SOME RESULTS FOR A PARTICLE IN A BOX AND THEIR SUPERSYMMETRIC PARTNERS

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Some physical restrictions and their influences on the boundary conditions for a particle in a one-dimensional box are pointed out. We discuss the invariance of the corresponding Hamiltonian under time-reversal $\hat{T}$ and its relation with the degeneracy of the energy eigenvalues. We also discuss the effect on the boundary conditions of requiring the invariance of the Hamiltonian under parity $\hat{P}$ and simultaneous space and time reflection $\hat{P}\hat{T}$. A condition, which depends only on the boundary values of an eigenfunction of the Hamiltonian and its derivative, determines if the corresponding eigenvalue satisfies the inequality $E > V(x) = \text{const}$, $V(x)$ being the potential inside the box. Once these results have been presented, we choose various representative analytically solvable examples of boundary conditions (Hamiltonians) and supersymmetrize the corresponding problems. We find real and complex valued supersymmetric partner potentials among all these systems.

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1. Introduction

In the last few years, supersymmetric quantum mechanics (SUSY QM) has become a very active field of research, especially because it has the ability to find new exactly solvable potentials with almost equal energy spectra [1]. For example, many exactly solvable potentials have been studied, nevertheless, until a short time ago, the supersymmetric version of the simplest model problem of quantum mechanics with bound states, the free particle inside a one-dimensional box (with Hilbert space $L^2(\Omega)$, where $\Omega \subset \mathbb{R}$), had been studied only when the ground state
eigenfunction for the Hamiltonian $\hat{H}$ satisfies the Dirichlet boundary condition [2]. Recently, a (non standard) complex boundary condition was considered for the same problem [3], also introducing an alternative approach to the general problem of factorization that uses the probability density and current corresponding to the ground-state eigenfunction of $\hat{H}$. As is well known, this eigenfunction is especially important in the SUSY QM procedure, peculiarly, the ground state eigenfunction for a particle in a box could be specifically complex and nondegenerate, or complex and degenerate, or simply real and nondegenerate or degenerate. More recently, in Ref. [4], other representative boundary conditions were studied again by applying the formalism introduced in Ref. [3]. (The approach used in Refs. [3, 4], with local observable quantities, is specially useful for the consideration of bound states; moreover, it complements other SUSY complexification procedures [5].) The SUSY quantum mechanical treatment of the infinite square well potential (with Hilbert space $L^2(\mathbb{R})$), has also been studied [6]. In that paper, the SUSY version of the finite square well potential was developed first, and then from these results, the corresponding infinite square well was obtained.

In this paper, we complement, extend and discuss the results obtained in Refs. [3, 4]. We supersymmetrize various interesting types of explicitly solvable boundary conditions that are included within a four-parameter general family of boundary conditions. By the way, some of these boundary conditions are physically rare or unusual and lead to unexpected, interesting and not so common results (for instance, as complex superpotentials, or two partner potentials corresponding to only one potential). For this reason, we also obtain and introduce here several results about boundary conditions for a particle in a box. These results have consequences on the type of ground state eigenfunction that one has at first – for the operator $\hat{H}$ – and, therefore, on the type of final energy eigenvalue problem, for its respective partner.

The plan of this paper is as follows. In the following section, we present the most general family of boundary conditions for the Schrödinger Hamiltonian that describes a free particle in a one-dimensional box. We discuss the invariance of this Hamiltonian under time-inversion $\hat{T}$ and its relation with the degeneracy of the energy eigenvalues. (We also have more results about this in section 4.) The requirements of space-reflection $\hat{P}$ and $\hat{P}\hat{T}$ symmetry also restrict the general family of boundary conditions, and this is discussed in this section as well. Likewise, we obtain a condition, which depends only on the boundary values of a Hamiltonian eigenfunction $u(x)$ and its derivative $u'(x)$, that determines does the corresponding energy eigenvalue satisfies the inequality $E > V(x) (= \text{const})$. The content of this section complements results previously obtained [7], moreover, all these results for boundary conditions for a particle in a box may be of an independent interest. In section 3, we briefly review our approach (introduced in Ref. [3]) to the problem of factorization of a self-adjoint Hamiltonian operator with (possibly) complex eigenfunctions. (We also establish notation with this content.) In section 4, we use this approach to supersymmetrize some representative Hamiltonians for a particle in a box. Finally, some concluding remarks are given in section 5.
2. Particle in a box

For a free particle in a one-dimensional box (i.e., null or constant potential inside a box) with walls at \( x = 0 \) and \( x = L \), the Hamiltonian (real and self-adjoint) is \( H = (-\hbar^2/2m)(d^2/dx^2) + V \), which is defined in the Hilbert space \( \mathbb{H} \) for functions \( u(x) \) such that \( ||u|| < \infty \), in \( \Omega = [0, L] \) (with the usual definition of the norm). This \( \hat{H} \) is an unbounded operator, and its domain \( D(\hat{H}) \) are all functions belonging to \( \mathbb{H} \) satisfying \( ||\hat{H}(u)|| < \infty \). (Also, \( u(x) \) and \( du/dx = u'(x) \) are absolutely continuous functions.) Furthermore, \( u(x) \) must satisfy some of the following boundary conditions \([7,8]\)

\[
\begin{pmatrix}
  u(L) - i\lambda u'(L) \\
  u(0) + i\lambda u'(0)
\end{pmatrix} = U \begin{pmatrix}
  u(L) + i\lambda u'(L) \\
  u(0) - i\lambda u'(0)
\end{pmatrix}.
\]

The primes in the preceding equation mean differentiation with respect to \( x \). The parameter \( \lambda \) is inserted for dimensional reasons and the matrix \( U \) belongs to \( U(2) \).

