# Bound states in the continuum and time evolution of the generalized eigenfunctions

D. Lohr[a], E. Hernández[a], A. Jáuregui[b], and A. Mondragón[a]
[a]*Instituto de Física, Universidad Nacional Autónoma de México, Apartado Postal 20-364, 01000 Ciudad de México, México.*
[b]*Departamento de Física, Universidad de Sonora, Apartado Postal 106, Hermosillo, Sonora, México.*

Received 14 March 2018; accepted 16 May 2018

We study the Jost solutions for the scattering problem of a von Neumann-Wigner type potential, constructed by means of a two times iterated and completely degenerated Darboux transformation. We show that for a particular energy the unnormalized Jost solutions coalesce to give rise to a Jordan cycle of rank two. Performing a pole decomposition of the normalized Jost solutions we find the generalized eigenfunctions: one is a normalizable function corresponding to the bound state in the continuum and the other is a bounded, non-normalizable function. We obtain the time evolution of these functions as pseudo-unitary, characteristic of a pseudo-Hermitian system. An explicit calculation of the cross section as a function of the wave number $k$ reveals no sign of the bound state in the continuum.

*Keywords:* Bound states in the continuum; Darboux transformations; Jordan chain.

PACS: 03.65.-w; 03.65.Ge; 03.65.Nk

## 1. Introduction

Bound states in the continuum (BICs) are a wave phenomenon that refers to states whose wave functions remain localized among a continuum of radiating waves with positive energies. This phenomenon of localized waves has been identified in atomic and molecular physics, optics, acoustics and other fields [1–5]. One review concerning this type of bound states was recently published [6].

BICs were first proposed by von Neumann and Wigner in 1929 [7], since then they have stimulated many experimental and theoretical research in various branches of physics. The first experimental evidence in this direction was reported by F. Capasso *et al*., they found an electronic bound state with energy greater than the barrier height in a semiconductor superlattice [8]. More recently, BICs have been observed in optical waveguide arrays [9–11]. M. Koirala *et al*. found a class of critical states embedded in the continuum in a one-dimensional arrangement of waveguides [12], and M. I. Molina *et al*. observed surface bound states in the continuum in a linear optical band of a discrete lattice [13].

In quantum physics, there exists a particular type of potentials that support BICs and are solely defined by their oscillatory asymptotic behaviour. Typically, a radial potential with an oscillatory asymptotic behaviour that falls to zero slowly,

$$V(r) = a\frac{\sin br}{r} + \mathcal{O}\left(\frac{1}{r^2}\right), \tag{1}$$

supports a BIC with energy $E = b^2/4$, if the parameters $a$ and $b$ satisfy the relation $|a| > |b|$ [14]. Potentials of the form (1) are known as von Neumann-Wigner potentials [7], and have been studied with methods of supersymmetric quantum mechanics (SUSY QM) [15], Darboux transformation [16] and the inverse scattering method (Gel'fand-Levitan equation) [17]. Further development in the techniques for this purpose was made in the following years. A. A. Andrianov and A. V. Sokolov studied a non-Hermitian Hamiltonian in the whole axis with complex von Neumann-Wigner type potential obtained with SUSY methods, and found the normalized eigenfunction and associated eigenfunction and their orthogonal relations; as the Hamiltonian is non-Hermitian and self-orthogonality of the normalized eigenfunction occurs, they related the BIC to an exceptional point [18]. A. Khelashvili and N. Kiknadze established a one to one correspondence between the decay law in von Neumann-Wigner type potentials and the asymptotic behaviour of the wave functions representing the bound states [19], while T. A. Weber and D. L. Pursey showed that by truncating a von Neumann-Wigner potential the BIC manifest itself as a resonance [20]. E. Hernández *et al*. studied a particular spectral singularity produced by the coalescence of two BICs [21].

In this paper, in an attempt to develop further results in this field, particularly concerning the nature of the eigenfunction corresponding to a BIC, we study the Jost solutions of a radial Hamiltonian with a real von Neumann-Wigner type potential and obtain the Jordan cycle of length two of generalized eigenfunctions, one of which is the BIC, and their respective time evolution. Although the exact model presented in this paper may not be readily applied to a real physical system, it may prove useful in determining further properties of more realistic Hamiltonians. The paper is organized as follows: In Sec. 2, by performing a two times iterated and completely degenerated Darboux transformation with initial Hamiltonian the free particle, a von Neumann-Wigner type potential is obtained supporting a BIC with energy $E = q^2$. In Sec. 3, the set of Jost solutions normalized to unit flux are explicitly constructed and it is shown that the unnormalized Jost solutions coalesce at $k = q$ to give rise to a Jordan

chain of rank two. In Sec. 4, the generalized eigenfunctions are found from the pole decomposition of the normalized Jost solutions and the corresponding Jordan chain is established. The time evolution of the generalized eigenfunctions is described in Sec. 5. In Sec. 6, the scattering matrix is obtained as a function of $k$ and the cross section is calculated. In Sec. 7, a summary of the results and conclusions is presented.

