{1/2}$$

Hence, the real part of the energy-pole position function, $Re\hat{\epsilon}_{n,n+1}(\xi_1, \xi_2)$, has an algebraic branch point of square root type (rank one) at the exceptional point 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

$$\mathcal{L}_R : \vec{I}\cdot\hat{\xi}_c = 0 \quad \text{and} \quad \vec{R}\cdot\hat{\xi}_c = -|\vec{R}\cdot\hat{\xi}_c|$$

Similarly,

$$Im\ \hat{\epsilon}_{n,n+1}(\xi_1, \xi_2) = \pm\frac{1}{2\sqrt{2}}\left[+\sqrt{\left(\vec{R}\cdot\vec{\xi}\right)^2 + \left(\vec{I}\cdot\vec{\xi}\right)^2} - \vec{R}\cdot\vec{\xi}\right]^{1/2}$$

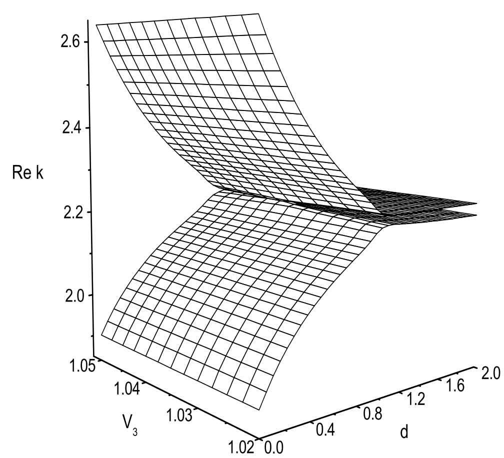
The imaginary part of the energy-pole position function, $Im\ \epsilon_{n,n+1}(\xi_1, \xi_2)$, also has an algebraic branch point of square root type (rank one) at the exceptional point in parameter space, and also has a branch cut along a line, $\mathcal{L}_I$, that starts at the exceptional point and extends in the negative direction defined by the unit vector $\hat{\xi}_c$ satisfying

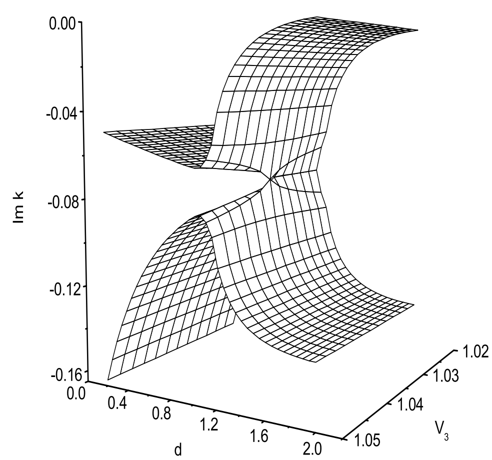
$$\mathcal{L}_I : \vec{I}\cdot\hat{\xi}_c' = 0 \qquad \text{and} \qquad \vec{R}\cdot\hat{\xi}_c' = -|\vec{R}\cdot\hat{\xi}_c'|$$

Unfolding a degeneracy point

Eigenwave Number Hypersurfaces

The surfaces, S_R and S_I, that represent the real and imaginary parts of the eigenwave numbers, k_1 and k_2 at the crossing, as functions of the control parameters (d, V_3)





Phenomenology of the exceptional point

Phenomenological manifestations of the geometrical properties of the energy surfaces close to a crossing of unbound states (close to the exceptional point).

- When one parameter is slowly varied keeping the other constant close to the exceptional point

  I Crossing and anticrossings of energies and widths

  II Change of identity of the pole trajectories of the scattering matrix in the E-plane

- When the system is slowly transported around the exceptional point in a double circuit in parameter space

  III The wave function acquires a geometric (Berry) phase

Sections of the energy surfaces

The intersection of the eigenenergy surface of the isolated doublet of unbound states, $S_{n,n+1}$, and the hyperplanes $\pi_i : \xi_2 = \bar{\xi}_2^{(i)}$, defines two-three-dimensional curves

$$S_{n,n+1} \bigcap \pi_i = \begin{cases} C_n(\pi_i) \\ C_{n+1}(\pi_i) \end{cases}$$

$$S_{n,n+1} : \frac{1}{2}\Big(\mathcal{E}_n(\xi_1,\xi_2) + \mathcal{E}_{n+1}(\xi_1,\xi_2)\Big) \pm \sqrt{\frac{1}{4}\big(\mathcal{E}_n(\xi_1,\xi_2) - \mathcal{E}_{n+1}(\xi_1,\xi_2)\big)^2}$$

$$\pi_i : \xi_2 = \bar{\xi}_2^{(i)}, \qquad\qquad i = 1, 2, 3$$

The sections, $C_n(\pi_i)$ and $C_{n+1}(\pi_i)$ are three dimensional curves traced by the points $\mathcal{E}_n(\xi_1, \bar{\xi}_2)$ and $\mathcal{E}_{n+1}(\xi_1, \bar{\xi}_2^{(i)})$ on the hypersurfaces $\epsilon_{n,n+1}(\xi_1, \xi_2)$ when the point $(\xi_1, \bar{\xi}_2^{(i)})$ moves along the straight line path π_i in parameter space.

Projections of the sections of the energy surfaces I

The projections of the sections $C_n(\pi_i)$ and $C_{n+1}(\pi_i)$ on the three orthogonal planes (Reϵ, ξ_i), (Imϵ, ξ_1) and (Reϵ, Imϵ) are accesible to experimental determination.

