THE INFINITE SQUARE WELL WITH A POINT INTERACTION:
A DISCUSSION ON THE DIFFERENT PARAMETRIZATIONS.

MANUEL GADELLA, MªÁNGELES GARCÍA-FERRERO, SERGIO GONZÁLEZ-MARTÍN,
AND FÉLIX H. MALDONADO-VILLAMIZAR

Abstract. The construction of Dirac delta type potentials has been achieved with the use of the theory of self adjoint extensions of non-self adjoint formally Hermitian (symmetric) operators. The application of this formalism to investigate the possible self adjoint extensions of the one dimensional kinematic operator \( K = -d^2/dx^2 \) on the infinite square well potential is quite illustrative and has been given elsewhere. This requires the definition and use of four independent real parameters, which relate the boundary values of the wave functions at the walls. By means of a different approach, that fixes matching conditions at the origin for the wave functions, it is possible to define a perturbation of the type \( a\delta(x) + b\delta'(x) \), thus depending on two parameters, on the infinite square well. The objective of this paper is to investigate whether these two approaches are compatible in the sense that perturbations like \( a\delta(x) + b\delta'(x) \) can be fixed and determined using the first approach.

1. Introduction

The question on whether a formally Hermitian operator is or it is not self adjoint has been completely solved by mathematicians decades ago. A very interesting presentation of this question from the physicists point of view is given in a paper by Bonneau, Faraut and Valent [1]. This paper discusses the notion of self adjoint extensions of the one dimensional momentum operator \( p = -i\frac{d}{dx} \) and the one dimensional kinetic operator \( K = -\frac{d^2}{dx^2} \) on the Hilbert space of square integrable functions on a bounded interval (we take \( m = 1/2 \) and \( \hbar = 1 \) along this Introduction and most of Section 2 for simplicity. Nevertheless, we shall reintroduce explicitly the mass in the final discussion). It is shown the existence of infinite self adjoint realizations of these operators each realization corresponding to one distinct self adjoint operator and therefore, according to the widely accepted interpretation, to one distinct quantum observable.

The crucial point resides in the fact that both \( p = -i\frac{d}{dx} \) and \( K = -\frac{d^2}{dx^2} \) belong to a special type of operators on Hilbert space, the closed unbounded operators. Most of observables (position, momentum, components of the angular momentum, most of Hamiltonians) are represented by self adjoint unbounded operators. Unbounded operators are not defined in general on the whole Hilbert space \( \mathcal{H} \), but on a dense subspace of \( \mathcal{H} \), the domain of the operator. An unbounded operator \( A \) on \( \mathcal{H} \) is determined by both its domain \( \mathcal{D}_A \) and the action of \( A \) on each \( \psi \in \mathcal{D}_A \), which is \( A\psi \).

Let us go back to the operator \( K = -\frac{d^2}{dx^2} \) this time as an operator on the Hilbert space \( L^2([-c, c]) \). This operator cannot be defined on the whole \( L^2([-c, c]) \) as we know the existence of functions on this space which either are not differentiable or do not have square integrable derivatives. In addition, even for domains such that both conditions are satisfied, \( K \) may not be even Hermitian, i.e., \( \langle K\psi|\varphi \rangle = \langle \psi|K\varphi \rangle \) for any pair of functions \( \psi, \varphi \) in the domain. Furthermore, Hermiticity does not imply self adjointness, when we deal with unbounded operators. In any case, \( K \) has an infinite number of self adjoint determinations each one characterized by its own domain. The action of all these

Key words and phrases. Point potentials, Parameterizations of self adjoint extensions
PACS 03.65Db · 03.65.Ge.
determinations on a given function always transform this function into minus its second derivative, but the spaces of functions on which they act are different.

In order to find the self adjoint determinations of \( K \) one uses the theory of extensions\(^1\) of Hermitian operators. It is not our intention to give here a review of this theory. For a presentation comprehensible to physicists, see \([1]\).

For the infinite square well, we have chosen a point perturbation of the type \( a\delta(x) + b\delta'(x) \), where \( \delta(x) \) is the Dirac delta and \( \delta'(x) \) its derivative in the distributional sense, on an infinite square well centered at the origin. In this case, the formal Hamiltonian takes the form:

\[
H = -\frac{1}{2m} \frac{d^2}{dx^2} + V(x) + a\delta(x) + b\delta'(x)
\]

with \( V(x) = \begin{cases} \infty & \text{if } x < -c \\ 0 & \text{if } -c \leq x \leq c \\ \infty & \text{if } x > c \end{cases} \).

In consequence, the time independent Schrödinger equation is

\[
-\frac{1}{2m} \frac{d^2f(x)}{dx^2} + \{V(x) + a\delta(x) + b\delta'(x)\}f(x) = Ef(x),
\]

which is an equation on distributions.