## 2. Von Neumann-Wigner potentials and Darboux transformations

A particular class of completely degenerated Darboux transformations, with initial Hamiltonian the free particle, generates new potentials of von Neumann-Wigner type supporting any number of bound states embedded in the continuum [16]. These transformations are obtained from Crum's theorem, a generalization of the Darboux transformation, which states that the function

$$\psi_E = \frac{W(\phi_1, \phi_2, \ldots, \phi_n, \phi_E)}{W(\phi_1, \phi_2, \ldots, \phi_n)} \tag{2}$$

is an eigenfunction of the Hamiltonian

$$H_n = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + U_n, \tag{3}$$

with eigenvalue $E$, and the potential $U_n$ is given by

$$U_n = V_0 - 2\frac{\mathrm{d}^2}{\mathrm{d}r^2} \ln W(\phi_1, \phi_2, \ldots, \phi_n). \tag{4}$$

The auxiliary or transformation functions $\phi_i$ are eigenfunctions of the initial Hamiltonian $H_0$ with eigenvalues $E_i$, $i = 1, \ldots, n$, and $\phi_E$ is also an eigenfunction of $H_0$ with eigenvalue $E$. In the above expressions $W(\phi_1, \phi_2, \ldots, \phi_n)$ is the Wronskian of the eigenfunctions $\phi_i$ [22, 23].

The completely degenerated case occurs when we take all $E_i$ energies close to each other, *i.e.* $E_i \to \bar{E} + \epsilon_i$ with $\epsilon_i \ll 1$, and later taking the limit $\epsilon_i \to 0$. After this procedure, all eigenfunctions $\phi_i$ coalesce in $\phi$ and the respective eigenvalues $E_i$ in $\bar{E}$. From Crum's theorem it follows that the function

$$\psi_E = \frac{W(\phi, \partial\phi, \ldots, \partial^{n-1}\phi, \phi_E)}{W(\phi, \partial\phi, \ldots, \partial^{n-1}\phi)} \tag{5}$$

is an eigenfunction of the Hamiltonian $H_n$, with eigenvalue $E$, and the potential $U_n$ is substituted by $V_n$ given as

$$V_n = V_0 - 2\frac{\mathrm{d}^2}{\mathrm{d}r^2} \ln W(\phi, \partial\phi, \ldots, \partial^{n-1}\phi). \tag{6}$$

The partial derivative is with respect to the energy $\bar{E}$.

From here on, we consider as the initial Hamiltonian the free particle in spherical coordinates with potential $V_0 = 0$, and auxiliary eigenfunction

$$\phi = \sin(qr + \delta(q)) \tag{7}$$

with eigenvalue $\bar{E} = q^2$ and $\delta(q)$ an arbitrary phase shift which sets the parameters of the system. In this case, differentiation with respect to the energy $\bar{E}$ is equivalent to differentiation with respect to wave number $q$ in expressions (5) and (6), and in what follows we derive with respect to $q$.

Let us consider now the simplest case that produces a von Neumann-Wigner potential: $n = 2$. The Hamiltonian $H_2$ is given in (3), with the potential $V_2$ obtained from (6) as

$$V_2(r) = -2\frac{\mathrm{d}^2}{\mathrm{d}r^2} \ln W(\phi, \partial\phi), \tag{8}$$

and calculating the Wronskian $W_2 \equiv W(\phi, \partial\phi)$ with (7) we obtain:

$$W_2(r) = \frac{1}{2}\left(\sin 2\theta - 2q\gamma\right), \tag{9}$$

where

$$\theta = qr + \delta(q), \tag{10}$$

$$\gamma = r + \delta'(q), \tag{11}$$

and as a convenient notation the prime in $\delta'(q)$ indicates the first derivative of $\delta(q)$.

Using (9) in (8) the potential obtained is:

$$V_2(r) = 32q^2 \frac{(\sin\theta - q\gamma\cos\theta)\sin\theta}{(\sin 2\theta - 2q\gamma)^2}, \tag{12}$$

with asymptotic behaviour given by:

$$V_2(r) = -4q\frac{\sin 2\theta}{r} + \mathcal{O}\left(\frac{1}{r^2}\right), \tag{13}$$

and comparing it with (1) we see that it is a potential of von Neumann-Wigner type and, given that $a = -4q$ and $b = 2q$, supports a bound state in the continuum with energy $E = q^2$.

A requirement for the validity of the Darboux transformation is the absence of singularities in the new potential not present in the initial potential. From (12) we see that the singularities of $V_2$ occur at the zeros of $W_2$. The Wronskian $W_2$ as a function of $r$ grows linearly with a negative slope, and has only one real zero.

As the Hamiltonian $H_2$ is defined in the positive semiaxis, we set the condition

$$W_2(0) < 0, \tag{14}$$

which locates the real zero for negative $r$ and therefore setting the potential $V_2$ an analytical function of $r$ in the physical space. Condition (14) provides a differential relation for the phase shift $\delta(q)$ as a function of $q$. Evaluating (9) in $r = 0$ we get,

$$W_2(0) = \frac{1}{2}\left(\sin 2\delta(q) - 2q\frac{\mathrm{d}\delta(q)}{\mathrm{d}q}\right),$$

and defining $t(q) = \tan\delta(q)$ we can write condition (14) as

$$q\frac{\mathrm{d}t(q)}{\mathrm{d}q} - t(q) > 0. \tag{15}$$

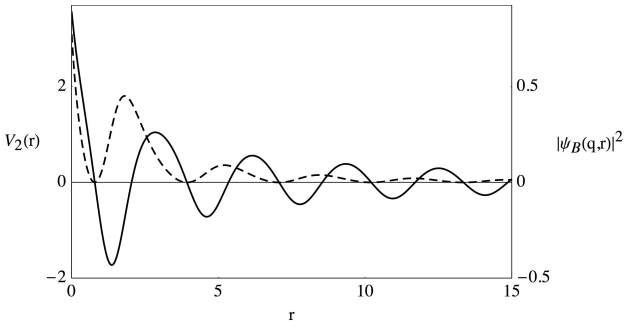


FIGURE 1. Potential $V_2$ (continuous line) and density probability of the eigenfunction of the bound state embedded in the continuum (dashed line) for parameters values $\alpha = 2$, $\beta = 3$ and $q = 1$.