I. The projections of $C_n(\pi_i)$ and $C_{n+1}(\pi_i)$ on the plane (Reϵ, ξ_1) shows the crossings or anticrossings of the energies

$$Re\big[C_n(\pi_i)\big] = -Re\big[C_{n+1}(\pi_i)\big] = -\sigma_n^{(R)} Re\big[\epsilon_{n,n+1}\big(\xi_1, \bar{\xi}_2^{(i)}\big)\big]$$

II. The projections of $C_n(\pi_i)$ and $C_{n+1}(\pi_i)$ on the plane $(Im\epsilon, \xi_1)$ show the crossings or anticrossings of the widths

$$Im\big[C_n(\pi_i)\big] = -Im\big[C_{n+1}(\pi_i)\big] = -\sigma_n^{(I)} Im[\epsilon_{n,n+1}\big(\xi_1, \bar{\xi}_2^{(i)}\big)]$$

III. The projections of $C_n(\pi_i)$ and $C_{n+1}(\pi_i)$ on the plane $(Re\epsilon, Im\epsilon)$ are the trajectories of the poles on the complex energy plane.

Projections of the sections of the energy surfaces II

Very accurate analytical approximations for the projections of the sections of the energy surfaces are obtained from the contact equivalent approximant at the exceptional point

I. The projections of the sections $\hat{C}_n(\pi_i)$ and $\hat{C}_{n,+1}(\pi_i)$ on the plane $(Re\epsilon, \xi_1)$ are

$$Re\Big[\hat{C}_n(\pi_i)\Big] = -Re\Big[\hat{C}_{n+1}(\pi_i)\Big] = -Re\hat{\mathcal{E}}_n(\xi_1, \bar{\xi}_2^{(i)})$$

where

$$Re\hat{\mathcal{E}}_n(\xi_1, \bar{\xi}_2^{(i)}) = \frac{\sigma_R^{(n)}}{2\sqrt{2}}|C_1^{(1)}|\Big[+\sqrt{\xi_1^2 + 2z_i\cos(\phi_1 - \phi_2)\xi_1 + z_i^2} + \Big(\cos\phi_1\xi_1 + \cos\phi_2 z_i\Big)\Big]^{1/2}$$

z_i, ϕ_1 and ϕ_2 are constants.

II. The projections of the sections $\hat{C}_n(\pi_i)$ and $\hat{C}_{n+1}(\pi_i)$ on the plane $(Im\epsilon, \xi_1)$ are

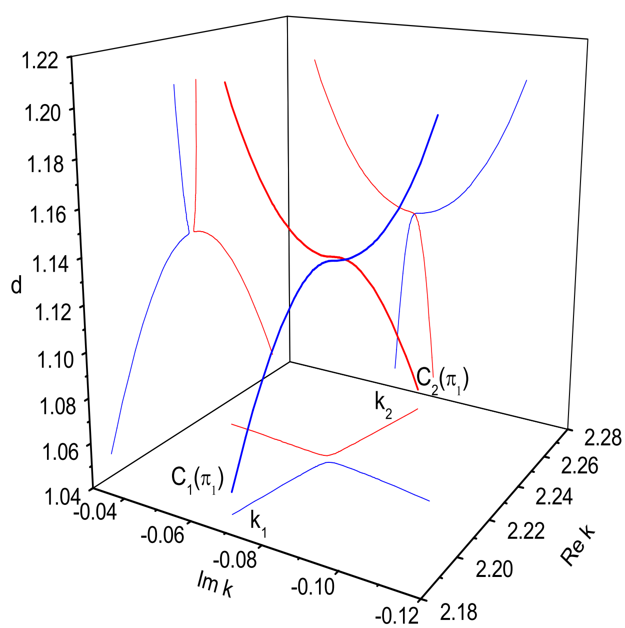
$$Im\Big[\hat{C}_n(\pi_i)\Big] = -Im\Big[\hat{C}_{n+1}(\pi_i)\Big] = Im\hat{\mathcal{E}}_n(\xi_1, \bar{\xi}_2^{(i)})$$

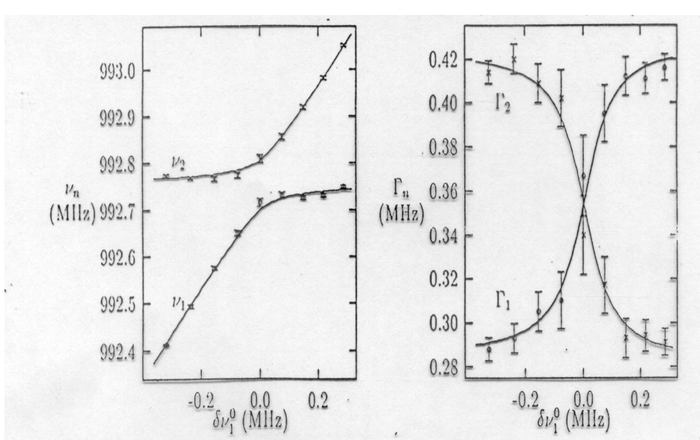
where

$$Im\hat{\mathcal{E}}_n(\xi_1, \bar{\xi}_2^{(i)}) = \frac{\sigma_I^{(n)}}{2\sqrt{2}}|c_1^{(1)}|\Big[+\sqrt{\xi_1^2 + 2z_i\cos(\phi_1 - \phi_2)\xi_i + z_i^2} - (\cos\phi_1\xi_1 + \cos\phi_2 z_i)\Big]^{1/2}$$

