Particular spectral singularity in the continuum energies: a manifestation as resonances

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Abstract
We study the coalescence of two bound energy eigenstates embedded in the continuous spectrum of a real Hamiltonian \( H_W \) and the singular point produced by this coalescence. At the singular point, the two unnormalized Jost eigenfunctions are no longer linearly independent but coalesce to give rise to a bound state eigenfunction embedded in the continuum. We disturb the potential \( V_W \) by means of a truncation; this perturbation breaks the singular point in two resonances. The phase shift shows a jump of magnitude \( 2\pi \) and the shape of the cross section shows two inverted peaks; this behaviour is due to the interference between the two nearly degenerate resonances and the background component of the Jost function.

Keywords: singularity theory, scattering theory, phases geometric, dynamics or topological

(Some figures may appear in colour only in the online journal)

1. Introduction
In recent years the development and progress of quantum physics with non-Hermitian operators has given rise to important accomplishments in different fields [1–9], and in particular in the study of the physics of exceptional points [2, 7, 10–13] and spectral singularities [14–19]. Many theoretical [11, 20–33] and experimental [34–41] works are related to exceptional points produced by an accidental degeneracy of resonant states. Exceptional points in the real and continuous spectrum of a Hamiltonian of infinite dimension [42–44] have received much less attention than the case of non-Hermitian Hamiltonians of finite dimension. These exceptional
points are associated with bound states embedded in the continuous energy of scattering states. Bound states embedded in the continuous energy were first proposed by von Neumann and Wigner in 1929 [45]. They showed that certain spatially oscillating potentials could support a bound state with energy above the potential barrier. Later Stillinger et al [46] proposed that these states could be found in certain atomic and molecular systems, and in ultra-thin layer structures of semiconductors. They showed [47] that lattices could be used to construct potentials that support bound states with positive energies. The first experimental evidence of these states was reported by Capasso et al [48] in a super lattice consisting of thin superconducting layers of AlInAs/GaInAs. Pappademos et al [49] showed that, with methods of supersymmetric quantum mechanics, one can construct potentials supporting bound states in the continuum. A great number of examples of potentials that support a bound state in the continuum have been studied [50]. Bound states embedded in the continuum have been recently observed in optical wave guide arrays [51–53]. The first observation of a bound state associated with an exceptional point (defect modes) in PT-symmetric optical lattice was done by Regensburger et al [54]. A possible way to observe a bound state embedded in the continuum is by perturbing the potential. Weber and Pursey [55] studied the s-wave scattering of a von Neumann–Wigner type potential and showed that, by truncating the potential, the bound state in the continuum manifests itself as a resonance. The Darboux transformation method is a powerful technique for the generation of bound states in the continuum associated with singularities in the spectrum of the Hamiltonian. These singularities may be of different nature [19], as poles of the scattering function or exceptional points of a non-Hermitian Hamiltonian [44].

According to Kato [56] the exceptional points are characterized by the coalescence of two eigenvalues and the corresponding eigenfunctions. Due to the coalescence of their eigenfunctions the scalar product vanishes. These points are the beginning of branch points and branch cuts on the energy surfaces as a function of the control parameters of the system [24, 57]. However, in very few cases [19, 58] emphasis is placed on the important role of the eigenvectors associated with these exceptional points.

A particular class of spectral singularity that has characteristics similar to the exceptional points is that associated with zero energy bound states. According to Newton [59] the problem of the scattering of a particle with a radial potential that admits bound states may have resonances close to zero energy for $\ell > 0$. Newton discusses the evolution of a resonant state through a zero energy eigenstate to a bound state, by increasing the intensity of the attractive potential. The resonance as well as the bound state are poles of the scattering function in the $k$-plane. He shows that a resonance gives rise to two poles in lower $k$-plane, which are symmetrically located with respect to the imaginary $k$-axis, by increasing the intensity of the potential the two poles move towards $k = 0$, and coalesce at this point and then continue moving along the imaginary $k$-axis in opposite directions. In 2011 Heiss et al [19] reanalysed the single particle scattering around zero energy in relation to some recent experiments: A Bose-Einstein condensate of neutral atoms with induced electromagnetic attractive interaction [60], in nanostructures [61] and optics using continuous media with complex refractive index [62, 63]. They studied the singular behaviour of the states of energy when the length of the interaction around a bound state to zero energy is varied. The scattering length $a_\ell$ is defined by an expansion for energy eigenvalues [19, 59] other than zero and has a first order pole when an eigenvalue at zero energy is produced. From a strength $v_0$ of the potential that produces a bound state at $k = 0$ for orbital angular momentum $\ell > 0$, they modify the potential at $v_0 + \epsilon$ and obtain new eigenvalues as an expansion in terms of the $\epsilon$ potential intensity, $k_{1,2} = \sum_{n=1} C_n^2 / n^2$, the square root in this expression is a clear reminiscence of an exceptional point. They illustrate these results for a square well of width $\pi$ and $\ell = 1$. Similarly, they also find the expansion of the scattering function around $k = 0$. However, when they analyse
the eigenstates and the scattering function they find that the behaviour is different from that of an exceptional point \[12\].

We present an analytical and numerical study of a particular type of spectral singularity of a Hamiltonian with a potential \( V_W \) generated by a four times iterated and completely degenerate Darboux transformation \[64\]. This spectral singularity is reminiscent of the zero energy bound state of a single particle scattering for angular momentum greater than zero \[19\]. The potential \( V_W \) explicitly depends on two free parameters. Perturbing the potential \( V_W \) we show that the particular spectral singularity manifests itself as two resonances in the complex \( k \)-plane.