The potential inside a box \( V \) is real. It can be shown that for every function \( u \in D(\hat{H}) \), the density current \( j(x) = (\hbar/m) \text{Im}(\bar{u}(x)u'(x)) \) (bar means the complex conjugation) satisfies \( j(0) = j(L) \). Some of these boundary conditions verify \( j(0) = j(L) = 0 \), which is the impenetrability condition at the walls of the box.

The unitary matrix in (1) can be written, for instance, as \([7]\)

\[
U = \exp(i\phi) \begin{pmatrix}
  m_0 - im_3 \\
  m_2 - im_1
\end{pmatrix} - m_1 + im_3,
\]

where \( \phi \in [0, \pi] \), and quantities \( m_k \in \mathbb{R} \) \( (k = 0, 1, 2, 3) \) satisfy \( (m_0)^2 + (m_1)^2 + (m_2)^2 + (m_3)^2 = 1 \).

Physically, one can classify the boundary conditions included in (1) in many ways; for example, only a subset of the boundary conditions always leads to real eigenfunctions (up to an inessential constant factor), and these are the conditions that are invariant under time-reversal \( \hat{T} \). In fact, if we suppose that the Hamiltonian operator \( \hat{H} \) is invariant under time-reversal \( \hat{T} \), we have \((\hat{T}^{-1}\hat{H}\hat{T}u)(x) = (\hat{H}u)(x)\), so that the operator \( \hat{T} \) commutes with \( \hat{H} \) and the time-reversal transformed function must satisfy \((\hat{T}u)(x) \in D(\hat{H})\). If we consider a stationary state of definite energy (in that situation, \( \hat{T} \) is also called the complex conjugation operator), this invariance implies that \( u(x) \) and \( (\hat{u})(x) \equiv (\hat{T}u)(x) \) are two eigenfunctions of \( \hat{H} \) with the same eigenvalue and they both satisfy the same boundary condition. Thus, the matrix \( U \) must satisfy \( U^+ = \bar{U} \), which implies \( m_2 = 0 \) \([7]\). Therefore, the number of the parameters in \( U \) is reduced to three, and the eigenfunctions for these \( \hat{T} \)-invariant Hamiltonians can be real functions. (This result has also been found in the problem of a particle on a line with a hole; see Ref. [9] and references therein.) If \( u(x) \) is complex, then \( \text{Re}(u) = (u + \bar{u})/2 \) and \( \text{Im}(u) = (u - \bar{u})/2i \) are the two real eigenfunctions of \( \hat{H} \) (within a phase).
It is important to emphasize that when \( u \) and \( \bar{u} \) are complex eigenfunctions of \( \hat{H} \) (or \( \text{Re}(u) \) and \( \text{Im}(u) \) belong to \( \mathbb{R} \)), there is a double degeneracy in the level energies, such that the usual proof that forbids the degeneracy for a one-dimensional system [10] cannot be applied to the problem of a particle inside a box. A necessary condition for the existence of degeneracy in the level energies in this problem is that the respective Hamiltonian be invariant under time-reversal. Hence, \( \hat{T} \)-invariant boundary conditions also exist that cannot lead to degeneracy in the energies, for example, the usual Dirichlet boundary condition \( u(0) = u(\pi) = 0 \), the Neumann boundary condition \( u'(0) = u'(\pi) = 0 \), and the so-called mixed boundary conditions \( u(0) = u'(\pi) = 0 \) and \( u'(0) = u(\pi) = 0 \). (All these boundary conditions are included in a subfamily of boundary conditions that is introduced in section 4.) In conclusion, if the (complex or real) eigenfunctions of the Hamiltonian \( \hat{H} \) are doubly degenerate, then the respective boundary condition is \( \hat{T} \)-symmetric. If the boundary condition is not \( \hat{T} \)-symmetric, then the eigenfunctions are necessarily complex and, in addition, they cannot be degenerate.