This relation is readily solved by considering a positive constant $\beta$ to eliminate the inequality, and solving the resulting differential equation yields the result

$$\delta(q) = \arctan(\alpha q - \beta), \tag{16}$$

with $\alpha$ and $\beta$ real constants, and $\beta > 0$.

The potential $V_2$ in (12) is now determined by the parameters $\alpha$ and $\beta$. Figure 1 shows the potential $V_2$ as a function of $r$ for a given choice of parameters.

## 3. Jost solutions of the Hamiltonian $H_2$

The Schrödinger equation for the scattering problem of potential $V_2$ is

$$H_2 f^{\pm}(k,r) = k^2 f^{\pm}(k,r), \tag{17}$$

for positive energies $E = k^2$, where $f^{\pm}(k,r)$ are the two linearly independent unnormalized Jost solutions of Hamiltonian $H_2$, which behave asymptotically as outgoing and incoming spherical waves [24]. They are obtained from the Darboux transformation in (5) with $n = 2$ and $\phi_E$ are the free particle wave solutions $e^{\pm ikr}$ with eigenvalue $E = k^2$:

$$f^{\pm}(k,r) = \frac{W(\phi, \partial\phi, e^{\pm ikr})}{W(\phi, \partial\phi)}.$$

As the last column of the Wronskian in the numerator is proportional to $e^{\pm ikr}$, the above expression can be written as

$$f^{\pm}(k,r) = \frac{w^{\pm}(k,r)}{W_2(r)} e^{\pm ikr}, \tag{18}$$

with $w^{\pm}(k,r)$ a complex function of real arguments $k$ and $r$ defined as

$$w^{\pm}(k,r) = -\frac{1}{2}(k^2+q^2)\sin 2\theta + (k^2-q^2)q\gamma \pm i2kq\sin^2\theta. \tag{19}$$

Using the expressions (9) and (19) in (18), we can write the unnormalized Jost solutions in explicit form as

$$f^{\pm}(k,r) = \Big[2(k^2-q^2)q\gamma - (k^2+q^2)\sin 2\theta \pm 4ikq\sin^2\theta\Big]\frac{e^{\pm ikr}}{\sin 2\theta - 2q\gamma}, \tag{20}$$

and from the linear behaviour of $\gamma$ in $r$ for large values of $r$ we find the asymptotic behaviour:

$$f^{\pm}(k,r) = \left[-(k^2-q^2) + \mathcal{O}\left(\frac{1}{r}\right)\right] e^{\pm ikr}. \tag{21}$$

Hence, to obtain the two Jost solutions of $H_2$ normalized to unit flux at infinity, we must divide (20) by the factor $-(k^2-q^2)$,

$$F^{\pm}(k,r) = -\frac{f^{\pm}(k,r)}{k^2-q^2}, \tag{22}$$

and the Jost solutions exhibit a simple pole at $k = q$.

In Appendix A, it is shown that the previous results can be obtained in an alternative way using the confluent case of the intertwining method of SUSY QM.

Hamiltonian $H_2$ has its spectrum defined for positive energies and, for each spectral point, there exist two linearly independent eigenfunctions. However, at the point $k = q$ the two unnormalized Jost solutions coalesce. The Wronskian of the unnormalized Jost solutions can be obtained with the asymptotic behaviour given in (21):

$$W(f^+, f^-) = -2ik(k^2-q^2)^2, \tag{23}$$

which vanishes at the point $k = q$ and therefore the unnormalized Jost solutions are linearly dependent at that spectral point. An eigenfunction is lost and the basis of linearly independent eigenfunctions of the Hamiltonian $H_2$ appears to be incomplete. In its place a Jordan chain of two generalized eigenfunctions is formed. The subspace spanned by the generalized eigenfunctions is in the domain of $H_2$ for $E = q^2$.

## 4. Poles of the Jost solutions and Jordan chain

To obtain the generalized eigenfunctions, we rewrite the normalized Jost solution as a decomposition of its pole in a sum of singular and regular parts. From (22) and using (20) we can write

$$F^{\pm}(k,r) = \left[1 + 4q\frac{(q\cos\theta \mp ik\sin\theta)\sin\theta}{(k^2-q^2)(\sin 2\theta - 2q\gamma)}\right] e^{\pm ikr}, \tag{24}$$

which can also be written as

$$F^{\pm}(k,r) = \frac{\psi_B(q,r)}{k^2-q^2} + \psi_R^{\pm}(k,r), \tag{25}$$

with the following defined functions:

$$\psi_B(q,r) = \lim_{k\to q}(k^2-q^2)F^{\pm}(k,r) = 4q^2\frac{\sin\theta}{\sin 2\theta - 2q\gamma}e^{\mp i\delta(q)} \tag{26}$$

and

$$\psi_R^{\pm}(k,r) = F^{\pm}(k,r) - \frac{\psi_B(q,r)}{k^2-q^2}, \tag{27}$$

where $\psi_B(q,r)$ is a square integrable function of $r$, while $\psi_R^{\pm}(k,r)$ are analytic functions of $k$, and behave asymptotically in $r$ as outgoing and incoming spherical waves. The explicit form of $\psi_R^{\pm}(k,r)$ obtained form (27) is

$$\psi_R^{\pm}(k,r) = e^{\pm ikr} + \left[ \frac{e^{\pm i(k-q)r} - \frac{2q}{k+q}}{k-q} - \frac{e^{\pm i((k+q)r+2\delta(q))}}{k+q} \right] \frac{\psi_B(q,r)}{2q}, \tag{28}$$

and its expression in $k = q$ is given by

$$\psi_R^{\pm}(q,r) = e^{\pm iqr} + \left[1 - e^{\pm 2i\theta} \pm i2qr\right] \frac{\psi_B(q,r)}{4q^2}. \tag{29}$$