Although this potential is obtained without reference to any specific field forces, it can be used to study some of the properties of Hamiltonian operators. The paper is organized as follows: In section 2 we generate a Hamiltonian \( H_W \) by means of a four times iterated and completely degenerated Darboux transformation. In section 3 we compute the Jost solutions of \( H_W \) normalized to unit probability flux at infinity and we show that, at \( E = q^2 \), the Wronskian of the two unnormalized Jost solutions of \( H_W \) vanishes, this property identifies this point as a particular spectral singularity in the spectrum of the Hamiltonian \( H_W \). In section 4 we perturb the potential \( V_W \) with a cut off at a finite value \( r = a \) and we show that the particular spectral singularity manifests as two resonances. In section 5 we study the interference between the two resonances and the background term, which comes from an infinite number of zeros of the Jost function. A summary of the main results and conclusions is given in section 6.

2. The Hamiltonian \( H_W \)

A Hamiltonian that has some kind of spectral singularity in its real and continuous spectrum may be generated by means of a four times iterated and completely degenerated Darboux transformation; this transformation results from the coalescence of two bound states embedded in the continuum \[64\]. The potential \( V_W \) obtained from the Darboux transformation should not have any singularities that are not present in the initial potential; this condition puts constraints on the potential \( V_W \) that fix the number of free parameters, as will be shown in this section.

The radial Schrödinger equation is given by

\[
\left( -\frac{\partial^2}{\partial r^2} + V_W \right) \psi(r) = k^2 \psi(r),
\]

with units \( 2m = 1, \hbar = 1 \) and is defined in \([0, \infty)\). We will compute the regular solutions that satisfy the boundary condition \( \psi(0) = 0 \).

According to Crum’s generalization of the Darboux theorem \[65\], the potential \( V_W \) is obtained with the Wronskian \( W(\phi, \partial_q \phi, \partial^2_q \phi, \partial^3_q \phi) \equiv W_1(q, r) \) and its derivatives with respect to \( r \). In \( W_1(q, r) \), the transformation function, \( \phi(q, r) \), is an eigenfunction of the free particle radial Hamiltonian with eigenvalue \( E = q^2 \):

\[
\phi(q, r) = \sin(qr + \delta(q)),
\]

and \( \partial_q \phi \) is shorthand for \( \partial \phi / \partial q \). The phase shift \( \delta(q) \) is a smooth function of the positive wave number \( q \).

The potential \( V_W \) is given by the equation

\[
V_W = -2 \frac{1}{W^2_1(q, r)} \left( W''_1(q, r)W_1(q, r) - W'^2_1(q, r) \right).
\]

where prime means differentiation with respect to \( r \).

An explicit expression for \( W_1(q, r) \) is the following \[66\].
\[ W_1(q, r) = 16(q^4 - 12(q^2) + 8(q^3 \gamma_2)(q \gamma) - 12(q^2 \gamma_1)^2 \\
+ 24[(q^2 \gamma_1)(q \gamma) - (q \gamma)^2] \cos 2 \theta + 3 \sin^2 2 \theta \\
+ [16(q^2 - 12q \gamma - 12q^2 \gamma_1 - 4q^3 \gamma_2) \sin 2 \theta], \]

where

\[ \theta(r) = qr + \delta(q), \quad \gamma(r) = \partial_q \theta = r + \gamma_0, \quad \gamma_0 = \partial_q \delta(q), \]

\[ \gamma_1 = \partial_q^2 \delta(q), \quad \gamma_2 = \partial_q^3 \delta(q). \]  

From equation (3) it follows that, if the Wronskian \( W_1(q, r) \) has a zero of order \( n \) at \( r = r_0 \), then the potential \( V_W \) has a centrifugal barrier of the form \( 2n/(r - r_0)^2 \) and diverges at that point. The potential \( V_W \) constructed from the coalescence of two bound states embedded in the continuum has two singularities \[67\], or, equivalently, there are two points, \( r_1 \) and \( r_2 \), where \( W_1(q, r) \) is zero.

From equation (4) the function \( W_1(q, r) \), for large values of \( r \), is positive and grows with \( r \) as \( r^4 \). However, if the phase \( \delta(q) \) is left unrestricted, \( W_1(q, r) \) could take a negative value at \( r = 0 \), in which case \( r_2 > 0 \) and \( r_1 < 0 \). Therefore, to avoid the above situation we impose the condition

\[ W_1(q, 0) > 0, \]  

which defines the phase \( \delta(q) \), and from expressions (5) the value of the functions \( \gamma_0, \gamma_1, \) and \( \gamma_2 \) is computed. An explicit demonstration is given in appendix A. From equation (A.10), we verify that the Wronskian \( W_1(q, r) \), for \( r = 0 \), is given by

\[ W_1(q, 0) = \frac{12 \beta^2}{(1 + (\alpha q - \beta)^2)^2}, \]  

where \( \alpha \) and \( \beta \) are real parameters that determine the potential \( V_W \). However, condition (6) does not exclude the possibility in which both \( r_1 \) and \( r_2 \) are positive; this occurs when \( W_1(q, r) \) has a negative slope at \( r = 0 \). Therefore, we impose the additional condition that the slope of \( W_1(q, r) \) at the origin must be positive,

\[ W_1'(q, 0) > 0. \]

The first derivative of \( W_1(q, r) \) with respect to \( r \) is obtained in equation (A.12) and, evaluating at \( r = 0 \), we get

\[ W_1'(q, 0) = 48 \beta q \frac{(\beta - 2 \alpha q)^2 + \alpha^2 q^2}{(1 + (\alpha q - \beta)^2)^2}, \]

which is always positive for \( \beta > 0 \), since we consider \( q > 0 \). Hence, the conditions given by equations (6) and (8) allow a choice of parameters \( \alpha, \beta \) and \( q \) locating both singularities of \( V_W \) for \( r < 0 \). Specifically, the potential, with parameters \( \alpha = 1, \beta = 3 \) and \( q = 1 \), is illustrated with a dashed line in figure 1.