Functions in the domain for which the Hamiltonian in (3) is self adjoint cannot be continuous and with continuous derivative at the origin \([2–4]\). Therefore, we need to define the distributions resulting from the products of \( \delta(x) \) and \( \delta'(x) \) times one function discontinuous at the origin. Henceforth, we shall the following definitions:

\[
f(x)\delta(x) = \frac{f(0-) + f(0+)}{2} \delta(x),
\]

\[
f(x)\delta'(x) = \frac{f(0-) + f(0+)}{2} \delta'(x) - \frac{f'(0-) + f'(0+)}{2} \delta(x),
\]

where,

\[
f(0-) = \lim_{x \to 0^-} f(x), \quad f(0+) = \lim_{x \to 0^+} f(x).
\]

Same for \( f'(0-) \) and \( f'(0+) \).

Concerning the derivative of the delta: It is not well known that the term in the form \( b\delta'(x) \) does not provide a unique perturbation of the Hamiltonian \(-\frac{1}{2m} \frac{d^2}{dx^2} + V(x) + a\delta(x)\). In fact, the introduction of the term \( b\delta'(x) \) often produces a certain degree of confusion. For instance, some authors say that if we add to a potential a term of this kind, then the potential is opaque, i.e., no transmission coefficient exists. On the other hand, other authors find a non-zero transmission coefficient for \( a\delta(x) + b\delta'(x) \). The reason of this disagreement lies on the use of different self adjoint extensions that provide different realizations for the perturbation \( b\delta'(x) \). See \([3–7]\). In this paper, we shall define a self adjoint realization of (1) having reasonable physical properties such as non-zero transmission and reflection coefficients through the \( a\delta(x) + b\delta'(x) \) barrier, as in \([8]\).

Self adjoint extensions of the kinetic operator \( K = -\frac{d^2}{dx^2} \) on the infinite square well have been discussed in \([1]\). These self adjoint extensions are parameterized by five real numbers having one

\(^1\)The operator \( B \) extends the operator \( A \) if \( D_A \subset D_B \) and \( A\psi = B\psi \) for all \( \psi \in D_A \). Then, we write \( A \prec B \).
relation among them, so that only four are independent. This means that each of the self-adjoint extensions of $K$ is characterized by the actual values of four real parameters. These parameters relate the boundary values of the wave functions and of their first derivatives as given at both walls of the well.

Our Hamiltonian $H$ in $(1)$ is given by a point perturbation added to $K$ depending on two real parameters. This perturbation is obtained by choosing a suitable self-adjoint extension of $K$. However, in this case, this self-adjoint extension is determined by some matching conditions imposed to the wave functions at the origin. Then, the question that we want to investigate here is how we could characterize this self-adjoint extension using the parameters relating the boundary conditions at the wall as discussed in $(1)$. As we shall see, this is not a trivial matter.

This paper is organized as follows: In Section 2, we introduce two possible parameterizations of self-adjoint extensions of the kinetic operator in a finite interval, just the parameterizations we want to compare. Section 3 contains the core of the present work. We use the results in $(1)$ to determine the parameters that produce the self-adjoint determination of $(1)$ that we are considering. The final conclusion shows that the relation between parameters is not one to one.

2. The infinite square well with a point perturbation

Let us consider the Hamiltonian of a one-dimensional free particle confined in the interval $[-c, c]$. Its Hamiltonian is given by $H = -\frac{d^2}{dx^2} + V(x)$, where $V(x)$ is given by $(2)$, the infinite square well potential. Along the present section, we shall usually take $m = 1/2$ for simplicity, although we shall explicitly show the mass $m$ whenever convenient.

As a matter of fact, the issue here is the analysis of the differential operator $K = -\frac{d^2}{dx^2}$, sometimes called the kinetic operator, on the interval $[-c, c]$. As is well known, this is an unbounded operator which is not completely determined until we define its domain, i.e., the space of vectors on which it acts. The Hilbert space of pure states for this interval is $L^2[-c, c]$. Therefore, the domain of $K = -\frac{d^2}{dx^2}$ should be contained in the space of square integrable functions on $[-c, c]$ which are twice differentiable (almost elsewhere, i.e., with the possible exception of points in a set of zero Lebesgue measure) and such that their first and second derivative are also square integrable on the same interval. We shall call this space $D^*$.

Now, the question is to find out the domains for which this operator is self-adjoint. Let us consider the functions $\psi(x)$ and $\varphi(x)$ in $D^*$. Then, integration by parts gives:

\begin{equation}
\langle \psi | -\frac{d^2}{dx^2} \varphi \rangle = -i\{\psi^* (\varphi' - \varphi' (-c)) + \psi^*' (\varphi - \varphi' (-c)) + \psi' (\varphi' (-c)) + \psi' (\varphi' (-c))\} + \langle \frac{d^2}{dx^2} \psi | \varphi \rangle .
\end{equation}

In $(7)$, the star denotes complex conjugation. Note that we demand the square integrability of the first derivatives of functions in $D^*$ in order to be able to integrate by parts.