After some algebraic manipulation the previous expression can be written as

$$\psi_R^{\pm}(q,r) = (1 \mp iq\delta') \frac{\psi_B(q,r)}{2q^2} + \psi_A(q,r), \tag{30}$$

and $\psi_A(q,r)$, the associated eigenfunction to $\psi_B(q,r)$, is defined as

$$\psi_A(q,r) = -\frac{2q\gamma\cos\theta}{\sin 2\theta - 2q\gamma} e^{\mp i\delta(q)}, \tag{31}$$

which is a bounded, non-normalizable function.

As eigenfunctions of the Hamiltonian $H_2$, the normalized Jost solutions satisfy the time independent Schrödinger equation

$$H_2 F^{\pm}(k,r) = k^2 F^{\pm}(k,r) \tag{32}$$

for all $k$, except $k = q$ where $F^{\pm}(k,r)$ is not defined. To explore the limit $k \to q$ we substitute (25) in (32):

$$H_2 \left( \frac{\psi_B(q,r)}{k^2-q^2} + \psi_R^{\pm}(k,r) \right) = k^2 \left( \frac{\psi_B(q,r)}{k^2-q^2} + \psi_R^{\pm}(k,r) \right). \tag{33}$$

Multiplying (33) by $(k^2-q^2)$ and taking the limit $k \to q$ we obtain:

$$H_2\psi_B(q,r) = q^2\psi_B(q,r), \tag{34}$$

the square integrable solution $\psi_B(q,r)$ representing the bound state embedded in the continuum is an eigenfunction of $H_2$ with energy $E = q^2$. Figure 1 shows $|\psi_B(q,r)|^2$ as a function of $r$.

Using the result (34) in (33) and taking the limit $k \to q$ we get

$$H_2\psi_R^{\pm}(q,r) = q^2\psi_R^{\pm}(q,r) + \psi_B(q,r). \tag{35}$$

However, as the additive term proportional to $\psi_B(q,r)$ in (30) satisfies (34) it can be omitted and we can write

$$H_2\psi_A(q,r) = q^2\psi_A(q,r) + \psi_B(q,r), \tag{36}$$

with $\psi_A(q,r)$ the associated eigenfunction. Thus, $\psi_B(q,r)$ and $\psi_A(q,r)$ are generalized eigenfunctions of the Hamiltonian $H_2$, and they form a Jordan chain of rank two for $E = q^2$. The Jordan chain is the result of the coalescence of two energy levels [25], for a direct proof see Appendix B.

## 5. Pseudo-unitary time evolution of the generalized eigenfunctions

The two generalized eigenfunctions $\psi_B(q,r)$ and $\psi_A(q,r)$ belong to the same spectral point, $E = q^2$; in consequence, they evolve in time together. Hence, it should be convenient to introduce a matrix notation to deal with the two together. From (34) and (36) we can write them as

$$H_2\Psi(q,r) = \mathcal{H}(q)\Psi(q,r), \tag{37}$$

where

$$\Psi(q,r) = \begin{pmatrix} \psi_B(q,r) \\ \psi_A(q,r) \end{pmatrix} \tag{38}$$

is the two component vector of the doublet, and

$$\mathcal{H}(q) = \begin{pmatrix} q^2 & 0 \\ 1 & q^2 \end{pmatrix} \tag{39}$$

is the $2 \times 2$ energy matrix.

The time dependent generalized eigenfunctions are

$$\Psi(r,t) = \mathcal{U}(q,t)\Psi(q,r), \tag{40}$$

where $\mathcal{U}(q,t)$ is the $2 \times 2$ matrix of time dependent coefficients and gives the time evolution of the wave function $\Psi(q,r)$.

Substitution of $\Psi(r,t)$ in the time dependent Schrödinger equation gives the following set of coupled equations written in matrix form

$$i\frac{\partial\mathcal{U}(q,t)}{\partial t}\Psi(q,r) = \mathcal{U}(q,t)H_2\Psi(q,r) = \mathcal{U}(q,t)\mathcal{H}(q)\Psi(q,r). \tag{41}$$

Making abstraction of $\Psi(q,r)$, we obtain

$$i\frac{\partial\mathcal{U}(q,t)}{\partial t} = \mathcal{U}(q,t)\mathcal{H}(q). \tag{42}$$

Integrating equation (42) we get

$$\mathcal{U}(q,t) = e^{-i\mathcal{H}(q)t}, \tag{43}$$

writing $\mathcal{H}(q)$ in explicit form in (43), and computing the exponential, we obtain

$$\mathcal{U}(q,t) = e^{-iq^2t} \begin{pmatrix} 1 & 0 \\ -it & 1 \end{pmatrix}. \tag{44}$$

Substitution of the expression (44) in (40) gives the evolution in time of the two generalized components of the doublet $\Psi(r,t)$:

$$\psi_B(r,t) = \psi_B(q,r)e^{-iq^2t} \tag{45}$$

and

$$\psi_A(r,t) = \psi_A(q,r)e^{-iq^2t} - it\psi_B(q,r)e^{-iq^2t}. \quad (46)$$

The component $\psi_B(r,t)$, describing the time evolution of the bound state eigenfunction embedded in the continuum, exhibits a unitary evolution in time, while the component $\psi_A(r,t)$ has a linear growth with time. Therefore, the wave function $\Psi(r,t)$ grows linearly with time $t$. This type of behaviour has been found by Longhi *et al.* [26] in a non-Hermitian Hamiltonian.