Crossings and anticrossings of $Re\ k_n(d, V_3)$ **and** $Im\ k_n(d, V_3)$

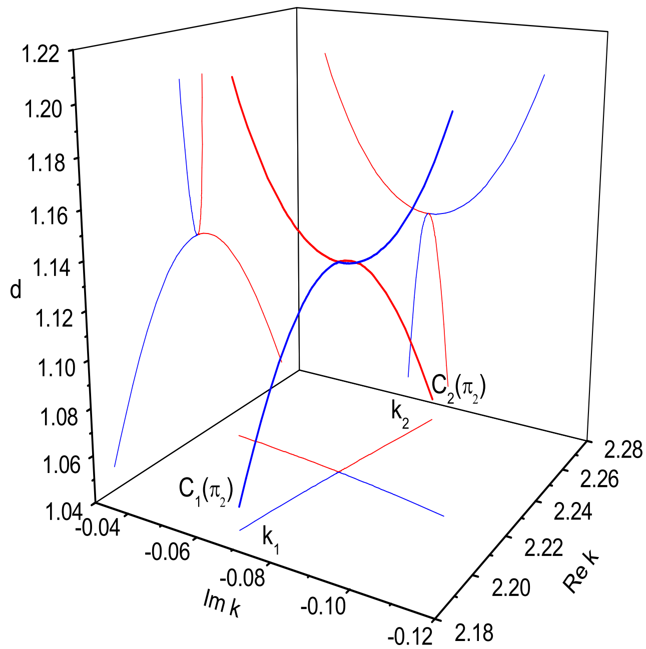
- **The projections of $\mathbf{C_1}$ and $\mathbf{C_2}$ on the plane (Re k, d) for fixed V_3 give the crossings or anticrossings of the energy levels. The projections of $\mathbf{C_1}$ and $\mathbf{C_2}$ on the plane (Re k, Im k) give the pole trajectories in the complex $k-$plane**





M. Phillipp, P. von Brentano, G. Pascovici and A. Richter. PRE 62, 1922,(2000)

Degeneracy point

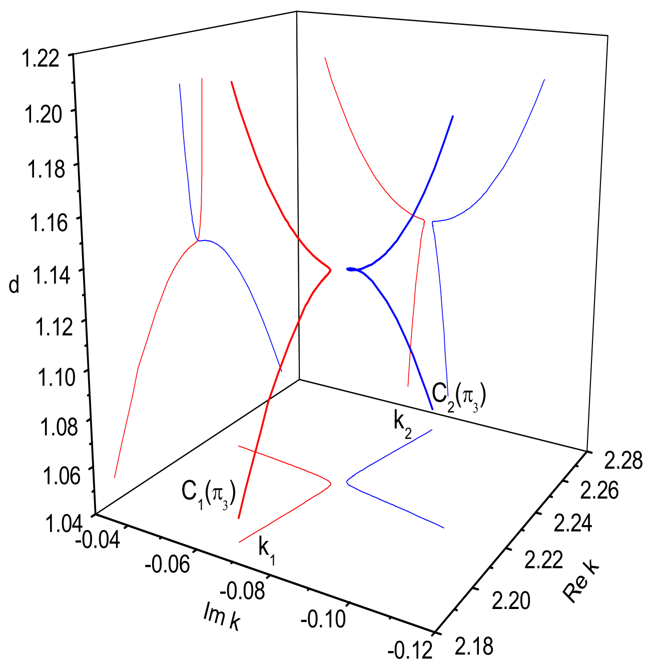


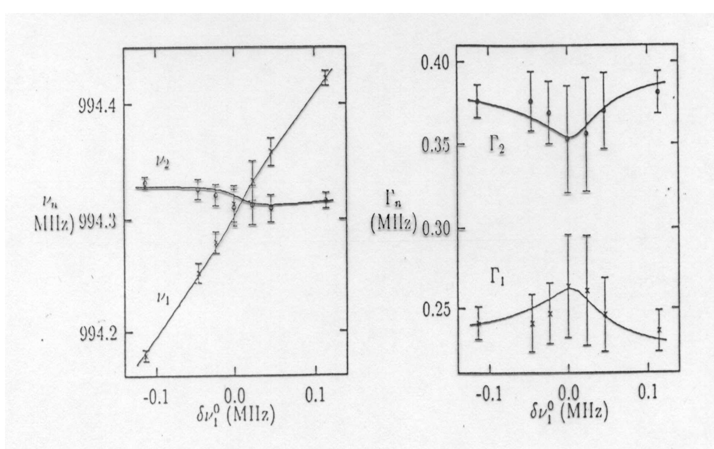
$$V_3^* = \mathbf{1.038235081}$$

$$d^* = \mathbf{1.1314661145}$$

- The projections of $\mathbf{C_1}$ and $\mathbf{C_2}$ on the plane **(Im k, d)** for V_3 fixed give the crossings or anticrossings of the widths

$$V_3 = \mathbf{1.0384}$$





M. Phillipp, P. von Brentano, G. Pascovici and A. Richter. PRE 62, 1922,(2000)

Real and Imaginary parts of $\mathcal{E}_{1,2}(d, \bar{V}_3)$ as a function of d, and $V_3 = 1.0381$ fixed