3. The Jost solutions of \( H_W \)

The two linearly independent unnormalized Jost solutions of \( H_W \), that belong to the energy eigenvalue \( E = k^2 \) and behave as outgoing and incoming waves for large values of \( r \), are obtained from the Wronskians \( W(\phi, ..., \partial_q^3 \phi, e^{\pm ikr}) \) and \( W_1(q, r) \) \[64, 66\].


Explicit expressions for the functions \(k_u k, r\) and \((v r)\) and \(\phi r^\gamma\). Hence, the unnormalized Jost solutions take the form

\[
f^\pm(k, r) = \frac{W(\phi, ..., \partial_q^2 \phi, e^{\pm ikr})}{W_1(q, r)} = \frac{1}{W_1(q, r)} w^\pm(k, r)e^{\pm ikr}, \tag{10}
\]

where the function \(w^\pm(k, r)\) is the reduced Wronskian which is a complex function of real arguments

\[
w^\pm(k, r) = u(k, r) \pm iv(k, r). \tag{11}
\]

Explicit expressions for the functions \(u(k, r)\) and \(v(k, r)\) are given by

\[
u(k, r) = 16q^4 (k^2 - q^2) \gamma_3 - 24q^2 (k^4 + 6q^2 k^2 + q^4) \gamma_4
+ 8q^2 (k^2 - q^2)^2 \gamma_3 - 12q^2 (k^2 - q^2)^2 \gamma_4
+ 24q^2 [(k^4 - 4q^2 k^2 - q^4) \gamma_3 + q_4 (k^4 - q^4) \gamma_4] \cos 2\theta
+ [16q^4 (k^4 - q^4) \gamma_3 - 12q (k^4 - 4q^2 k^2 - q^4) \gamma_4
- 4q^2 (k^4 - q^4) - 12q_4 q^2 (k^4 - 4q^2 k^2 - q^4)] \sin 2\theta
+ 3 (k^4 + 6q^2 k^2 + q^4) \sin^2 2\theta, \tag{12}
\]

and

\[
v(k, r) = 64q^4 k(k^2 - q^2) \gamma_3 - 24q^2 k(k^2 + q^2) \gamma + 8q^2 q^4 k(k^2 - q^2)
- 48q^3 q + [32q^2 k(k^2 - q^2) \gamma_3 + 24q^2 (k^2 + q^2) \gamma - 8q^2 q^4 k
\times (k^2 - q^2) + 48q_4 q^2 k] \cos 2\theta + [96q^3 k \gamma - 48q_4 q^4 k(k^2 - q^2) \gamma
- 12q k(k^2 + q^2)] \sin 2\theta + 6q k(k^2 + q^2) \sin 4\theta. \tag{13}
\]

\textbf{Figure 1.} The graph shows, with a dashed line, the potential \(V_w\) for values of the parameters \(\alpha = 1, \beta = 3\) and \(q = 1\). The potential oscillates with an amplitude which decreases as \(r^{-1}\) with increasing \(r\), in the origin takes the value 19.55 and the maximum of the first oscillation is at a height of 4.43. The probability density of the normalized bound state solution as a function of \(r\) is shown with a solid line. Note the difference of scale with the potential. The bound state is confined in the first well of the potential. The inset illustrates the rapid growth and the absence of zeros of \(W_1(q, r)\) for these parameters.
For large values of \( r \), the behaviour of \( w^{\pm}(k, r) \) is dominated by the highest power of \( r \). From equations (11)–(13) we get

\[
 w^{\pm}(k, r) = 16(k^2 - q^2)^2(qr)^4 + O(r^3),
\]

and from equation (A.10) it is clear that

\[
 W_1(q, r) = 16(qr)^4[1 + O(r^{-1})],
\]

hence, for large values of \( r \) the unnormalized Jost solutions are given by

\[
 f^{\pm}(k, r) = [(k^2 - q^2)^2 + O(r^{-1})]e^{\pm iqr}.
\]

At infinity the Jost solutions are incoming and outgoing waves, and at the origin they have a finite value [59]. The factor \( (k^2 - q^2)^2 \) is the flux of probability current at infinity of the unnormalized Jost solutions. Therefore, the Jost solutions of \( H_w \) normalized to unit probability flux at infinity are

\[
 F^{\pm}(k, r) = \frac{f^{\pm}(k, r)}{(k^2 - q^2)^2} = \frac{1}{(k^2 - q^2)^2 W_1(q, r)}w^{\pm}(k, r)e^{\pm iqr}, k^2 \neq q^2.
\]

Each pair of linearly independent Jost solutions belongs to a point \( E = k^2 \), with \( k^2 \neq q^2 \), in the spectrum of \( H_w \).