The above result is a direct consequence of the pseudo-Hermiticiy of Hamiltonian $H_2$ at $E = q^2$, represented as the matrix $\mathcal{H}(q)$ in (39). An operator is pseudo-Hermitian if there exists a linear, invertible, Hermitian operator $\eta$ such that [27]

$$\mathcal{H}^\dagger = \eta\mathcal{H}\eta^{-1}. \quad (47)$$

The general form of $\eta$ satisfying (47) for $\mathcal{H}(q)$ in (39) is

$$\eta = \begin{pmatrix} a & b \\ b & 0 \end{pmatrix}, \quad (48)$$

with $a$ and $b$ any real parameters. In turn, $\mathcal{U}(q,t)$ is pseudo-unitary because Hamiltonian $H_2$ at $E = q^2$ is a pseudo-Hermitian operator. An operator is pseudo-unitary if its inverse and its adjoint satisfy the transformation [27]

$$\mathcal{U}^\dagger = \eta\mathcal{U}^{-1}\eta^{-1}, \quad (49)$$

as it may be verified by substitution of (44) and (48).

Therefore, the generalized eigenfunctions $\psi_B(q,r)$ and $\psi_A(q,r)$ in the Jordan cycle have a pseudo-unitary time evolution.

## 6. Cross section and scattering matrix

In this section, we will show that the scattering matrix has no singularities at the corresponding spectral point $k = q$, contrary to the case of conventional bound states with negative energies.

The scattering solution is defined as [24]:

$$\psi_s(k,r) = \frac{i}{2}[F^-(k,r) - S(k)F^+(k,r)], \quad (50)$$

where $F^\pm(k,r)$ are the Jost solutions in (22) and $S(k)$ is the scattering matrix defined as

$$S(k) = \frac{F^-(k,0)}{F^+(k,0)}, \quad (51)$$

and $F^+(k,0)$ is the Jost function.

From (20) and (22) evaluated at $r = 0$ we obtain $F^\pm(k,0)$ and a direct substitution in (51) gives:

$$S(k)=\frac{2(k^2-q^2)q\delta'-(k^2+q^2)\sin 2\delta-4ikq\sin^2\delta}{2(k^2-q^2)q\delta'-(k^2+q^2)\sin 2\delta+4ikq\sin^2\delta} \quad (52)$$

which can be written as

$$S(k) = e^{2i\Delta(k)}, \quad (53)$$

where $\Delta(k)$ is the phase shift and is given by

$$\Delta(k)=-\arctan\left(\frac{4kq\sin^2\delta}{2(k^2-q^2)q\delta'-(k^2+q^2)\sin 2\delta}\right). \quad (54)$$

Taking the limit $k \to q$ we get $\Delta(q) = \delta$. Hence, the scattering matrix evaluated at $k = q$ is finite and equal to

$$\lim_{k\to q} S(k) = e^{2i\delta(q)}. \quad (55)$$

However, there can be singularities of $S(k)$ for different values of $k$. The singularities of $S(k)$ are the zeros of the Jost function $F^+(k_0,0) = 0$:

$$(2q\delta' - \sin 2\delta)k_0^2 + (4iq\sin^2\delta)k_0 - (2q\delta' + \sin 2\delta)q^2 = 0, \quad (56)$$

which is a quadratic equation for $k_0$. In terms of $\alpha$ and $\beta$ we have

$$\beta k_0^2 + 2iq(\alpha q - \beta)^2 k_0 - 2\alpha q + \beta = 0. \quad (57)$$

The zeros in the fourth quadrant of the complex $k$-plane near the real axis may be resonances, while zeros on the imaginary positive axis correspond to bound states with negative energy.

The cross section is defined as

$$\sigma(k) = \frac{4\pi}{k^2}\sin^2\Delta(k), \quad (58)$$

and with the explicit form of $\Delta(k)$ in (54) we are able to observe its behaviour and dependence on $k$. Figure 2 shows $\sigma(k)$ as a function of $k$ and for the chosen values of parameters $\alpha$ and $\beta$ a resonance shape is found, belonging to the value $k_0 = \sqrt{2}/3 - i/3$, far from the value $k = q = 1$ of the BIC. The BIC has no effect in the cross section, only when the system is perturbed the BIC may manifest itself as a resonance [20].

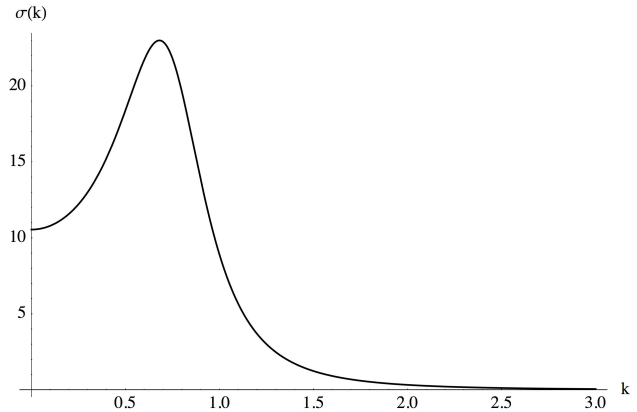


FIGURE 2. Cross section $\sigma(k)$ for parameters values $\alpha = 2$, $\beta = 3$ and $q = 1$. The Breit-Wigner peak in $\sigma(k)$ corresponds to a resonance, far from the value $k = q = 1$ of the BIC, located at $k_0 = \sqrt{2}/3 - i/3$.