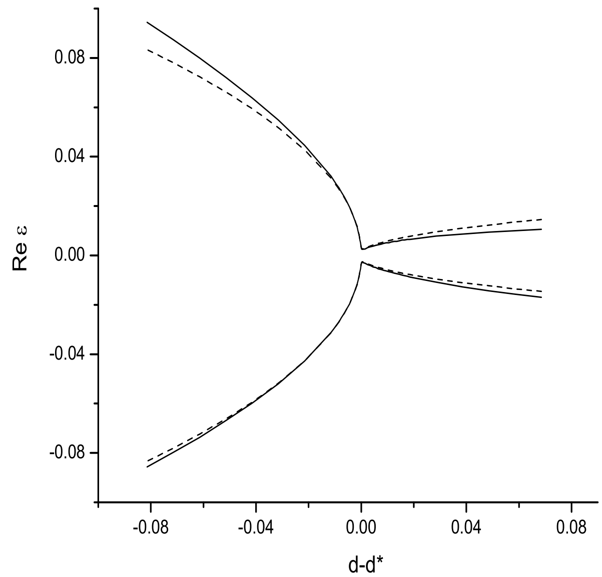


Figure 1:

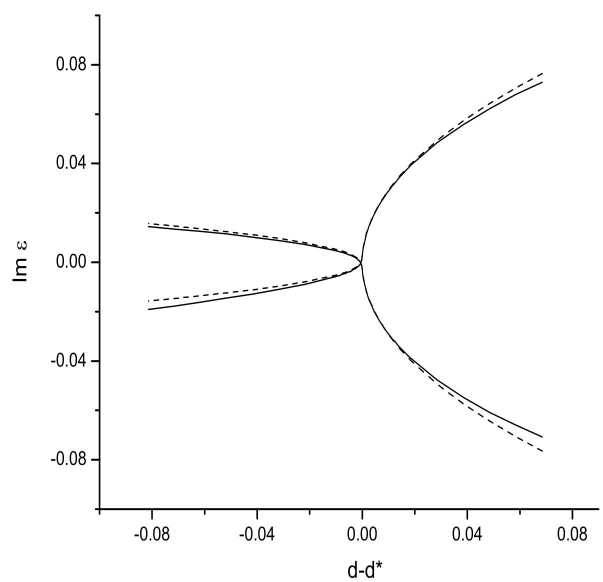


Figure 2: $V_3 = 1.0381$

- - - - - - contact equivalent approximant

———————— numerically exact

Real and Imaginary parts of $\mathcal{E}_{1,2}(d, \bar{V}_3)$ as a function of d, and $V_3 = 1.038235081$ fixed

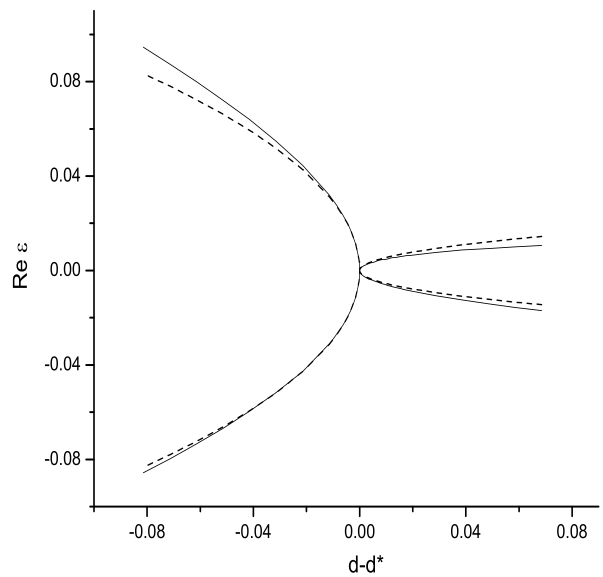


Figure 3: $V_3 = 1.038235081$

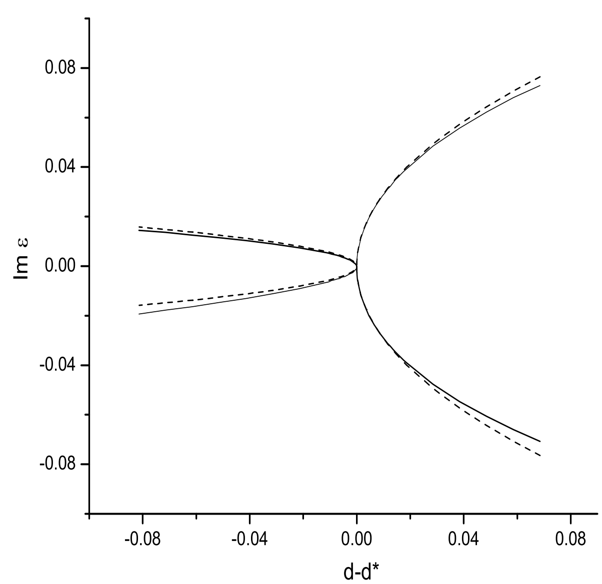


Figure 4: $V_3 = 1.038235081$

- - - - - - contact equivalent approximant

—————— numerically exact

Real and Imaginary parts of $\mathcal{E}_{1,2}(d, \bar{V}_3)$ as a function of d, and $V_3 = 1.0384$ fixed