One can also require that the boundary conditions be invariant under parity \( \hat{P} \). That is, by supposing that the Hamiltonian operator \( \hat{H} \) is invariant under the parity operator \( \hat{P} \), we have \( (\hat{P}^{-1} \hat{H} \hat{P} u)(x) = (\hat{H} u)(x) \) so that \( \hat{P} \) commutes with \( \hat{H} \) and the parity transformed function must additionally satisfy \( (\hat{P} u)(x) \in D(\hat{H}) \). Thus, \( (\hat{P} u)(x) \equiv u(L - x) \) must satisfy the same boundary condition that \( u(x) \) satisfies. By making use of this last relation and also of the following \( (\hat{P} u)'(x) = \frac{d}{dx} u(L - x) = -\frac{d}{dx} u(\bar{x}) \bigg|_{\bar{x} = L - x} \), it can be seen that the matrix \( U \) must satisfy \( \sigma_x U = U \sigma_x \), and this requires that \( m_2 = m_3 = 0 \). So, we see that any \( \hat{P} \)-invariant boundary condition is at the same time \( \hat{T} \)-invariant. (This result has also been found in the problem of a particle on a line with a hole [11].)

Likewise, if we require that the boundary conditions be invariant under simultaneous space (\( \hat{P} \)) and time (\( \hat{T} \)) reflection, that is, by supposing that the Hamiltonian operator \( \hat{H} \) is invariant under the operator \( \hat{P} \hat{T} \), we have \( ((\hat{P} \hat{T})^{-1} \hat{H} \hat{P} \hat{T} u)(x) = (\hat{H} u)(x) \) so that \( \hat{P} \hat{T} \) commutes with \( \hat{H} \) and the \( \hat{P} \hat{T} \)-transformed function must additionally satisfy \( (\hat{P} \hat{T} u)(x) \in D(\hat{H}) \). Thus, the function \( (\hat{P} \hat{T} u)(x) \equiv \bar{u}(L - x) \) must obey the same boundary condition that \( u(x) \) satisfies. By using this fact and the corresponding expression for the derivative \( (\hat{P} \hat{T} u)'(x) = \frac{d}{dx} \bar{u}(L - x) = -\frac{d}{dx} \bar{u}(\bar{x}) \bigg|_{\bar{x} = L - x} \), it can be demonstrated that the matrix \( U \) satisfies \( \sigma_x U^+ = \bar{U} \sigma_x \), which requires that \( m_3 = 0 \). (Several results about the \( \hat{P} \hat{T} \)-symmetric second derivative operators with point interactions can be found in Ref. [12].) Clearly, the set of boundary conditions invariant under the parity operator is also invariant under the operator \( \hat{P} \hat{T} \).

Finally, given a boundary condition, we can easily obtain a useful condition that determines if an energy eigenvalue satisfies the inequality \( E > V(x) (= \text{const}) \), or else if \( E > 0 \) in the case that \( V = 0 \). (For a particle in a box, the existence of energy eigenvalues for which \( E < V \) is somewhat surprising; as a matter of fact, at
the most, two of these eigenvalues might appear \(^7\).) Certainly, \(E\) being the eigenvalue and \(u(x)\) the corresponding eigenfunction of \(\hat{H}\), we multiply the Schrödinger equation \((\hat{H}u)(x) = Eu(x)\) by \(\bar{u}(x)\) and integrate it between the boundaries of the box. Now, by integrating by parts (once) the term that contains \(u''(x)\), we obtain the following result. If an eigenfunction satisfies the inequality \(\bar{u}(L)u'(L) - \bar{u}(0)u'(0) \leq 0\), then its corresponding energy verifies \(E > V\). It is worth mentioning that the condition \(j(0) = j(L)\) implies that \(\text{Im}(\bar{u}(L)u'(L) - \bar{u}(0)u'(0)) = 0\), so that the inequality we have obtained here, in fact, takes the form

\[
\text{Re}(\bar{u}(L)u'(L) - \bar{u}(0)u'(0)) \leq 0. \tag{3}
\]

This condition is automatically satisfied for some typical boundary conditions, and therefore, all their corresponding eigenfunctions also satisfy this inequality. (Notice that, generally, quantities \(u(x)\) and derivatives \(u'(x)\), evaluated at \(x = 0\) or \(x = L\), depend on the respective eigenvalue.)

In this paper we will consider various examples of boundary conditions that are included within the four parameter family (1) (see Table 1).