## 7. Summary and conclusions

In this work, we presented a von Neumann-Wigner type potential $V_2$ constructed by means of a two times iterated and completely degenerated Darboux transformation. The Hamiltonian $H_2$ and the free particle Hamiltonian $H_0$ are isospectral, and to each point in their continuous spectrum corresponds two linearly independent Jost solutions, which behave at infinity as incoming and outgoing waves. However, we have shown that in the continuous spectrum of $H_2$ there is a singular point, with energy $E = q^2$, such that the two unnormalized Jost solutions are linearly dependent and coalesce to give rise to a Jordan chain of rank two of generalized eigenfunctions and a Jordan block representation of the Hamiltonian $H_2$. The normalized Jost solutions have a simple pole at wave number $k = q$ and after a pole decomposition the Jordan chain and respective generalized eigenfunctions are obtained. One of the generalized eigenfunctions is normalizable and corresponds to the BIC, the other is a bounded, non-normalizable function associated with the BIC. Finally, we obtained the time evolution of the generalized eigenfunctions: the BIC has a unitary time evolution, while the associated eigenfunction has a linear growth in time. Together, they exhibit a pseudo-unitary behaviour characteristic of a pseudo-Hermitian system. Finally, we have shown that the BIC is not associated with a singularity of the scattering matrix $S(k)$ and, as a result, the BIC is not observed in the cross section $\sigma(k)$.

## Appendix

## A. Equivalence with the confluent case of SUSY QM

The completely degenerated case of the Darboux transformation and the confluent case of SUSY QM are equivalent methods for obtaining new, completely solvable, quantum systems from previously solved ones.

In SUSY QM of second order the relation between the initial Hamiltonian $H_0$ and the transformed Hamiltonian $H_2$ is given by [28]

$$H_2 B_2 = B_2 H_0 \tag{A.1}$$

where

$$H_2 = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_2 \tag{A.2}$$

$$H_0 = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_0 \tag{A.3}$$

$$B_2 = \frac{\mathrm{d}^2}{\mathrm{d}r^2} + g(r)\frac{\mathrm{d}}{\mathrm{d}r} + h(r). \tag{A.4}$$

Operator $B_2$ is known as the intertwining operator, and is a differential operator of second order, with $g(r)$ and $h(r)$ functions to be determined.

Therefore, by applying (A.1) and using $V_2$, given in (12), we can find an explicit expression for the corresponding intertwining operator for the present problem. With $V_0 = 0$ we obtain the following equations:

$$-2\frac{\mathrm{d}g(r)}{\mathrm{d}r} + V_2 = 0 \tag{A.5}$$

$$-\frac{\mathrm{d}^2 g(r)}{\mathrm{d}r^2} - 2\frac{\mathrm{d}h(r)}{\mathrm{d}r} + V_2 g(r) = 0 \tag{A.6}$$

$$-\frac{\mathrm{d}^2 h(r)}{\mathrm{d}r^2} + V_2 h(r) = 0. \tag{A.7}$$

We notice that $h(r)$ in (A.7) satisfies the equivalent equation $H_2 h(r) = 0$; thus, $h(r)$ is readily obtained from (20) by taking $k = 0$:

$$h(r) = -q^2 \frac{\sin 2\theta + 2q\gamma}{\sin 2\theta - 2q\gamma}. \tag{A.8}$$

Using (A.5) in (A.6) we write:

$$\frac{\mathrm{d}}{\mathrm{d}r}\left(-\frac{1}{2}V_2 + g^2(r) - 2h(r)\right) = 0,$$

and as we know both $V_2$ and $h(r)$ we get $g(r)$ as:

$$g(r) = \pm\sqrt{\frac{1}{2}V_2 + 2h(r) + c},$$

with $c$ an arbitrary integration constant. Using $V_2$ and $h(r)$ given in (12) and (A.8), respectively, we get

$$g(r) = \pm\sqrt{16q^2\frac{\sin^4\theta}{(\sin 2\theta - 2q\gamma)^2} + 2q^2 + c},$$

and choosing $c = -2q^2$ the function $g(r)$ is simplified to

$$g(r) = \pm 4q\frac{\sin^2\theta}{\sin 2\theta - 2q\gamma}. \tag{A.9}$$

Differentiating (A.9) once with respect to $r$ and substituting in (A.5), we conclude that we must take the positive root. Hence, with (A.8) and (A.9) the intertwining operator $B_2$ in (A.4) is given by

$$B_2 = \frac{\mathrm{d}^2}{\mathrm{d}r^2} + 4q\frac{\sin^2\theta}{\sin 2\theta - 2q\gamma}\frac{\mathrm{d}}{\mathrm{d}r} - q^2\frac{\sin 2\theta + 2q\gamma}{\sin 2\theta - 2q\gamma}. \tag{A.10}$$

If $\phi_k$ is an eigenfunction of $H_0$ with energy eigenvalue $E = k^2$, satisfying the eigenvalue equation $H_0\phi_k = k^2\phi_k$, then $B_2\phi_k$ is an eigenfunction of $H_2$ for the same eigenvalue

$$H_2 B_2\phi_k = k^2 B_2\phi_k. \tag{A.11}$$

Using the same eigenfunctions for the free particle of outgoing and incoming waves $\phi_k^{\pm} = e^{\pm ikr}$ we get the following eigenfunctions for $H_2$:

$$B_2\phi_k^{\pm} = \left[2(k^2 - q^2)q\gamma - (k^2 + q^2)\sin 2\theta \pm 4ikq\sin^2\theta\right] \times \frac{e^{\pm ikr}}{\sin 2\theta - 2q\gamma}, \tag{A.12}$$

which are exactly the same Jost solutions in (20) obtained with the method of Darboux transformation, thus proving the equivalence of both methods.