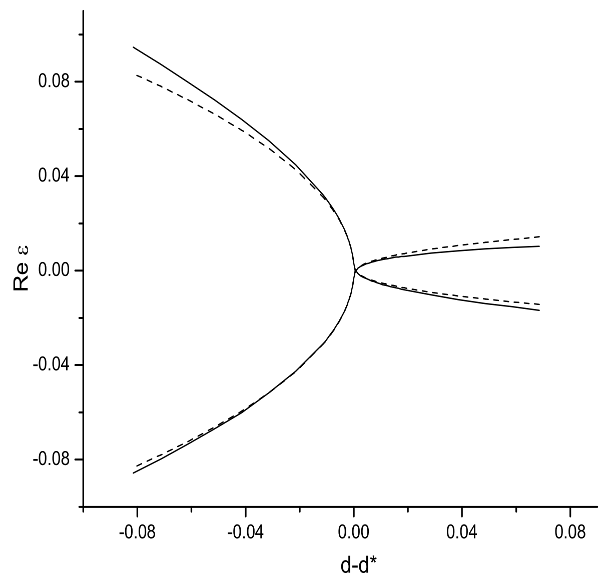


Figure 5: $V_3 = 1.0384$

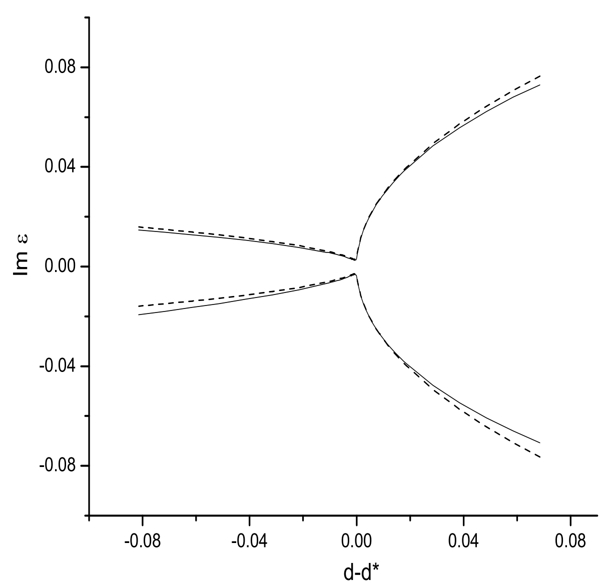


Figure 6: $V_3 = 1.0384$

- - - - - - contact equivalent approximant

————— numerically exact

Crossings and anticrossings of energies and widths I

Standard notation: $\mathcal{E}_n = E_n - i\frac{1}{2}\Gamma_n$

Crossings of energies

$$\Delta E = E_n - E_{n+1} = 0 \quad \rightarrow \quad Re\left[\hat{C}_n(\pi_i)\right]\Big|_{\vec{\xi}=\vec{\xi}_c} = Re\left[\hat{C}_{n+1}(\pi_i)\right]\Big|_{\vec{\xi}=\vec{\xi}_c}$$

if and only if $\vec{I}\cdot\vec{\xi}_c = 0$ **and**

$$\left[+\sqrt{\left(\vec{R}\cdot\vec{\xi}_c\right)^2 + \left(\vec{I}\cdot\vec{\xi}_c\right)^2} + \vec{R}\cdot\vec{\xi}_c\right]\Big|_{\xi_2=\bar{\xi}_2^{(i)}} = 0$$

A crossing of energies, $\Delta E = 0$**, occurs at the intersection of the hyperplane,** $\xi_2 = \bar{\xi}_2^{(i)}$**, and the branch cut line** $\mathcal{L}_R$

Crossings of widths:

$$\Delta\Gamma = \Gamma_n - \Gamma_{n+1} = 0 \quad \rightarrow \quad Im\left[\hat{C}_n(\pi_i)\right]\Big|_{\vec{\xi}'=\vec{\xi}'_c} = Im\left[\hat{C}_{n+1}(\pi_i)\right]\Big|_{\vec{\xi}'=\vec{\xi}'_c}$$

if and only if $\vec{I}\cdot\vec{\xi}_c = 0$ **and**

$$\left[+\sqrt{\left(\vec{R}\cdot\vec{\xi}'_c\right)^2 + \left(\vec{I}\cdot\vec{\xi}'_c\right)^2} - \vec{R}\cdot\vec{\xi}'_c\right]\Big|_{\xi'_2=\bar{\xi}_2^{(i)}} = 0$$

A crossings of widths, $\Delta\Gamma = 0$**, occurs at the intersection of the hyperplane** $\xi'_2 = \bar{\xi}_2^{(i)}$ **and the branch cut line** $\mathcal{L}_I$

Crossings and anticrossings of energies and widhts II

A generalization of the level repulsion theorem (von Neumann and Wigner) from bound to unbound states.

From our previous expressions

$$\Delta E \Delta \Gamma = -\frac{1}{2}\Big(\vec{I}\cdot\vec{\xi}\Big)\Big|_{\xi_2=\bar{\xi}_2^{(i)}}$$

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

For $(\vec{I}\cdot\vec{\xi}_c)_{\bar{\xi}_2^{(i)}} = 0$**, we find three cases:**

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** $\Delta\Gamma = 0$**,**
a joint energy and width crossings, that is, exact 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.