The Wronskian of the unnormalized Jost solutions is readily computed from (10) and equations (11)–(13)

\[
 W(f^+(k, r), f^-(k, r)) = -2ik(k^2 - q^2)^4.
\]

At the points \( k^2 = q^2 \), the Wronskian of the two unnormalized Jost solutions of \( H_w \) vanishes, then the two unnormalized Jost solutions are no longer linearly independent and coalesce in the function

\[
 f^{\pm}(q, r) = 4q^2 \frac{24q^2}{W_1(q, r)}[-2q^2\gamma^2 \cos \theta + (q\gamma + q^2\gamma_1) \sin \theta
 + \sin^2 \theta \cos \theta + e^{\mp i\theta},
\]

which is obtained from equation (10) when \( k = q \). From equation (19), the asymptotic behaviour of the function \( f^{\pm}(q, r) \) follows, and goes to zero as \( r^{-3} \). Hence, \( f^{\pm}(q, r) \) can be normalized and represents a bound state eigenfunction embedded in the continuum and can be written as

\[
 \psi_b(q, r) = \frac{24q^2}{W_1(q, r)}[-2q^2\gamma^2 \cos \theta + (q\gamma + q^2\gamma_1) \sin \theta + \sin^2 \theta \cos \theta],
\]

where \( \gamma_0, \gamma_1 \) and \( \gamma_2 \), as functions of \( q \), are given explicitly in appendix A. The wave function of the bound state is zero at \( r = 0 \); this condition is guaranteed if the parameters satisfy the relation \( \beta = 3\alpha q \). The normalized probability density of the bound state solution \( \psi_b(q, r) \) and the potential \( V_w \), as functions of \( r \), for the parameters \( \alpha = 1, q = 1 \) and \( \beta = 3 \) are shown in figure 1. The bound state is confined in the first well of the oscillating potential for energy \( E = q^2 \).

The Wronskian of the unnormalized Jost solutions, equation (18), goes to zero as the fourth power of \( (k - q) \) as a result of the coalescence of four functions. This property identifies \( E = q^2 \) as a point associated with a particular spectral singularity in the spectrum of the Hamiltonian \( H_w \). The singular point is formed by the coalescence of two bound states.
embedded in the continuum; each one is constructed from the coalescence of two eigenvalues and their respective eigenfunctions by means of a Darboux transformation. This procedure is totally contained in the four times iterated and completely degenerate Darboux transformation [66]. The particular spectral singularity is associated with a double pole in the normalization factor of the Jost solutions $F^\pm(k, r)$, see equation (17), but they are not associated with a double pole in the scattering matrix. The scattering matrix and the cross section are regular analytical functions of the wave number $k$ and the Green function has a first order pole [66]. The square root behaviour that characterizes an exceptional point is not present in this kind of singularity.

4. Truncated $V_W$ potential

The bound state in the continuum associated with the type of spectral singularity presented in this paper is not related to the poles of the scattering matrix and, therefore, it is not possible to perform a direct measurement. However, this state is formed in the first well of the oscillating potential, its binding energy is $E = q^2$, so it is a fragile state and any disturbance can break the equilibrium necessary for its formation, thus showing its presence in the complex $k$-plane [55]. The advantage of this method of perturbation is that, although it may seem artificial, it allows for an analytical study of the solutions. In this section we disturb the potential by cutting off its range at a value $r = a$. A cut off value of $a = 5000$ means that the perturbation is very small; however, it is enough to show the breaking of the bound state in the continuum into two resonances.

The radial Schrödinger equation is

$$\left[-\frac{d^2}{dr^2} + V(r)\right] \varphi(k, r) = k^2 \varphi(k, r), \quad (21)$$

with the potential

$$V(r) = \begin{cases} V_W(r) & r \leq a \\ 0 & r > a \end{cases} \quad (22)$$

and $\varphi(k, r)$ is the regular wave function that is uniquely defined by the boundary condition at $r = 0$ [59]

$$\lim_{r \to 0} r^{-1} \varphi(k, r) = 1. \quad (23)$$

The regular wave function is given by [59]

$$\varphi(k, r) = \begin{cases} \Phi(k, r) & r \leq a \\ \frac{1}{2i} \left[F(-k)e^{-ikr} - F(k)e^{ikr}\right] & r > a. \end{cases} \quad (24)$$

For $r \leq a$, $\varphi(k, r)$ is a linear combination of the unnormalized Jost solutions, equation (10). From the boundary condition (23) we get

$$\Phi(k, r) = \frac{1}{h(k)} \frac{W_1(q, 0)}{W_1(q, r)} \left[u(k, r) \left(u(k, 0) \sin kr - v(k, 0) \cos kr\right) + v(k, r) \left(v(k, 0) \sin kr + u(k, 0) \cos kr\right)\right], \quad (25)$$
where
\[ h(k) = u(k,0) \left( \frac{\partial v(k,r)}{\partial r} \right)_{r=0} - v(k,0) \left( \frac{\partial u(k,r)}{\partial r} \right)_{r=0} + k\left( u^2(k,0) + v^2(k,0) \right). \] (26)

For \( r > a \), \( \varphi(k,r) \) is a linear combination of a free incoming spherical wave and a free outgoing spherical wave. In equation (24), the Jost function of the perturbed potential is the coefficient \( F(-k) \) of the incoming wave \([59]\).

### 4.1. Resonant state eigenfunctions

To complete this study in this section we give a brief description of resonant state eigenfunctions or Gamow state eigenfunctions.