**TABLE 1. Some boundary conditions (BC).**

<table>
<thead>
<tr>
<th>BC</th>
<th>Name of boundary condition</th>
<th>Boundary condition</th>
<th>(m_0)</th>
<th>(m_1)</th>
<th>(m_2)</th>
<th>(m_3)</th>
<th>(\phi)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>Dirichlet</td>
<td>(u(0) = u(L) = 0)</td>
<td>1 (-1)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>(\pi(0))</td>
</tr>
<tr>
<td>(b)</td>
<td>Neumann</td>
<td>(u'(0) = u'(L) = 0)</td>
<td>1 (-1)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0 ((\pi))</td>
</tr>
<tr>
<td>(c)</td>
<td>Mixed</td>
<td>(u(0) = u'(L) = 0)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>(\pi/2)</td>
</tr>
<tr>
<td>(d)</td>
<td>Another mixed</td>
<td>(u'(0) = u(L) = 0)</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>-1</td>
<td>(\pi/2)</td>
</tr>
<tr>
<td>(e)</td>
<td>Periodic</td>
<td>(u(0) = u(L), \ u'(0) = u'(L))</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>(\pi/2)</td>
</tr>
<tr>
<td>(f)</td>
<td>Antiperiodic</td>
<td>(u(0) = -u(L), \ u'(0) = -u'(L))</td>
<td>0</td>
<td>-1</td>
<td>0</td>
<td>0</td>
<td>(\pi/2)</td>
</tr>
<tr>
<td>(g)</td>
<td>“Complex”</td>
<td>(u(0) = iu(L), \ u'(0) = -iu'(L))</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>(\pi/2)</td>
</tr>
<tr>
<td>(h)</td>
<td>“Unusual”</td>
<td>(\lambda u(0) = -iu(L), \ \lambda u'(L) = -iu(0))</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Boundary conditions (a), (b), (c), (d), (e) and (f) are \(\hat{T}\)-invariant. The conditions (a), (b), (e), (f), (g) and (h) are \(\hat{P}\hat{T}\)-invariant but only (a), (b), (e) and (f) are \(\hat{P}\)-invariant. All eigenfunctions for the boundary conditions: (a), (b), (c), (d), (e) (f) and (g) satisfy relation (3) for their respective potentials. The ground state for the boundary condition (h) does not satisfy the inequality (3), as we will see in section 4.
3. Factorization with local observable quantities

For completeness, in this section we briefly review our approach to the problem of factorization of a real (self-adjoint) Hamiltonian operator $\hat{H}$ that has a purely discrete spectrum $E_n$ and (possibly complex) eigenfunctions $u_n(x)$ with $n = 0, 1, 2, \ldots$. The ground-state eigenfunction is $u_0(x)$, and its corresponding energy is $E_0 = 0$. Consequently, we write

$$\left(\hat{H}u_0\right)(x) = \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)\right)u_0(x) = 0,$$

(4)

with

$$V(x) = \frac{\hbar^2}{2m} \frac{(u_0)'(x)}{u_0(x)} = w^2(x) - \frac{\hbar}{\sqrt{2m}} w'(x),$$

(5)

where the complex quantity

$$w(x) = -\frac{\hbar}{\sqrt{2m}} \frac{(u_0)'(x)}{u_0(x)} = \frac{\hbar}{\sqrt{2m}} \left(-\frac{(R_0)'(x)}{R_0(x)} - \frac{m j_0}{\hbar} \frac{1}{(R_0)^2(x)}\right),$$

(6)

is the so-called superpotential and the probability density for the ground-state eigenfunction $R_0(x)$ and its corresponding probability current density $j_0$ are given by

$$R_0(x) = \sqrt{|u_0|^2}, \quad j_0(x) = \frac{\hbar}{m} \text{Im}(\bar{u}_0(x)u_0'(x)) = \text{const}.$$

(7)

The potential in (5) is real because $\hat{H}$ is self-adjoint [3, 4], however, as we have explained previously, the eigenfunction $u_0(x)$ is not always real. For example, the ground-state eigenfunction associated to the boundary condition (g), which was mentioned in Section 2, is complex.

The Hamiltonian $\hat{H}$ defined in Eq. (4) can be factorized as

$$\hat{H} = \hat{b} \hat{a},$$

(8)

where we have defined the following linear differential operators

$$\hat{a} \equiv \frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + w(x), \quad \hat{b} \equiv -\frac{\hbar}{\sqrt{2m}} \frac{d}{dx} + w(x).$$

(9)

If the typical case of $j_0 = 0$ is considered, for example, if we are using a real ground-state eigenfunction or an eigenfunction verifying $u_0(x) \propto \bar{u}_0(x)$, which implies that $u_0(x)$ can always be written real, one has (formally) $\hat{b}^+ = \hat{a}$. (As a matter of fact, the probability current density is constant for a stationary state, the external potential being a real function. This constant is zero, for example, if the
A new SUSY partner Hamiltonian \( \hat{H}_S \) (with eigenvalues and eigenfunctions denoted by \( E_S \) and \( u_S \), respectively) can be constructed as

\[
\hat{H}_S = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_S = \hat{a} \hat{b},
\]

where the complex potential \( V_S(x) \) is

\[
V_S(x) = w^2(x) + \frac{\hbar}{\sqrt{2m}} w'(x).
\]

From Eqs. (8) and (10), it is clear that there is an intertwining between the operators \( \hat{H} \) and \( \hat{H}_S \),

\[
\hat{H}_S \hat{a} = \hat{a} \hat{H},
\]

\[
\hat{b} \hat{H}_S = \hat{H} \hat{b}.
\]

Equation (13) is equivalent to

\[
(\hat{a})^+ \hat{H}_S = \hat{H} (\hat{a})^+,
\]

and it is obtained by taking the complex conjugation of Eq. (12), and then its formal adjoint (it must be recalled that \( \hat{H} \) is real, but, in general, \( \hat{H}_S = (\hat{H}_S)^+ \) is complex). Remarkably, if \( u(x) \) is a solution of the Schrödinger eigenvalue equation \( \hat{H}u(x) = Eu(x) \), then \( u_S(x) \sim (\hat{a}u)(x) \neq 0 \) is a solution of the equation \( \hat{H}_S u_S(x) = Eu_S(x) \) with the same energy \( E \). The solutions \( u \) and \( u_S \) can only be considered eigenfunctions of \( \hat{H} \) and \( \hat{H}_S \), respectively, if they are physically adequate, i.e., if they satisfy proper boundary conditions and are normalizable.