Trajectories of the S-matrix poles and changes of identity

Eliminating ξ_1 between $Re\hat{\mathcal{E}}_n(\xi_i, \bar{\xi}_2^{(i)})$ and $Im\hat{\mathcal{E}}_n(\xi_i, \bar{\xi}_2^{(i)})$ we obtain the equation of the trajectories of the poles

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

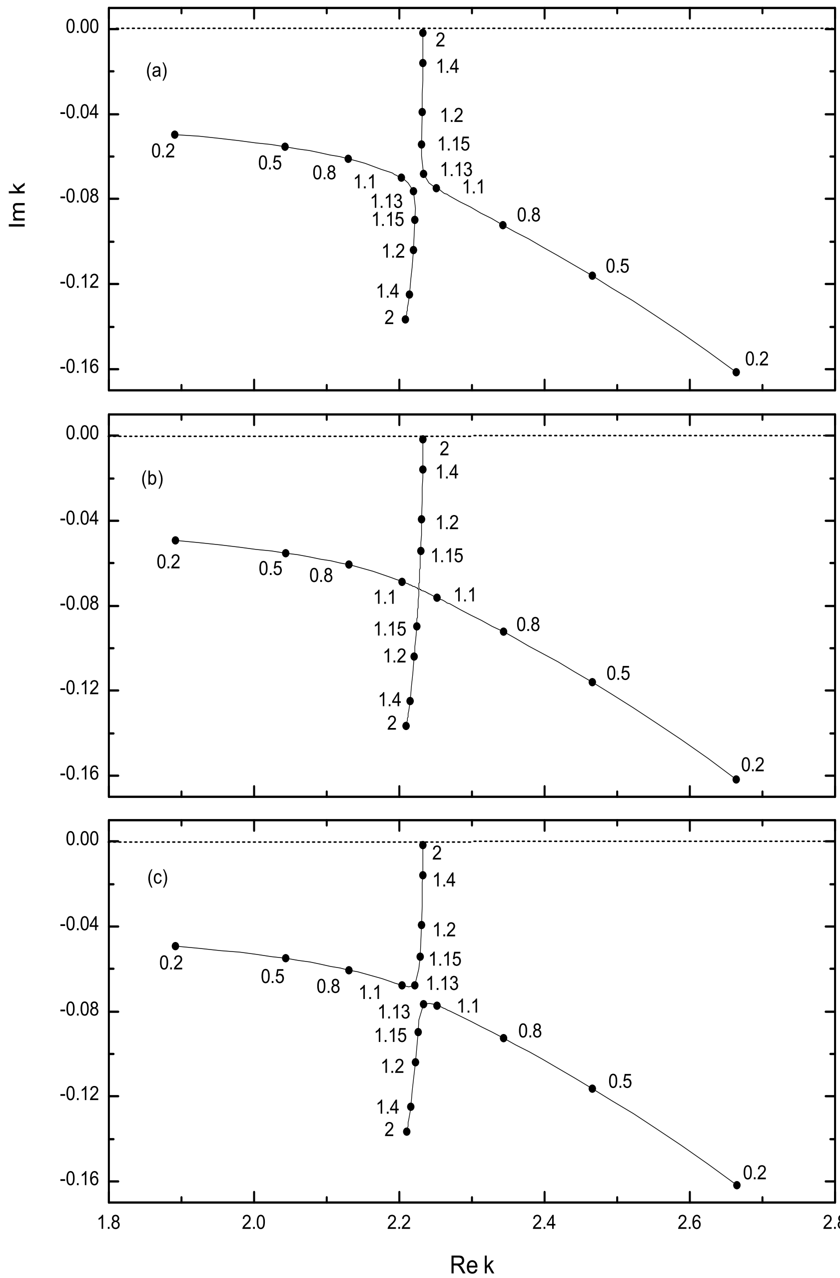
Close to the crossing point, the trajectories of the S-matrix poles of an IDUS in the complex energy plane are the branches of a hyperbola

1. $\left(\vec{R}\cdot\vec{\xi}_c\right)\big|_{\xi_2=\bar{\xi}_2^{(i)}} > 0$ **Anticrossing of energies and crossing of widths**

2. $\left(\vec{R}\cdot\vec{\xi}_c\right)\big|_{\xi_2=\bar{\xi}_2^{(i)}} = 0$ **Joint crossing of energies and widths**

3. $\left(\vec{R}\cdot\vec{\xi}_c\right)\big|_{\xi_2=\bar{\xi}_2^{(i)}} < 0$ **Crossing of energies and anticrossing of widths**

"Change of identity" of the poles' trajectories close to a degeneracy



This plot shows the poles' trayectories of the scattering matrix $S(k)$ in the complex $k-$ plane, for fixed V_3 and 1.02 $\leq d \leq$ 1.2; $V_3^{(1)} =$ 1.0381, $V_3^{(2)} =$1.038235081, $V_3^{(3)} =$ 1.0384