## B. Explicit coalescence of two energy levels and Jordan chain

In Sec. 2 the completely degenerated case of the Darboux transformation generalized in Crum's theorem was presented, and the case $n = 2$ was studied. An equivalent way of approaching the problem consists in performing the Darboux transformation with two different transformation functions

$$\phi_1 = \sin(q_1 r + \delta(q_1)) \tag{B.1}$$

$$\phi_2 = \sin(q_2 r + \delta(q_2)) \tag{B.2}$$

with respective energy eigenvalues $E_1 = q_1^2$ and $E_2 = q_2^2$, and then consider the limit when both energy eigenvalues coalesce.

The potential $U_2$ is given by (4) with $n = 2$ and $V_0 = 0$. A calculation of the Wronskian of $\phi_1$ and $\phi_2$ gives

$$W(\phi_1, \phi_2) = q_2 \sin\theta_1 \cos\theta_2 - q_1 \cos\theta_1 \sin\theta_2, \tag{B.3}$$

with $\theta_i = q_i r + \delta(q_i)$. And the potential is

$$U_2(r) = -2\frac{(q_1^2 - q_2^2)(q_2^2 \sin^2\theta_1 - q_1^2 \sin^2\theta_2)}{(q_2 \sin\theta_1 \cos\theta_2 - q_1 \cos\theta_1 \sin\theta_2)^2}. \tag{B.4}$$

Now we calculate the eigenfunctions of the Hamiltonian with potential (B.4) and study the limit when $q_2 \to q_1$. From (2) with $n = 2$ and the free particle solutions $\phi_E = e^{\pm ikr}$, the eigenfunctions are obtained as

$$\varphi^{\pm}(k, r) = \frac{q_1(k^2 - q_2^2)\cos\theta_1 \sin\theta_2 - q_2(k^2 - q_1^2)\sin\theta_1 \cos\theta_2 \mp ik(q_1^2 - q_2^2)\sin\theta_1 \sin\theta_2}{q_2 \sin\theta_1 \cos\theta_2 - q_1 \cos\theta_1 \sin\theta_2} e^{\pm ikr}. \tag{B.5}$$

The Wronskian of the eigenfunctions is directly calculated and has the form

$$W(\varphi^+, \varphi^-) = -2ik(k^2 - q_1^2)(k^2 - q_2^2), \tag{B.6}$$

and we see that for eigenvalues $E = q_1^2$ and $E = q_2^2$ the Wronskian vanishes. In the limit $q_2 \to q_1 = q$ expression (23) is recovered.

The respective eigenfunctions for the energies mentioned above are calculated by direct substitution $k = q_1$ and $k = q_2$ in (B.5) and we obtain

$$\varphi^{\pm}(q_1, r) = \frac{q_1(q_1^2 - q_2^2)\sin\theta_2\, e^{\mp i\delta(q_1)}}{q_2 \sin\theta_1 \cos\theta_2 - q_1 \cos\theta_1 \sin\theta_2} \tag{B.7}$$

and

$$\varphi^{\pm}(q_2, r) = \frac{q_2(q_1^2 - q_2^2)\sin\theta_1\, e^{\mp i\delta(q_2)}}{q_2 \sin\theta_1 \cos\theta_2 - q_1 \cos\theta_1 \sin\theta_2}. \tag{B.8}$$

For $q_1 \neq q_2$, the eigenfunctions $\varphi^{\pm}(q_1, r)$ and $\varphi^{\pm}(q_2, r)$ are linearly independent.

In order to study the coalescence of the two energy levels we denote $q_1 = q$ and $q_2 = q + \epsilon$, and take the limit $\epsilon \to 0$. Because $\epsilon \ll 1$ we consider the following series expansions

$$\sin\theta_2 = \sin\theta + \epsilon\gamma\cos\theta + \frac{\epsilon^2}{2}\left(\delta''\cos\theta - \gamma^2\sin\theta\right) + \ldots$$

$$\cos\theta_2 = \cos\theta - \epsilon\gamma\sin\theta - \frac{\epsilon^2}{2}\left(\delta''\sin\theta + \gamma^2\cos\theta\right) + \ldots,$$

with $\gamma = r + \delta'(q)$.

Substituting both series in (B.7) and (B.8), we get the following expressions

$$\varphi^{\pm}(q, r) = -\frac{4q^2\sin\theta + 2q\epsilon(2q\gamma\cos\theta + \sin\theta) + \mathcal{O}(\epsilon^2)}{\sin 2\theta - 2q\gamma - \epsilon(q\delta'' + 2\gamma\sin^2\theta) + \mathcal{O}(\epsilon^2)} e^{\mp i\delta(q)} \tag{B.9}$$

and

$$\varphi^{\pm}(q + \epsilon, r) = -\frac{4q^2\sin\theta + 6q\epsilon\sin\theta + \mathcal{O}(\epsilon^2)}{\sin 2\theta - 2q\gamma - \epsilon(q\delta'' + 2\gamma\sin^2\theta) + \mathcal{O}(\epsilon^2)} e^{\mp i\delta(q+\epsilon)}, \tag{B.10}$$

and taking the limit $\epsilon \to 0$ we get, respectively,

$$\lim_{\epsilon\to 0}\varphi^{\pm}(q, r) = -\frac{4q^2\sin\theta\, e^{\mp i\delta(q)}}{\sin 2\theta - 2q\gamma} = -\psi_B(q, r) \tag{B.11}$$

and

$$\lim_{\epsilon\to 0}\varphi^{\pm}(q + \epsilon, r) = -\frac{4q^2\sin\theta\, e^{\mp i\delta(q)}}{\sin 2\theta - 2q\gamma} = -\psi_B(q, r), \tag{B.12}$$

which means that both eigenfunctions coalesce to the same square integrable function $\psi_B(q, r)$, defined in (26) and representing the bound stated embedded in the continuum.