Resonant states energy eigenfunctions \( \psi_n(k_n, r) \) are solutions of equation (21), that vanish at the origin,
\[ \psi_n(k_n,0) = 0, \] (27)
and asymptotically behave as purely outgoing waves,
\[ \lim_{r \to \infty} \left[ \frac{1}{\psi_n(k_n, r)} \frac{d\psi_n(k_n, r)}{dr} \right] = 0, \] (28)
that oscillate between envelopes that increase exponentially with \( r \), where \( k_n \) are the zeros of the Jost function,
\[ F(-k_n) = 0, \] (29)
that are in the fourth quadrant of the complex \( k \)-plane, \( k_n = \kappa_n - i\Gamma_n/2 \) with \( \kappa_n > \Gamma_n/2 > 0 \).

The Gamow state eigenfunctions are given by \([68]\)
\[ \psi_n(k_n, r) = \frac{1}{N_n} \varphi(k_n, r), \] (30)
where \( N_n \) is the normalization constant written as \([69]\)
\[ N_n^2 = \frac{1}{14k_n^2} F(k_n) \left( \frac{dF(-k)}{dk} \right)_{k=k_n}. \] (31)
The features described are illustrated in the following section, where a graphic representation of the Gamow state eigenfunctions that characterizes the resonances coming from the breakdown of the particular spectral singularity in the complex \( k \)-plane is shown.

### 4.2. The phase shift and the cross section

In this section we compute the phase shift \( \delta(k) \) and the cross section \( \sigma(k) \).

By matching the function \( \varphi(k,r) \) and its derivative at the boundary \( r = a \) we get the following expression for the Jost function
\[ F(-k) = e^{ika} \left[ \Phi'(k,a) - ik\Phi(k,a) \right] \] (32)
and
\[ F(k) = e^{-ika} \left[ \Phi'(k,a) + ik\Phi(k,a) \right], \] (33)
where $\Phi'(k,a) = (\partial \Phi(k,r)/\partial r)_{r=a}$.

From equation (25) the derivative of the regular solution is
\[
\Phi'(k,r) = \frac{1}{i(k)} \frac{W_i(q,0)}{W^*_i(q,0)} \left\{ \left[ u'(k,r)W_i(q,r) - u(k,r)W^*_i(q,r) \right]
\right. \\
- kv(k,r)W_i(q,r) \left[ u(k,0) \sin kr - v(k,0) \cos kr \right]
+ \left[ v'(k,r)W_i(q,r) - v(k,r)W^*_i(q,r) + ku(k,r)W_i(q,r) \right]
\left. \times (v(k,0) \sin kr + u(k,0) \cos kr) \right\}. 
\]
(34)

Substituting (25) and (34) in (32) we get for the Jost function the expression
\[
F(-k) = \frac{1}{i(hk)} \frac{W_i(q,0)}{W^*_i(q,a)} e^{ik\alpha} [d(k) + ig(k)]
\]
(35)
and for the function $F(k)$
\[
F(k) = \frac{1}{i(hk)} \frac{W_i(q,0)}{W^*_i(q,a)} e^{-ik\alpha} [d(k) - ig(k)],
\]
(36)
with
\[
d(k) = \left[ u'(k,a)W_i(q,a) - u(k,a)W^*_i(q,a) - kv(k,a)W_i(q,a) \right]
\times \left( u(k,0) \sin ka - v(k,0) \cos ka \right)
\times W^*_i(q,a) + ku(k,a)W_i(q,a) \left[ u(k,0) \cos ka + v(k,0) \sin ka \right],
\]
(37)
and
\[
g(k) = -kW_i(q,a) \left[ u(k,a)(u(k,0) \sin ka - v(k,0) \cos ka) \right]
\times \left[ v(k,a)(v(k,0) \sin ka + u(k,0) \cos ka) \right].
\]
(38)

The scattering matrix $S(k)$ is given by:
\[
S(k) = \frac{F(k)}{F(-k)}. 
\]
(39)

The zeros of the Jost function $F(-k)$ are the poles of $S(k)$. Substituting equations (35) and (36) in (39), we obtain
\[
S(k) = \frac{e^{-ik\alpha} [d(k) - ig(k)]}{e^{ik\alpha} [d(k) + ig(k)]}. 
\]
(40)

From equation (40) the poles of the $S(k)$ matrix, in the neighbourhood of the singular point $E = q^*$, are obtained from the equation
\[
d(k) + ig(k) = 0.
\]
(41)

We solved this equation numerically for potential parameters $\alpha = 1$, $\beta = 3$ and the cut off parameter $a = 5000$, and found two zeros of the Jost function in the fourth quadrant of the complex $k$–plane close to $q = 1$, which correspond to the resonances in which the particular spectral singularity is broken by disturbing the system. These zeros are plotted in figure 2 with black points. There are other zeros of the Jost function more distant of the real axis of the complex $k$–plane. In figure 2 we show these zeros with small squares.

As the cut off parameter increases, the two resonances plotted with black points approach the real axis to coalesce at the point representing the particular spectral singularity.
In figure 3 we show, on the same scale of the potential $V_W$, the probability densities of the normalized eigenfunctions of resonant states corresponding to the resonances closest to the real $k$-axis, for the parameter values of the perturbed potential with $a = 5000$ and resonances $\kappa_1 = 0.998\,984\,4032$, $\Gamma_1/2 = 0.000\,173\,0065$ and $\kappa_2 = 1.001\,015\,5756$, $\Gamma_2/2 = 0.000\,173\,1296$. The resonances coming from the breaking of the point representing the particular spectral singularity are formed in the first well of the potential. The resonances are nearly degenerate, as we can see from the values of the real parts $\kappa_1$ and $\kappa_2$ of wave numbers and their half-widths $\Gamma_1/2$ and $\Gamma_2/2$ and therefore the probability densities of resonant states eigenfunctions are almost indistinguishable. In this figure the tunneling of the probability densities of resonant state eigenfunctions through the oscillating potential is observed.

