Resonances in piecewise potentials and Supersymmetric Quantum Mechanics (SUSY-QM) for the construction of optical potentials.

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Abstract. A method to obtain the general solution of any constant piecewise potential is presented, this is achieved by means of the analysis of the transfer matrices in each cutoff. The resonance phenomenon together with the supersymmetric quantum mechanics technique allow us to construct a wide family of complex potentials which can be used as theoretical models for optical systems. The method is applied to the particular case for which the potential function has six cutoff points.

1. Introduction
The study of one-dimensional potentials in quantum mechanics remains an interest topic to address problems in contemporary physics. Indeed, the square well potential is discussed in each elementary book and it can be used as start model in many fields of science: to describe the motion of an electron in the field of a linear molecule such as acetylene [1], as a simple model of the deuteron [2, 3] and recently for studying the energy levels of the electrons in the graphene [4]. Thus, it is still studying a wide range of one-dimensional potentials that can serve as simple models of physical systems (see for example [5, 6, 7]). On the other hand, the first-order Supersymmetric Quantum Mechanics is a simple but very powerful technique to generate solvable Hamiltonians from a given initial one, whose solution is completely known. This technique is based on the first-order intertwining relationship and it is closely related to the Darboux transformation and with the widely used factorization method [8, 9, 10, 11].

The resonance phenomenon is one of the most surprising phenomena in nature, quantum mechanics is not the exception, in fact, the resonance states (or resonances) are associated with quasi-bound states, that is, systems which have the sufficient energy to break up into two or more subsystems. Mathematically the resonances can be understood as solutions of the Schrödinger equation with complex eigenvalue that fulfill a purely outgoing boundary condition [12, 13] (for the latest information check [14] and references therein). In this work we are interested in obtaining the general solution of piecewise potentials of any number of steps, thus, together with the supersymmetric quantum mechanics, by using as transformation function a resonant state, a wide family of complex potential can be constructed [18, 19]. The structure of this paper is the following: Section 2 is dedicated to obtain the general solution for a general piecewise potential for any number of steps. In Section 3, by means of our method, the discrete spectrum for a piecewise potential of seven steps (asymmetric square well) is obtained. In Section 4 the
resonance spectrum is obtained for the same particular case. Section 5 is devoted to construct some complex potentials by means of the first order supersymmetric quantum mechanics; it is important to mention that these complex potentials probably can be used for describing optical systems, this last due that there is an analogy between the Helmholtz equation and the Schrödinger equation (see [20] and references therein). Finally, some concluding remarks are exposed.

2. Piecewise potential for any finite number of steps.

Let us consider the one-dimensional stationary Schrödinger equation, which is defined as follows

\[-\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x),\]  

(1)

where the type of potential we are interested in, for an arbitrary finite number of steps, can be written as follows

\[V(x) = V_1 + \sum_{j=2}^{n} (V_j - V_{j-1})\eta(x - a_{j-1}), \quad \eta(y) = \begin{cases} 1 & y \geq 0 \\ 0 & y < 0 \end{cases} \]

(2)

each \(V_j\) \((j = 1, ..., n)\) is constant but it changes from one step to the next; and \(a_j\) \((j = 1, ..., n-1)\) is the cutoff point which connect the regions \(j\) and \(j+1\) (a schematic graphic for \(n = 7\) is presented in Figure 1). The solution to the equation (1) for the potential (2), in each of the regions, is simply

\[\psi_j(x) = A_j e^{ik_j x} + B_j e^{-ik_j x}, \quad \text{with} \quad k_j^2 = (E - V_j), \quad (j = 1, ..., n).\]

(3)

![Figure 1. Schematic Figure of the potential (2) for \(n = 7\) with all the \(a_j > 0, V_1 = V_7 = 0\) and \(V_j < 0\) \((j = 2, ..., 6)\).](image)

According to the foundations of quantum mechanics, the above solutions must fulfill the following continuity conditions

\[
\begin{align*}
\psi_j(x = a_j) &= \psi_{j+1}(x = a_j), & j = 1, 2, ..., n - 1, \\
\psi'_j(x = a_j) &= \psi'_{j+1}(x = a_j), & \equiv \frac{d}{dx}.
\end{align*}
\]

(4)

(5)

The last relationships can be written in matrix form as follows:

\[M_j|j > = M_{j+1}|j + 1 >,\]