When two eigenfunctions and their respective eigenvalues coalesce, a Jordan chain of rank two is formed and the associated eigenfunction, completing the Jordan chain, is given by [25]

$$\psi_G^{\pm}(q, r) = \left.\frac{\frac{\partial\varphi^{\pm}(q,r)}{\partial\epsilon} - \frac{\partial\varphi^{\pm}(q+\epsilon,r)}{\partial\epsilon}}{\frac{\partial}{\partial\epsilon}q^2 - \frac{\partial}{\partial\epsilon}(q+\epsilon)^2}\right|_{\epsilon=0}. \tag{B.13}$$

Differentiating (B.9) and (B.10) with respect to $\epsilon$ and plugging the results in (B.13) we obtain the following expression for the generalized eigenfunction

$$\psi_G^{\pm}(q,r) = (-1 \pm iq\delta')\,\frac{\psi_B(q,r)}{2q^2} - \psi_A(q,r), \qquad \text{(B.14)}$$

with $\psi_A(q,r)$ defined in (31). In expressions (B.11), (B.12) and (B.14), obtained from the explicit coalescence of two energy levels, we notice a global sign difference to their counterparts in (26) and (30). This comes from the normalization factor $-(k^2 - q^2)$ used to normalize the Jost solutions (22) to unit flux at infinity.

## Acknowledgements

We would like to thank C. Calcáneo for his interest in this paper. E. Hernández would like to thank Professor A. Mondragón for his advice and suggestions on this kind of problems and for his great human quality.

1. F. H. Stillinger and T. A. Weber, *Phys. Rev. A* **10** (1974) 1122.
2. F. H. Stillinger and D. R. Herrick, *Phys. Rev. A* **11** (1975) 446.
3. H. Friedrich and D. Wintgen, *Phys. Rev. A* **31** (1985) 3964.
4. S. Longhi, *Opt. Lett.* **39** (2014) 1697.
5. A. A. Lyapina, D. N. Maksimov, A. S. Pilipchuk, and A. F. Sadreev, *J. Fluid Mech.* **780** (2015) 370.
6. C. W. Hsu, B. Zhen, A. D. Stone, J. D. Joannopoulos, and M. Soljačić, *Nat. Rev. Mater.* **1** (2016) 16048.
7. J. von Neumann and E. P. Wigner, *Phys. Z.* **30** (1929) 465.
8. F. Capasso, C. Sirtori, J. Faist, D. L. Sivco, S.-N. G. Chu, and A. Y. Cho, *Nature* **358** (1992) 565.
9. Y. Plotnik *et al*., *Phys. Rev. Lett.* **107** (2011) 183901.
10. G. Corrielli, G. Della Valle, A. Crespi, R. Osellame, and S. Longhi, *Phys. Rev. Lett.* **111** (2013) 220403.
11. S. Weimann *et al*., *Phys. Rev. Lett.* **111** (2013) 240403.
12. M. Koirala, A. Yamilov, A. Basiri, Y. Bromberg, H. Cao, and T. Kottos, *New J. Phys.* **17** (2015) 013003.
13. M. I. Molina, A. E. Miroshnichenko, and Y. S. Kivshar, *Phys. Rev. Lett.* **108** (2012) 070401.
14. M. Klaus, *J. Math. Phys.* **32** (1991) 163.
15. J. Pappademos, U. Sukhatme, and A. Pagnamenta, *Phys. Rev. A* **48** (1993) 3525.
16. A. A. Stahlhofen, *Phys. Rev. A* **51** (1995) 934.
17. T. A. Weber and D. L. Pursey, *Phys. Rev. A* **50** (1994) 4478.
18. A. A. Andrianov and A. V. Sokolov, *SIGMA* **7** (2011) 111.
19. A. Khelashvili and N. Kiknadze, *J. Phys. A: Math. Gen.* **29** (1996) 3209.
20. T. A. Weber and D. L. Pursey, *Phys. Rev. A* **57** (1998) 3534.
21. E. Hernández, A. Jáuregui, D. Lohr, and A. Mondragón, *J. Phys. A: Math. Theor.* **50** (2017) 265301.
22. M. M. Crum, *Q. J. Math.* **6** (1955) 121.
23. V. B. Matveev and M. A. Salle, *Darboux Transformations and Solitons* (Springer, Berlin, 1991).
24. R. G. Newton, *Scattering Theory of Waves and Particles* (Springer, Berlin, 2014).
25. A. A. Andrianov, F. Cannata, and A. V. Sokolov, *Nucl. Phys. B* **773** (2007) 107.
26. S. Longhi and G. Della Valle, *Phys. Rev. A* **89** (2014) 052132.
27. A. Mostafazadeh, *J. Math. Phys.* **45** (2004) 932.
28. D. Bermudez, D. J. Fernández, and N. Fernández-García, *Phys. Lett. A* **376** (2012) 692.