“Change of identity” of the poles’ trajectories close to a degeneracy

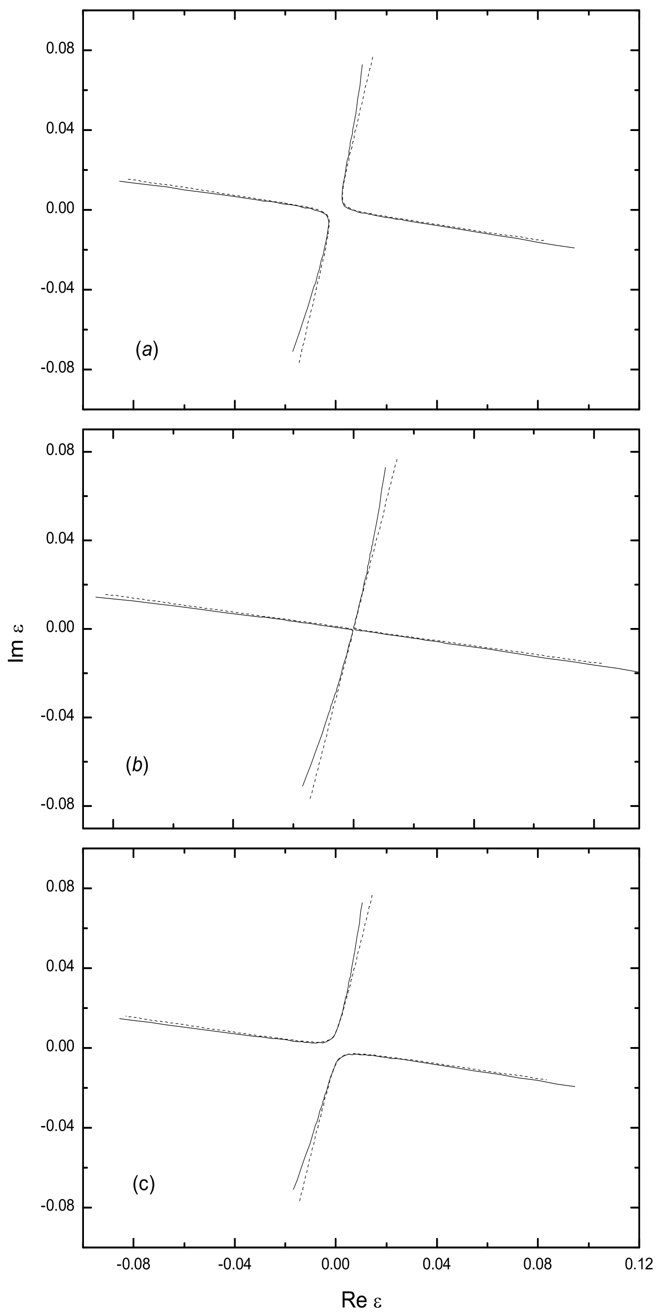


Figure 7: $V_3 = 1.0384$

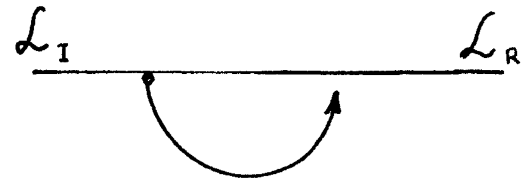
- - - - - - contact equivalent approximant

———————— numerically exact

Going around the exceptional point

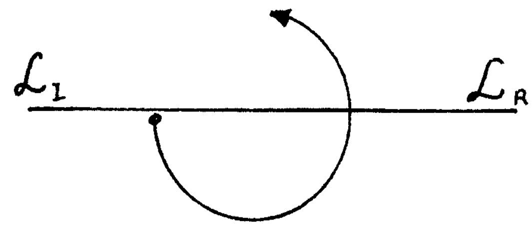
$k_{1i} = Rek^{I} + iImk^{I}$

$k_{2i} = Rek^{II} + iImk^{II}$



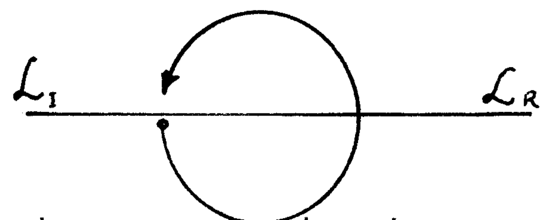
$k_1 = Rek^{II} + iImk^{I}$

$k_2 = Rek^{I} + iImk^{II}$



$k_{1f} = Rek^{II} + iImk^{II}$

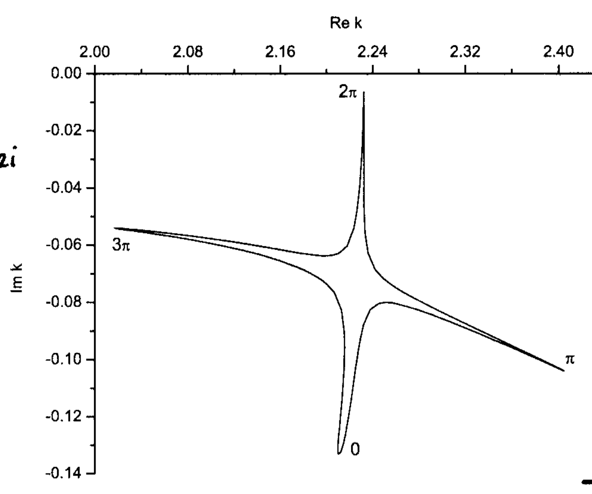
$k_{2f} = Rek^{I} + iImk^{I}$

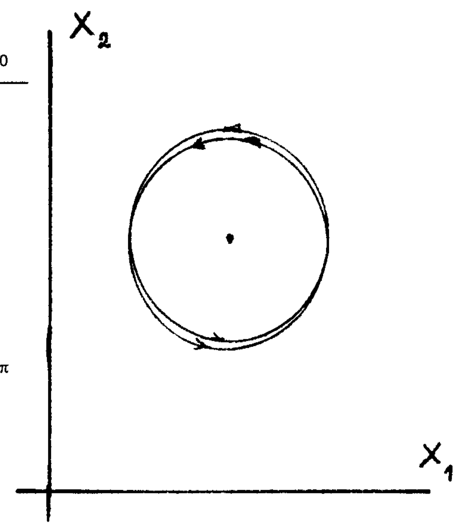


When the system goes around the exceptional point once, the eigenvalues and eigenfunctions are exchanged !