### 4. Examples

In this section, we sum up the results we have obtained, that is to say, we present the potentials \( V(x) \) (or Hamiltonians \( \hat{H} \) with \( E_0 = 0 \)) for a particle in a box (the diverse examples of boundary conditions were introduced in section 2, Table 1), the supersymmetric partner potentials \( V_S(x) \), the respective energy eigenvalues, and
the superpotentials (some of these results are also given in Table 2). From now on we write \( h^2 = 2m = 1 \). The box width has been chosen to be \( L = \pi \). The quantities \( R_0 \) and \( j_0 \) are always written for normalized \( u_0 \), and \( n \) is a positive integer \((n \geq 0)\) except where otherwise indicated.

Since boundary conditions (a), (b), (c), (d), (e) and (f) are \( \hat{T} \)-invariant, all their respective eigenfunctions can always be written real; nevertheless, we only have degenerate and complex eigenfunctions for boundary conditions (e) and (f). Actually, these two boundary conditions describe a free particle that is not really confined in the box (i.e., the walls are transparent to the particle) and we do not necessarily have a zero probability current density at the walls. In fact, we can obtain an expression for the probability current density at the walls of the box where

\[
\begin{align*}
\frac{\sin(\mu)}{\cos(\mu)} \cos(\phi) + \cos(\phi) = 0.
\end{align*}
\]

We have to note that all boundary conditions included in (16) are automatically \( \hat{T} \)-invariant as well, and neither of these conditions leads to degenerate eigenfunctions. Certainly, let \( u_a(x) \) and \( u_b(x) \) be two eigenfunctions of \( \hat{H} \) with the same eigenvalue \( E \). By making certain common operations with these solutions and the two respective eigen-equations, we obtain \( u_a'j_a - u_b'j_b = c = \text{const} \) [13]. Then, by evaluating this relation, for example, at \( x = 0 \), we write \( u_a(0)u_b'(0) - u_b(0)u_a'(0) = 0 \), and by using (16) we can write here \( u_a' \) and \( u_b' \) as functions of \( u_a(0) \) and \( u_b(0) \), respectively. We finally obtain \( c = 0 \), which implies \( u_a \propto u_b, \forall x \in [0, \pi] \), i.e., we do not have degenerate eigenfunctions. On the other hand, neither of the six boundary conditions (a) – (f) leads to states with energy eigenvalues for which \( E < V \). 

We obtain the following results for examples (a) – (f):

(a) We have \( V(x) = -1 \) and \( E_n = n(n+2) \). Then \( j_0 = 0, R_0(x) = \sqrt{2/\pi} \sin(x) \) and the superpotential is \( v(x) = -\cot(x) \). From these results, we obtain \( V_S(x) = 2 \csc^2(x) - 1 \) with eigenvalues \( (E_S)_n = (n+1)(n+3) \). The eigenfunctions \( (u_S)_n \) are easily obtained from \( u_n(x) \sim \sin((n+1)x) \) using \( u_S \sim \tilde{u} \). All these are the usual results for this well known problem [2].

(b) We have \( V = 0, E_n = n^2 \) and \( u_n(x) \sim \cos(nx) \). Then \( j_0 = 0, R_0(x) = \sqrt{1/\pi} \) and the superpotential vanishes \( w(x) = 0 \). From all these results, we obtain \( V_S(x) = 0 \) and \( (E_S)_n = (n+1)^2 \). The eigenfunctions of \( V_S(x) \) are \( (u_S)_n \sim \sin((n+1)x) \) which are precisely those corresponding to the free particle inside a box with the Dirichlet boundary condition. That is, the standard supersymmetric partner potential \( V_S(x) \)
of $V(x) = 0$ with the Neumann boundary condition is the potential for the infinite square well [4] and, in this way, the respective Hamiltonians are only essentially isospectral. (Note that another interesting situation is also met if one starts from the first excited eigenfunction $u_1(x)$, that is, from its corresponding probability density $R_1(x) = \sqrt{2/\pi} |\cos(x)|$ and probability current $j_1 = 0$, which implies $w(x) = \tan(x)$. For these choices, the partner potentials and the corresponding eigenvalues are $V(x) = -1$ and $E_n = n^2 - 1$, so that $E_0 = -1$ and $E_1 = 0$. Likewise, we obtain the potential $V_S(x) = 2 \sec^2(x) - 1$ with spectra $(E_S)_n = 4(n + 1)(n + 2)$ and eigenfunctions $(u_S)_n \sim (2n + 3) \sin((2n + 3)x) - \tan(x) \cos((2n + 3)x)$. In this last factorization, the superpotential is singular at $x = \pi/2$, which requires the wave function to vanish there. Thus, the almost absolute equality for the spectra of $V(x)$ and $V_S(x)$ is not valid. It is worth noting that the physical solutions $u_S$ we have obtained obey $u_S(0) = u_S(L) = 0$. We believe this is a somewhat unexpected result since $V_S(x)$ is finite at the walls of the box.)