The scattering matrix $S(k)$ given in equation (40) is written as:

$$S(k) = e^{2i\delta(k)} ,$$

where

$$\delta(k) = - \arctan \frac{d(k) \sin ka + g(k) \cos ka}{d(k) \cos ka - g(k) \sin ka} ,$$

is the phase shift of the perturbed potential.

In figure 4 we show the phase shift $\delta(k)$ as a function of the wave number $k$, and its behaviour in the neighbourhood of $k = 1$ for the cut off parameter $a = 5000$, where it shows a jump of $2\pi$, characteristic of the case where there are two nearly degenerate resonances [23]. The jump starts near $-\pi/2$ and ends near $-5\pi/2$. In this case, as in any other potential that ends abruptly, the phase shift is influenced by the cut off through the exponential factor that appears in the Jost function, see equation (32). This factor provides the term $-ka$ which dominates the increasing contribution of the phase shift in its passage through each resonance resulting in a negative phase shift, as in figure 4.
The cross section is defined as
\[
\sigma(k) = \frac{4\pi}{k^2} \sin^2 \delta_a(k).
\] (44)

Figure 5 shows the cross section as a function of the wave number \(k\). The inverted double peak is a feature of the two nearly degenerate resonances. Minima in the cross section are mainly produced by interference effects in the first potential well and tunneling through the oscillating potential, which is known as the Ramsauer–Townsend effect [59]. Extremal points
occur when the phase shift passes through the values $-\pi$ and $-2\pi$, where $\sigma(k)$ is a minimum; whereas the peak around $k = 1.0001$ is due to $\delta_a(k)$ passing through $-3\pi/2$, where $\sigma(k)$ is a maximum.

5. Interference of two close resonances

In this section we show the shape of the cross section, previously obtained, with the structure of two inverted peaks, as a result of the interference of the two resonances closest to the real axis of the complex $k$–plane and the background made up of distant resonances and other non-resonant phenomena.

When the first and second absolute momenta of the potential exist, and the potential decreases at infinity faster than any exponential, or if it vanishes identically beyond a finite radius, the Jost function $F(-k)$ is an entire function of $k$ [59]. The entire function of $k$, $F(-k)$, may be written in a form of an infinite product of zeros according to Hadamard’s form of the Weierstrass factorization theorem [70] and, by using a theorem of Pfluger [71], we get

\[ F(-k) = F(0) \exp(iR) \prod_{n=1}^{\infty} \left(1 - \frac{k}{k_n}\right), \]

where $R$ is the range of the potential, $F(0) = Ak$ with $A$ a constant and $\{k_n\}$ are the zeros of $F(-k)$ [59].

In order to show the interference of the two resonances and the background, we write the Jost function $F(-k)$ in the explicit form of a product of two zeros

\[ F(-k) = \left(k - \kappa_1 + i\frac{\Gamma_1}{2}\right) \left(k - \kappa_2 + i\frac{\Gamma_2}{2}\right) \exp(ika)D(k), \]

where $\kappa_1$ and $\kappa_2$ are the positions of the two resonances and $\Gamma_1$ and $\Gamma_2$ are their widths.
where the product \( \exp(ik a) D(k) \) corresponds to the background component of the Jost function with
\[
D(k) = F(0) \frac{1}{(\kappa_1 - ik_1)(\kappa_2 - ik_2)} \prod_{n=1}^{\infty} \left(1 - \frac{k}{\kappa_n}\right). \tag{47}
\]

We consider a small perturbation of the potential by taking a large value of the cut off parameter \( a \). This guarantees that the doublet of isolated resonances is close to the real axis of the complex \( k \)-plane. The other zeros of \( F(-k) \), contained in \( D(k) \), are farther away from the real axis and also from the first pair of resonances and correspond to distant resonances or other non-resonant phenomena; thus the infinite product of zeros on the right hand side of equation (47) has a smooth behaviour of \( k \), which can be written as
\[
D(k) = \mu(k)(1 + i\lambda(k)), \tag{48}
\]
where \( \mu(k) \) and \( \lambda(k) \) are real and smooth functions of \( k \). From equations (46)–(48), the Jost function takes the form
\[
F(-k) = \mu(k) \left\{ (Y(k) - \lambda(k)Z(k)) \cos ka - (\lambda(k)Y(k) + Z(k)) \sin ka 
+ i[(Y(k) - \lambda(k)Z(k)) \sin ka + (\lambda(k)Y(k) + Z(k)) \cos ka] \right\}, \tag{49}
\]
where
\[
Y(k) = (k - \kappa_1)(k - \kappa_2) - \frac{\Gamma_1\Gamma_2}{4}, \tag{50}
\]
\[
Z(k) = \frac{1}{2} [(k - \kappa_1)\Gamma_2 + (k - \kappa_2)\Gamma_1]. \tag{51}
\]

The Jost function is written in terms of the phase shift as
\[
F(-k) = |F(k)| e^{-i\delta(k)}, \tag{52}
\]
and the phase shift is given by
\[
\delta(k) = -\arctan \frac{(Y(k) - \lambda(k)Z(k)) \sin ka + (\lambda(k)Y(k) + Z(k)) \cos ka}{(Y(k) - \lambda(k)Z(k)) \cos ka - (\lambda(k)Y(k) + Z(k)) \sin ka}. \tag{53}
\]

The cross section \( \sigma(k) \) is given by the expression
\[
\sigma(k) = \frac{4\pi}{k^2(1 + \lambda^2(k))} \frac{[Y(k) - \lambda(k)Z(k)] \sin ka + (\lambda(k)Y(k) + Z(k)) \cos ka]^2}{Y^2(k) + Z^2(k)}. \tag{54}
\]

From the expressions for the phase shift and the cross section we can see that the function \( \lambda(k) \) gives a measure of the interference between the two resonances and the background term.