$k_{1i} \longrightarrow k_{1f} = k_{2i}$

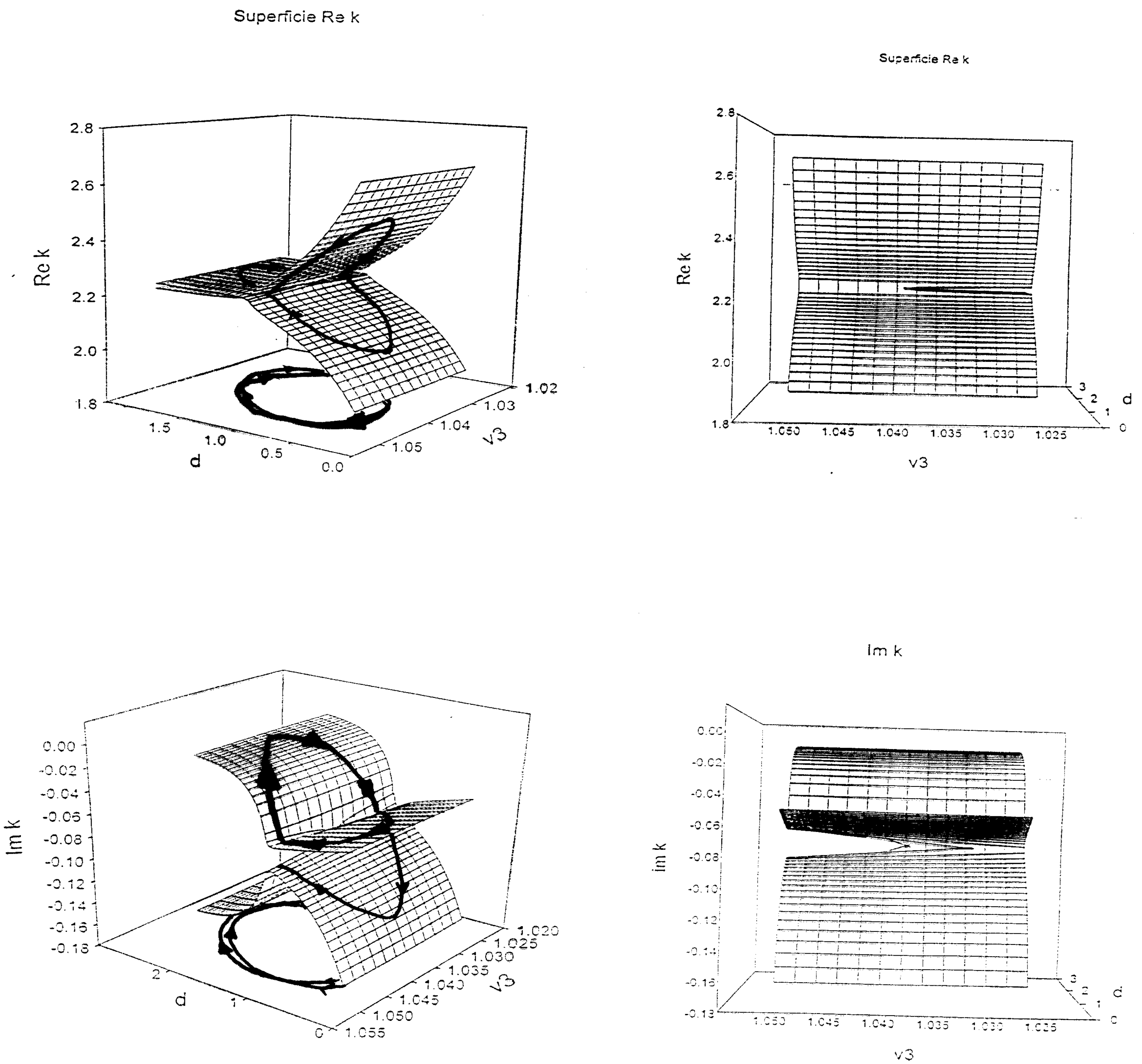
$k_{2i} \longrightarrow k_{2f} = k_{1i}$





When the system goes around the exceptional point twice, the eigenvalues return to their initial values. The eigenfunctions also return to their initial values but acquire a geometric phase !!.

Going around the exceptional point II



Conclusions

The local topological properties of the eigenenergy surfaces close to an exceptional point in parameter space, fully explain:

- **The rich phenomenology of crossings and anticrossings of energies and widths**
- **The very large and sudden change of shape of the trajectories of the S-matrix poles, also called "change of identity", observed in an isolated doublet of unbound energy eigenstates (resonances) when one control parameter is varied while the others are kept constant.**

  When the system goes around the exceptional point in parameter space, these same topological properties also fully explain:

- **The exchange of the poles' positions in the complex energy plane, and the exchange of the wave functions when the system goes around the exceptional point once.**
- **The geometric (Berry) phase acquired by the wave function when the system makes a double cyclic excursion around the exceptional point in parameter space.**