(6)

where

\[M_j = \begin{pmatrix} e^{ik_j x} & e^{-ik_j x} \\ ik_j e^{ik_j x} & -ik_j e^{-ik_j x} \end{pmatrix}_{x=a_j} \quad \text{and} \quad |j > = \begin{pmatrix} A_j \\ B_j \end{pmatrix}.\]

(7)
Hence, the coefficients of each of the solutions may be written in terms of the preceding one through the following relationships

\[ |j + 1> = T_j |j> \] (8)

where

\[
T_j = (M_{j+1})^{-1} M_j = \frac{1}{2} \left( \begin{array}{cc}
\left(1 + \frac{k_j}{k_{j+1}}\right) e^{-i(k_{j+1}-k_j)x} & \left(1 - \frac{k_j}{k_{j+1}}\right) e^{-i(k_{j+1}+k_j)x} \\
\left(1 - \frac{k_j}{k_{j+1}}\right) e^{i(k_{j+1}+k_j)x} & \left(1 + \frac{k_j}{k_{j+1}}\right) e^{i(k_{j+1}-k_j)x}
\end{array} \right) \bigg|_{x=a_j}
\] (9)

thus, the transfer matrix which connects the last coefficients with the initial ones (\(|n> = T_l |1>\)) is written as the next matrices product

\[
T_l = T_{n-1} T_{n-2} \cdots T_2 T_1.
\] (10)

In the next sections the discrete and resonance spectrums will be found for an asymmetric square well of seven steps (\(n = 7\)).

3. Bound states in the asymmetric square well of seven steps.

Let us consider a piecewise constant potential of seven steps with the following constrains on the values of the parameters (see Figure 1):

- \(a_j > 0\) for \(j = 1, ..., 7\).
- \(V_1 = V_7 = 0\).
- \(V_j < 0\) for \(j = 2, ..., 6\).

In this section we restrict our analysis to the case of negative energies. Thus, the kinetic terms in regions 1 and 7 are given by

\[ k_1 = k_7 = i\kappa = i\sqrt{|E|} \] (11)

Therefore, the asymptotic behaviors of the solution can be analyzed as follow

\[
\lim_{x \to -\infty} \psi_1(x) = \lim_{x \to -\infty} A_1 e^{-\kappa x} + B_1 e^{\kappa x} = \lim_{x \to -\infty} A_1 e^{-\kappa x} \to \infty,
\] (12)

\[
\lim_{x \to \infty} \psi_7(x) = \lim_{x \to \infty} A_7 e^{-\kappa x} + B_7 e^{\kappa x} = \lim_{x \to \infty} B_7 e^{\kappa x} \to \infty.
\] (13)

Since we are interested in solutions of square integrable, associated with the discrete spectrum of the system, we must pay attention only on those solutions for which it holds that \(A_1 = B_7 = 0\).

On the other hand, we know that

\[ |7> = T_l |1>, \quad \text{with} \quad T_l = T_6 \cdots T_1, \] (14)

or equivalently

\[
A_7 = (T_l)_{11} A_1 + (T_l)_{12} B_1, \\
B_7 = (T_l)_{21} A_1 + (T_l)_{22} B_1.
\] (15)
Table 1. Discrete spectrum for the conventional square well \((V_0 = -10\) and width \(a=4\)) and for the asymmetric square well with \(V_1 = V_7 = 0, V_2 = -12, V_3 = -4, V_4 = -10, V_5 = -5, V_6 = -11, a_1 = 1, a_2 = 2, a_3 = 3, a_4 = 3.7, a_5 = 4.3\) and \(a_6 = 5\).

| Energies          | Square well | Asymmetric well |
|-------------------|-------------|-----------------|
| Ground state:     | -9.541064761177934 | -8.572298254015104 |
| First excited state: | -8.176899605890787 | -7.292325563181705 |
| Second excited state: | -5.953924724417183 | -5.180401667805235 |

Figure 2. Square well (dashed line) and asymmetric square well (continuous line), for the parameters shown in Table 1.

Figure 3. Ground states of the square well (dashed line) and of the asymmetric square well (continuous line).

In accordance with the previous analysis about the square integrable solutions, we take \(A_1 = 0\), whence the last equation is reduced to

\[
A_7 = (T_t)_{12}B_1, \quad B_7 = (T_t)_{22}B_1, \quad (16)
\]

but \(B_7\) must be zero, then, the equation that allows us to find the discrete spectrum of the system is simply

\[
(T_t)_{22} = 0. \quad (17)
\]

The explicit expression for \((T_t)_{22}\) can be calculated from the general expressions for the transfer matrices presented previously. However, this expression is very long and therefore is not presented, instead, the Table 1 shows the negative energies associated with the discrete spectrums of our piecewise constant potential (asymmetric square well) and of the conventional square well for some particular values of the parameters.