For the computation of the cross section \( \sigma(k) \) of the approximation given by equation (54), we take the resonance wave numbers obtained from the numerical calculation of the Jost function zeros equation (41) for a cut off parameter \( a = 5000 \):
\[
\kappa_1 = 0.998\,984\,4032, \quad \Gamma_1/2 = 0.000\,173\,0065 \tag{55}
\]
\[
\kappa_2 = 1.001\,015\,5756, \quad \Gamma_2/2 = 0.000\,173\,1296 \tag{56}
\]
The assumption of the resonances being well isolated allows us to parametrize the function \( \lambda(k) \) as a linear polynomial of \( k \),

\[
\lambda(k) = \frac{1}{\kappa_1 \kappa_2} \left( \frac{\kappa_2 - k}{\kappa_2 - \kappa_1} \right),
\]

where the linear polynomial is determined by the factorization of the terms in the numerator and denominator.
\[ \lambda(k) = \lambda_0 + \lambda_1 k, \]  

the parameter values \( \lambda_0 = 1311.3931 \) and \( \lambda_1 = -1312.2167 \) are obtained from fitting the minima of the approximated cross section to the minima of the exact cross section.

After the substitution of \( \lambda(k) \) at equation (53), the phase shift \( \delta(k) \) in the neighbourhood of \( k = 1 \) exhibits a value near \(-\pi/2\) for \( k = 0.999 \) and then the known jump of \( 2\pi \), as can be seen from the graph for the phase shift in the lower part of figure 6. The jump of \( 2\pi \) of the phase shift is due to the interference between the two nearly degenerate resonances and the background parametrized through the \( \lambda(k) \) function. In the upper part of figure 6 we show the cross section as function of \( k \), exhibiting the same resonant structure as the exact cross section.

**Figure 6.** The cross section \( \sigma(k) \) and the phase shift \( \delta(k) \) as function of \( k \), calculated for the values of the resonances \( \kappa_1 = 0.9989844032 \), \( \Gamma_1/2 = 0.0001730065 \), \( \kappa_2 = 1.0010155756 \), \( \Gamma_2/2 = 0.0001731296 \), and the parameters \( \lambda_0 = 1311.3931 \), \( \lambda_1 = -1312.2167 \) and a cut off \( a = 5000 \).
Figure 7 shows the comparison of the results for the cross section, as a function of the wave number $k$, obtained from the numerically exact calculation with equation (44) and the results computed with the approximation given by equation (54) in the neighbourhood of the resonances. The fit to the cross section using the approximation of equation (54) is good enough in the sense that it reproduces the shape of the resonant structure shown in the exact calculation and allows us to give an explanation of this phenomenon.

6. Summary and conclusions

A study of a particular spectral singularity in the continuous spectrum of a real Hamiltonian $H_W$ has been presented and discussed. The Hamiltonian $H_W$ and the free particle Hamiltonian are isospectral. In the general case, to each point in this continuous spectrum correspond two linearly independent Jost solutions which behave at infinity as incoming and outgoing waves. However, here we have shown that in the continuous spectrum of $H_W$ there is a point corresponding to a particular spectral singularity at $E = q^2$; this particular spectral singularity is associated with a double pole in the normalization factor of the Jost solutions normalized to unit flux at infinity. At the singular point, the two unnormalized Jost solutions are no longer linearly independent and coalesce becoming a quadratically integrable eigenfunction of a bound state embedded in the continuum. The bound state is formed in the first well of the potential $V_W$. The perturbation of the potential $V_W$, with a cut off value $r = a$, manifests this particular spectral singularity as two resonant states in the complex $k$–plane. The two resonances are formed in the first well of the perturbed potential. The phase shift shows a jump
of magnitude $2\pi$, and the cross section shows two inverted peaks, where it vanishes, for the values of $k$ where the phase shift is $-\pi$ and $-2\pi$; and it has a local maximum at the value of $k$ where the phase shift is $-3\pi/2$. The shape of the cross section with two inverted peaks in the neighbourhood of $k = q$ is due to the interference between the two nearly degenerate resonances and the background component of the Jost function. This phenomenon is the Ramsauer–Townsend effect.

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Appendix. Computation of the Wronskian $W_1(q, r)$

In this appendix we compute the explicit expression for the Wronskian $W_1(q, r)$.