(c) We have $V(x) = -1/4$, $E_n = n(n + 1)$ and $u_n(x) \sim \sin((2n + 1)x/2)$. Then $j_0 = 0$ and $R_0(x) = \sqrt{2/\pi} \sin(x/2)$. The superpotential is $w(x) = -(1/2) \cot(x/2)$. From these results, we obtain $V_S(x) = (1/2) \csc^2(x/2) - (1/4)$ with spectra $(E_S)_n = (n + 1)(n + 2)$ and eigenfunctions $(u_S)_n \sim -(2n + 3) \cos((2n + 3)x/2) + \cot(x/2) \sin((2n + 3)x/2)$.

(d) We have in this case similar results for $V(x)$, $E_n$ and $j_0$ as in the last case, but $u_n \sim \cos((2n + 1)x/2)$ and $R_0(x) = \sqrt{2/\pi} \cos(x/2)$, which implies $w(x) = (1/2) \tan(x/2)$. We obtain the partner potential $V_S(x) = (1/2) \sec^2(x/2) - (1/4)$, with the same spectra we obtained before for $V_S(x)$ as in example (c) ($(E_S)_n = (n + 1)(n + 2)$) and eigenfunctions $(u_S)_n \sim -(2n + 3) \sin((2n + 3)x/2) + \tan(x/2) \cos((2n + 3)x/2)$.

(e) In this case $V(x) = 0$ and $E_n = 4n^2$. All eigenfunctions, with the exception of $u_0(x)$, are doubly degenerate. The complex eigenfunctions can be written as $u_n(x) \sim \exp(\pm 2nx)$, and then $j_0 = 0$, $R_0(x) = \sqrt{1/\pi}$ and $w(x) = 0$. We also obtain $V_S(x) = 0$ and $(E_S)_n = 4(n + 1)^2$. The eigenfunctions $(u_S)_n$, which can also be obtained from $u_n(x)$ making the change $n \rightarrow n + 1$, are almost equal to those of $\hat{H}$ but none of these is a constant function like $u_0(x)$. In fact, $(u_S)_0 \sim \exp(\pm 2x)$. The real eigenfunctions of $\hat{H}$ can be written as $u_0(x) \sim 1$, $u_n(x) \sim \sin(2nx)$ and $u_n(x) \sim \cos(2nx)$, with $n \geq 1$. Then the eigenfunctions of $\hat{H}_S$ are respectively $(u_S)_0 \sim \cos(2(n + 1)x)$ and $(u_S)_n \sim \cos(2(n + 1)x)$. This set of functions, as well as the complex set, is not complete in $\Omega = [0, \pi]$.

(f) We have in this case $V(x) = -1$ and $E_n = 4n(n + 1)$. All eigenfunctions, including the one corresponding to the ground state, are doubly degenerate $u_n(x) \sim \exp(\pm i(2n + 1)x)$ (these are the complex ones), and $j_0 = \pm 2/\pi$, $R_0(x) = \sqrt{1/\pi}$ and $w(x) = \mp i$. However, we obtain only one partner potential $V_S(x) = -1$. Furthermore, $(E_S)_n = 4(n + 1)(n + 2)$ and $(u_S)_n \sim \exp(\pm i(2n + 3)x)$. As in the periodic boundary condition, the set of complex functions $(u_S)_n$ is not complete. We found an unusual situation when we use the real eigenfunctions of $\hat{H}$. In fact, these functions are $u_n(x) \sim \sin((2n + 1)x)$ and $u_n(x) \sim \cos((2n + 1)x)$.
but then $j_0 = 0$ (since $\sin(x)$ and $\cos(x)$ are real functions), and furthermore $R_0(x) = \sqrt{2/\pi} \sin(x)$ and $R_0(x) = \sqrt{2/\pi} |\cos(x)|$, respectively. Obviously, from these results we obtain two superpotentials ($w(x) = -\cot(x)$ and $w(x) = \tan(x)$) and two partner potentials ($V_S(x) = 2 \csc^2(x) - 1$ and $V_S(x) = 2 \sec^2(x) - 1$). Clearly, we must have only one potential $V_S(x)$ corresponding to $V(x)$, but this is so if there is only one function corresponding to the ground state of $\hat{H}$. Finally, real eigenfunctions for these two potentials can be obtained from $u_S \sim \tilde{a} u$ with energies $(E_S)_{n} = 4(n + 1)(n + 2)$.