Figure 2 shows a comparison between the square well (dashed line) and the asymmetric square well (continuous line) for the parameters showed in Table 1. Furthermore, Figures 3, 4 and 5 make clear that the wave functions corresponding to the discrete spectrum inherited the asymmetry of the piecewise potential. Moreover, the wave function of the ground state shows that any particle in this energy state, has a higher probability to be in the region where the potential is deeper, that is, to the left of the center of the potential. However, as the energy increases the wave function approaches the wave functions of the conventional square well (see Figure 5).
4. Resonances in the asymmetric square well of seven steps.

The resonances or resonant states are widely used to describe scattering processes, and they are defined as solutions of the Schrödinger equation with complex eigenvalues, which fulfill a purely outgoing boundary condition. For short range one dimensional potentials, this boundary condition can be written as follows (see [18])

\[
\lim_{x \to \pm \infty} [\psi'(x) \mp ik\psi(x)] = 0, \quad \text{with} \quad k^2 = E. \tag{18}
\]

Therefore, as happened to the discrete spectrum, we must analyze the asymptotic behavior of the solution. For this purpose, we start from

\[
A_7 = (T_t)_{11} A_1 + (T_t)_{12} B_1, \\
B_7 = (T_t)_{21} A_1 + (T_t)_{22} B_1. \tag{19}
\]

If we assume that a single particle source is located far to the left of the interaction region, we have to take \(B_7 = 0\), then

\[
B_1 = -\frac{(T_t)_{21}}{(T_t)_{22}} A_1 \tag{20}
\]

substituting the last expression into (19), a relation of \(A_7\) in terms of \(A_1\) is obtained

\[
A_7 = \frac{\text{Det}[T_t]}{(T_t)_{22}} A_1. \tag{21}
\]

It is not difficult to show that the remaining coefficients \(A_j\) and \(B_j\) \((j = 2, \ldots, 6)\), can be written in terms of \(A_1\) and all them have as common factor to 1/(\(T_t)_{22}\). Thus, the zeros of the function \((T_t)_{22}\) lead to a singular solution. Nevertheless, this singularity can be removed if the solution is renormalized by means of the redefinition of the arbitrary constant \(A_1\) as follows

\[
A_1 = (T_t)_{22} A, \tag{22}
\]

where \(A\) is the new normalization constant. Thus, with this assumption we have a nonsingular solution and the zeros of the function \((T_t)_{22}\) are justly the complex energy eigenvalues which fulfill the purely outgoing boundary condition (18); moreover, these zeros are simple poles of the transmission coefficient (for more details see for example [18]), which in this case is defined as

\[
T = \left| \frac{A_7}{A_1} \right|^2 = \left| \frac{\text{Det}[T_t]}{(T_t)_{22}} \right|^2 \tag{23}
\]
Table 2. Resonant states found by the parameters: $V_1 = V_7 = 0$, $V_2 = -1000$, $V_3 = -930$, $V_4 = -980$, $V_5 = -950$, $V_6 = -1010$, $a_1 = 10$, $a_2 = 15.6$, $a_3 = 19.3$, $a_4 = 22$, $a_5 = 26.7$, $a_6 = 30$.

| Elements      | Resonance energies                                      |
|---------------|---------------------------------------------------------|
| First resonance | 3.04386926392625 - 0.339066907380203i                 |
| Second resonance | 12.9822853595348 - 0.704447767786007i                  |
| Third resonance | 22.8975576232267 - 0.959431583552292i                  |
| Fourth resonance | 32.6650005179265 - 1.144896448819466i                  |
| Fifth resonance  | 42.8024271749718 - 1.308763165361565i                  |
| Sixth resonance  | 52.7270667854136 - 1.462783086145259i                  |
| Seventh resonance | 62.8514355221570 - 1.587975668791163i                  |
| Eighth resonance  | 72.9718969834342 - 1.700247690561512i                  |

Figure 6. Superposition between the transmission coefficient and the Breit-Wigner distribution.

and can be approximated by a superposition of Breit-Wigner distributions of the form

$$\omega(E, \epsilon_R, \Gamma) = \frac{\frac{\Gamma}{2}}{\left(\epsilon_R - E\right)^2 + \left(\frac{\Gamma}{2}\right)^2}. \quad (24)$$

The complex zeros of $(T_t)^{22}$ for the present case can be computed numerically. The Table 2 shows the resonance spectrum for the asymmetric square well of seven steps, for some specific parameters values. Figure 6 shows a schematic comparison between the transmission coefficient and a superposition of Breit-Wigner distribution, this last defined in terms of the resonances presented in the Table 2. It is important to note that, according to the results presented in this work, both the discrete spectrum as the spectrum of resonances are obtained from the same condition $(T_t)^{22} = 0$, this is why we can understand the resonant states as bound states with finite lifetime and vice versa. In the next section we will use the supersymmetric quantum mechanics technique for constructing a wide family of complex potentials, which can be used as theoretical models of optical systems [20].