From equations (4) and (5) we have

$$W_1(q, 0) = 16 \left( q \frac{d\delta(q)}{dq} \right)^4 - 12 \left( q \frac{d\delta(q)}{dq} \right)^2 + 8 \left( q^3 \frac{d^3\delta(q)}{dq^3} \right) \left( q \frac{d\delta(q)}{dq} \right) - 12 \left( q^3 \frac{d^2\delta(q)}{dq^2} \right)^2 + 24 \left[ \left( q^3 \frac{d^2\delta(q)}{dq^2} \right) \left( q \frac{d\delta(q)}{dq} \right) + \left( q^3 \frac{d\delta(q)}{dq} \right)^2 \right] \cos 2\delta(q) + 3 \sin^2 2\delta(q) + 16 \left( q \frac{d\delta(q)}{dq} \right)^3 - 12 \left( q \frac{d\delta(q)}{dq} \right)$$

$$- 12 \left( q^2 \frac{d^2\delta(q)}{dq^2} \right) - 4 \left( q^3 \frac{d^3\delta(q)}{dq^3} \right) \sin 2\delta(q). \quad (A.1)$$

To simplify the notation, we define a new function $t(q)$ as

$$t(q) := \tan \delta(q), \quad (A.2)$$

then

$$\sin 2\delta(q) = \frac{2t(q)}{1 + t^2(q)} \quad \text{and} \quad \cos 2\delta(q) = \frac{1 - t^2(q)}{1 + t^2(q)}. \quad (A.3)$$

Written in terms of $t(q)$, equation (A.1) takes the form

$$W_1(q, 0) = \frac{4 \left( -t(q) + qt_1(q) \right)}{\left( 1 + t^2(q) \right)^2} \left[ 3(-t(q) + qt_1(q)) + 6q^2 t_{11}(q) \right.$$

$$+ 2q^3 t_{111}(q) \left. - 3q^4 \left( \frac{d}{dq}(-t(q) + qt_1(q)) \right)^2 \right]. \quad (A.4)$$
where \( t_q \) is shorthand for \( dt/dq \).

Now it is evident from (A.4) that if \( t(q) \) satisfies
\[
-t(q) + q t_q(q) = \beta,
\]
the equation (A.4) becomes an identity, and the condition given in (6) is satisfied provided that
\[
W_1(q,0) = \frac{12 \beta^2}{(1 + P(q))^2}.
\]

Integrating (A.5) we get
\[
t(q) = \alpha q - \beta,
\]
and according to equation (A.2) the phase shift is given by
\[
\delta(q) = \arctan(\alpha q - \beta),
\]
in these expressions \( \alpha \) and \( \beta \) are free parameters, but \( \beta \neq 0 \).

Once the phase shift \( \delta(q) \) is known as an explicit function of \( q \), the functions \( \gamma_0, \gamma_1 \) and \( \gamma_2 \) are obtained from its first, second and third derivative, respectively,
\[
\begin{align*}
\gamma_0 & = \frac{\alpha}{1 + (\alpha q - \beta)^2}, \\
\gamma_1 & = -\frac{2 \alpha^2 (\alpha q - \beta)}{(1 + (\alpha q - \beta)^2)^2}, \\
\gamma_2 & = -\frac{2 \alpha^3 (1 - 3 (\alpha q - \beta)^2)}{(1 + (\alpha q - \beta)^2)^3}.
\end{align*}
\]

With the help of these expressions and equation (4) we get for \( W_1(q, r) \) the following expression
\[
W_1(q, r) = \frac{12 \beta^2}{\Omega^2} + \frac{24 \beta \alpha q}{\Omega^2} (\cos 2qr - 1) + \frac{12 \alpha q (\alpha^2 q^2 + \beta^2 - 1)}{\Omega^2} \sin 2qr
\]
\[
+ 16 \left[ (qr)^4 + \frac{4 \alpha q}{\Omega} (qr)^3 + \frac{6 \alpha^2 q^2}{\Omega^2} (qr)^2 + \frac{3 \alpha^3 q^3}{\Omega^2} (qr) \right]
\]
\[
- 12 \left[ (qr)^2 + \frac{2 \alpha q}{\Omega} (qr) \right]
\]
\[
+ 24 \left[ (qr)^2 + \frac{2 \alpha q (1 - \beta (\alpha q - \beta))}{\Omega^2} (qr) \right] \cos 2(qr + \delta(q))
\]
\[
+ \left[ 16 (qr)^3 + \frac{3 \alpha q}{\Omega} (qr)^2 + \frac{3 \alpha^2 q^2}{\Omega^2} (qr) \right] - 12 (qr) \sin 2(qr + \delta(q))
\]
\[
+ 3 \left[ 1 - 6 (\alpha q - \beta)^2 + (\alpha q - \beta)^4 \right] \sin^2 2qr
\]
\[
+ \frac{4 (\alpha q - \beta)(1 - (\alpha q - \beta)^2)}{\Omega^2} \sin 2qr \cos 2qr,
\]
where
\[
\Omega = 1 + (\alpha q - \beta)^2.
\]

Then, the derivative of \( W_1(q, r) \) with respect to \( r \) is given by
\[
W_i(q,r) = 48\beta q \left( \frac{\beta - 2\alpha q}{\Omega^2} + 24q \left[ \cos(2(qr + \delta(q))) - 1 \right]
+ \frac{4\alpha^2 q^2 (\alpha - \beta)}{\Omega^2} \sin(2(qr + \delta(q))) \right)
+ 24\beta q \left[ 1 + \frac{\beta - 2\alpha q}{\Omega^2} + \alpha^2 q^2 (\cos 2qr - 1) \right]
+ 32q \left[ (qr)^3 + \frac{3\alpha q}{\Omega^2} (qr)^2 + \frac{3\alpha^2 q^2}{\Omega^2} (qr) (2 + \cos 2(qr + \delta(q))) \right]
+ 12q \left[ \frac{1 - 6(\alpha q - \beta)^2 + (\alpha q - \beta)^4}{\Omega^2} \cos 2qr
- \frac{4(\alpha q - \beta)(1 - (\alpha q - \beta)^2)}{\Omega^2} \sin 2qr
- \frac{1 + 4\alpha q(\alpha q - \beta) - (\alpha q - \beta)^4}{\Omega^2} \right] \sin 2qr. \]

(A.12)

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