$\textbf{TABLE 2. Some potentials, their boundary conditions (BC) and partners.}$ The box width has been chosen to be $L = \pi$ in units $\hbar^2 = 2m = 1$. The complex (CE) and real eigenfunctions (RE) in example (f) give some different results.

\begin{center}
\begin{tabular}{|c|c|c|c|}
\hline
BC & $V(x)$ & $w(x)$ & $V_S(x)$ \\
\hline
(a) & -1 & $-\cot(x)$ & $2 \csc^2(x) - 1$ \\
(b) & 0 & 0 & 0 \\
(c) & $-1/4$ & $-(1/2)\cot(x/2)$ & $(1/2)\csc^2(x/2) - (1/4)$ \\
(d) & $-1/4$ & $(1/2)\tan(x/2)$ & $(1/2)\sec^2(x/2) - (1/4)$ \\
(e) & 0 & 0 & 0 \\
(f)CE & -1 & $\mp i$ & -1 \\
(f)RE & -1 & $-\cot(x)$ and $\tan(x)$ & $2 \csc^2(x) - 1$ and $2 \sec^2(x) - 1$ \\
(g) & $-1/4$ & $i/2$ & $-1/4$ \\
(h) & $(1/\lambda)^2$ & \begin{align*}
\text{Re}(w(x)) = & - (1/\lambda) \tanh((2x - \pi)/\lambda) \\
\text{Im}(w(x)) = & (1/\lambda) \text{sech}((2x - \pi)/\lambda)
\end{align*} & \begin{align*}
\text{Re}(V_S(x)) = & (1/\lambda)^2 \\
\text{Im}(V_S(x)) = & (1 - 4 \text{sech}^2((2x - \pi)/\lambda)) \times \text{sech}((2x - \pi)/\lambda) \\
\text{Im}(V_S(x)) = & -4(1/\lambda)^2 \\
\text{Im}(V_S(x)) = & \tanh((2x - \pi)/\lambda) \text{sech}((2x - \pi)/\lambda)
\end{align*}
\hline
\end{tabular}
\end{center}

Since the boundary conditions (g) and (h) are not $\hat{T}$-invariant, all respective eigenfunctions are necessarily complex and none of them are degenerate. Thus, we have the following results for these two physically rare boundary conditions:

(g) In this case $V(x) = -1/4$, $E_n = n(n + 1)$ and $u_n(x) \sim \exp(i(-1)^{n+1}(2n + 1)x/2)$. Then $j_0 = -1/\pi$, $R_o(x) = \sqrt{1/\pi}$ and $w(x) = i/2$. We also obtain $V_S(x) = -1/4$ and $(E_S)_{n} = (n + 1)(n + 2)$ with eigenfunctions $(u_S)_{n}$, which can be obtained from $u_n(x)$ making the change $n \to n + 1$. The complex set of functions $(u_S)_{n}$ is obviously not complete. By the way, we can find very similar results for the “twinned” boundary condition $u(0) = -iu(L)$, $u'(0) = -iu'(L)$.

(h) We have in this case $V(x) = (1/\lambda)^2$ and $E_0 = 0$, $E_n = n^2 + (1/\lambda)^2$, with $n \geq 1$ (note that $E_0 < V(x)$). The complex eigenfunctions are respectively:

\begin{align*}
\text{u}_0(x) = c_0 \left[ \exp(x/\lambda) + \frac{1 + i \exp(\pi/\lambda)}{1 - i \exp(-\pi/\lambda)} \exp(-x/\lambda) \right],
\end{align*}

(17a)
which does not verify the inequality (3), and
\[ u_n(x) = c_n \left[ \exp(inx) + \frac{n\pi + (-1)^n(\pi/\lambda)}{n\pi - (-1)^n(\pi/\lambda)} \exp(-inx) \right]. \] (17b)

From \( u_0(x) \) we obtain
\[ j_0 = -8 \left| c_0 \right|^2 \frac{\cosh(\pi/\lambda)}{\lambda} \frac{1}{1 + \exp(-2\pi/\lambda)}, \quad R_0(x) = |c_0|\sqrt{\exp(2x/\lambda) + \exp(2(\pi-x)/\lambda)}. \] (18)

The real and imaginary parts of the complex superpotential are
\[ \text{Re}(w(x)) = -(1/\lambda) \tanh((2x-\pi)/\lambda), \quad \text{Im}(w(x)) = (1/\lambda)\text{sech}((2x-\pi)/\lambda). \] (19)

We also obtain
\[ \text{Re}(V_S(x)) = (1/\lambda)^2(1 - 4\sech^2((2x - \pi)/\lambda)), \] (20a)
\[ \text{Im}(V_S(x)) = -4(1/\lambda)^2 \tanh((2x - \pi)/\lambda) \text{sech}((2x - \pi)/\lambda). \] (20b)

Complex eigenfunctions (normalizable) for this complex potential could be obtained from \( u_S \sim \hat{u}u \) with energies \( (E_S)_n \) obtained from \( E_n \), making the change \( n \rightarrow n + 1 \). By the way, it is interesting to note that by making \( \lambda \rightarrow \infty \), we obtain the results corresponding to the Neumann boundary condition (by starting from the ground-state eigenfunction \( u_0(x) \)). Finally, the boundary condition (h) was also studied in the framework of SUSY QM in Ref. [3], but therein the first excited eigenfunction \( u_1(x) \) was used (inadvertently) instead of \( u_0(x) \). This is not wrong, but the almost absolute equality of the spectra of \( V(x) \) and the complex potential \( V_S(x) \) is certainly not valid.