5. First-order Supersymmetric Quantum Mechanics.

This technique is based on the first order operatorial intertwining and allows us to generate exact analytical solutions for new potentials from one whose complete solution is known. Then, the starting relationship is

$$H_1A_1^+ = A_1^+H_0 \quad \quad (25)$$
with
\[ H = -\frac{d^2}{dx^2} + V_i(x), \quad i = 0, 1. \] (26)
\[ A^+ = \left( -\frac{d}{dx} + \alpha(x) \right). \] (27)

Here, we are assuming that the solution to the Schrödinger equation corresponding to the Hamiltonian \( H_0 \) is known and \( \alpha(x) \) is a function to be determined. Developing both sides of the intertwining relationship and equating coefficients of the same order in the derivatives, the following pair of equations is obtained:
\[ V_1 = V_0 - 2\alpha' \] (28)
\[ \alpha V_1 - \alpha'' = \alpha V_0 - V_0 \] (29)

after substituting (28) into (29) and integrating, the next Riccati equation for \( \alpha \) is obtained
\[ \alpha' + \alpha^2 = V_0 - \varepsilon. \] (30)

The above equation can be linearized by means of the following change \( \alpha = \frac{\psi(0)'}{\psi(0)} \), which leads the Riccati equation to a Schrödinger equation type for the potential \( V_0 \)
\[ \psi(0)'' + V_0 \psi(0) = \epsilon \psi(0). \] (31)

Therefore, function \( \alpha \) can be found in terms of a general solution of the last equation, in this context, the function \( \psi(0) \) is known in the literature as transformation function and \( \epsilon \) is the factorization constant. From equation (25) can be easily shown that if
\[ H_0 \psi_\lambda = \lambda \psi_\lambda \] (32)
then
\[ H_1 \psi_\lambda[1] = \lambda \psi_\lambda[1], \] (33)
where
\[ V_1 = V_0 - 2 \left( \frac{\psi(0)'}{\psi(0)} \right)' \quad \text{and} \quad \psi_\lambda[1] = A^\dagger \psi_\lambda. \] (34)

The last expressions are also known as Darboux transformation, which is equivalent to the supersymmetric quantum mechanics technique. In this paper we are interested in a special case of this transformation: one in which the transformation function is a resonant state, as this allows us to construct a wide variety of complex potentials that can be used to model optical systems (for details see [19]).

Figures 7 and 8 show respectively the real and imaginary parts of the first-order SUSY partner of the piecewise potential of seven steps, here we have taken the first resonance as transformation function. The real part of the supersymmetric partner shows a sequence of non divergent wells, which are very deep but in turn so narrow. It is not difficult to verify that the number of wells that appears in the supersymmetric partners increases as the resonance we have used for implementing the transformation is more excited (the real part of the complex eigenvalue is bigger). On the other hand, the sign of the imaginary part of the SUSY partner dictates if we have a source (positive values) or sink (negative values) of probability. Furthermore, we can see that there is a symmetry in the system, ie, everything that is absorbed in some region is emitted in another one, so that the net effect of the system is that there is a conservation of probability. This can be demonstrated if the area under the curve of the imaginary part is computed. This last result could be of interest for those involved in the ongoing discussion on PT-symmetry and the possible extension or generalization of Quantum Mechanics, see for example [21].
6. Concluding Remarks.
Based on the analysis of the transfer matrices, we have found general expressions for obtaining the complete solution of any piecewise potential. This method is applied to an asymmetric square well of seven steps, where the discrete and resonance spectrums were obtained. Moreover, a general expression for the transmission coefficient was also presented, which gives the dynamics of the scattering process. On the other hand, the supersymmetric quantum mechanics by using a resonance as transformation function, permit us to construct complex potentials, which could be used as theoretical models of optical systems. The method is so general that could be implemented for any number of steps and even keeping as arbitrary all the parameters.

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