On the other hand, since our potential is complex but the bound-state energy eigenvalues are real, we could be interested in the answer to the following question: Is the corresponding Hamiltonian operator \( \hat{H}_S \) \( \hat{P}\hat{T} \)-symmetric? For one-dimensional potentials in \( \Omega = [0, L] \), the \( \hat{P}\hat{T} \)-invariance of \( V_S(x) \) (and also of \( \hat{H}_S \)) requires that \( V_S(x) = V_S(L - x) \), thus, \( \text{Re}(V_S(x)) = \text{Re}(V_S(L - x)) \) and \( \text{Im}(V_S(x)) = -\text{Im}(V_S(L - x)) \). In fact, it can be easily checked that our \( V_S(x) \) is invariant under the combined \( \hat{P}\hat{T} \) reflection and that the eigenfunctions \( u_S \sim \hat{u}u \) are eigenfunctions of \( \hat{P}\hat{T} \). Therefore, the spectrum of \( H_S \) must be real (see, for example, Ref. [14] for an excellent account of the subject).

5. Concluding remarks

We have complemented, discussed and extended the results obtained in Refs. [3,4] by supersymmetrizing several (usual and unusual) interesting examples of explicitly solvable boundary conditions, which are included within a four-parameter general family of boundary conditions for the Hamiltonian that describes
a free particle inside a one-dimensional box. We also discussed the invariance of this Hamiltonian under time-reversal (and its relation to the degeneracy of the energy eigenvalues), parity and simultaneous space and time reflection, as well as its influence on the boundary conditions. As we have seen, for a particle in a box, the eigenfunctions (and particularly the ground state eigenfunction) could be specifically complex and nondegenerate, or complex and degenerate, or simply real and degenerate or nondegenerate. It is precisely all this variety that gives unexpected and not so common results (for instance, as complex superpotentials). Recently, a more complete study about this issue has been made [15].

We indeed discovered some interesting facts. The standard supersymmetric partner Hamiltonian ($\hat{H}_S$) of $\hat{H}$ with $V(x) = 0$ and Neumann boundary conditions is precisely the Hamiltonian for the standard infinite square well. It must be noticed that when we apply a boundary condition like $u(0) = 0$ or $u(L) = 0$, the same condition is fulfilled (there) by the function $u_S$ and its derivative $u'_S$. This last result was verified in examples (a), (c) and (d). Likewise, when we impose $u' = 0$ at one wall, the function $u_S$ is zero there (see examples (b), (c) and (d)). On the other hand, the set of functions $(u_S)_n$ for an operator $\hat{H}_S$ may not be complete when we have complex eigenfunctions for $\hat{H}$ and also real eigenfunctions with a degenerate or nondegenerate ground state (see the examples (e), (g) and (f)). Moreover, we noticed in example (f) two different partner potentials corresponding to only one potential $V(x)$. Finally, we can obtain complex valued potentials $V_S(x)$ with real spectra (which are SUSY partners of real potentials with real discrete energy spectra) if $j_0 \neq 0$ and $(R_0)' \neq 0$ (because of the fact that $\text{Im}(V_S(x)) = 2\hbar j_0(R_0)'(x)/(R_0)^3(x)$, see Ref. [3]). In all these cases, $u_0$ must be a non-trivial complex solution (i.e. different from $\exp(\pm iCx)$, with $C = \text{const}$) of the eigenvalue equation ($\hat{H}u_0)(x) = E_0u_0(x) = 0$, with $V(x) = \text{const} \neq 0$ ($u_0(x)$ may be an explicitly solvable analytical solution). For example, in the boundary condition (h), $u_0(x)$ is a linear combination of two real functions with complex constants (and is dependent on parameter $\lambda$). In this way, a free particle (although inside a box) may be in a partnership relation with a particle in a complex potential.

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References


NEKI REZULTATI ZA ČESTICU U KUTIJI I NJIHOVI SUPERSIMETRIČNI PAROVI

Ističemo neka fizikalna ograničenja i njihov utjecaj na granične uvjete za česticu u jednodimenzionalnoj kutiji. Raspravljamo invarijantnost odnosnog hamiltonijana pri vremenskoj inverziji $\hat{T}$ i njen odnos s degeneracijom energijskih svojstvenih vrijednosti. Raspravljamo i učinak zahtjeva za invarijantnost hamiltonijana pri zrcaljenju $\hat{P}$ i istovremenom zrcaljenju i vremenskoj inverziji $\hat{P}\hat{T}$ na granične uvjete. Jedan uvjet, koji ovisi samo o graničnim uvjetima neke svojstvene funkcije hamiltonijana i njenih derivacija, određuje zadovoljava li odnosna svojstva vrijednost nejednakost $E > V(x) = const$, gdje je $V(x)$ potencijal u kutiji. Nakon izlaganja gornjih rezultata odabrali smo niz oglednih i analitički rješivih graničnih uvjeta (hamiltonijana) i pronašli smo njihovu supersimetričnu inačicu. Našli smo realne i kompleksne supersimetrične parove potencijala za sve razmatrane slučajeve.