Obviously, $K = -\frac{d^2}{dx^2}$ on $D^*$ is not Hermitian. By Hermiticity, we mean that $\langle \varphi | K \psi \rangle = \langle K \varphi | \psi \rangle$ for any pair of functions $\varphi \equiv \varphi(x), \psi \equiv \psi(x) \in D^*$. We note that the necessary and sufficient condition for the Hermiticity of $K = -\frac{d^2}{dx^2}$ is that

\begin{equation}
\psi^* (\varphi' - \varphi' (-c)) + \psi^*' (\varphi - \varphi' (-c)) + \psi' (\varphi' (-c)) + \psi' (\varphi' (-c)) = 0 .
\end{equation}

We need to choose a domain $D$ for $K = -\frac{d^2}{dx^2}$ with the obvious condition that $D \subset D^*$, also fulfilling $(8)$. In order to define $D$ one may choose all functions $\varphi(x) \in D^*$ such that $\varphi(-c) = \varphi(c) = \varphi'(-c) = \varphi'(c) = 0$. Let us denote by $D_0$ the space of the functions in $D^*$ with this property. Any function $\varphi(x) \in D_0$ and its first derivative are continuous at the well borders $c$ and $-c$. Clearly, $K = -\frac{d^2}{dx^2}$ is Hermitian in $D_0$. However, $K$ is not self adjoint. Due to the Hermiticity of $K$, 

\footnote{Technically, $D^*$ is the space of absolutely continuous functions in $L^2[-c, c]$ with first absolutely continuous derivative and such that $\int_{-c}^{c} (|f(x)|^2 + |f''(x)|^2) \, dx < \infty$.}
K \prec K^\dagger$, i.e., the adjoint of $K$, $K^\dagger$ extends $K$. One can easily prove that this extension is strict, so that $K \neq K^\dagger$ and therefore $K$ cannot be self-adjoint.

The search for self-adjoint extensions of $K$ is nothing else than the search for domains $\mathcal{D}$ for $K$ with the condition that any $\psi(x) \in \mathcal{D}$ satisfies \[ (\frac{2c\psi'(c) - i\psi(-c)}{2c\psi'(c) + i\psi(c)}) = \mathbf{U} \begin{pmatrix} 2c\psi'(-c) + i\psi(-c) \\ 2c\psi'(-c) - i\psi(c) \end{pmatrix}, \] where the matrix $\mathbf{U}$ depends on four real parameters and has the form \[ \mathbf{U} = e^{i\Phi} \begin{pmatrix} m_0 - im_3 & -m_2 - im_1 \\ m_2 - im_1 & m_0 + im_3 \end{pmatrix}, \]

with

\[ m_0^2 + m_1^2 + m_2^2 + m_3^2 = 1 \quad \text{and} \quad \Phi \in [0, \pi]. \]

We see that there are five parameters and one relation between them, so that there are indeed four independent parameters. Each set of fixed values of these parameters gives a self adjoint extension of $K = -d^2/dx^2$. Each of the self adjoint extensions is a different operator with purely discrete spectrum.

As we have already remarked, there is another possibility, another characterization of the domains of the different self adjoint extensions of $K = -d^2/dx^2$, which consists in fixing matching conditions at the origin in the spirit of \[ \frac{\psi'(x)}{\psi(x)} = \frac{\psi'(x)}{\psi(x)} \text{ for } x \in L^2[-c, c]. \] We would like to know how the correspondence between these two approaches are and particularly how the correspondence between the parameters that label the self adjoint extensions of $K$ looks like. In general, this seems a rather cumbersome task. We shall limit our analysis to the case of the extensions of $K$ producing the $a\delta + b\delta'$ perturbation in the Hamiltonian $H = -\frac{1}{2m} d^2/dx^2 + V(x)$ with $V(x)$ as in \[ \frac{\psi'(x)}{\psi(x)} = \frac{\psi'(x)}{\psi(x)} \text{ for } x \in L^2[-c, c]. \] This will give enough relevant information on how this kind of correspondence between the parameters defining the self adjoint determination (extension) in two different settings work. In addition, the problem in its full generality is not tractable. It is important to remark that two different self adjoint extensions of $K$ are different operators and have different eigenvalues \[ \ref{footnote}. \]

2.1. The one dimensional infinite square well with a point perturbation of the type $a\delta(x) + b\delta'(x)$. Next let us make a brief excursion into the operator $-d^2/dx^2$ on $L^2(\mathbb{R})$. One possible domain, $\mathcal{D}_{0,\infty}$, for $-d^2/dx^2$ is the vector space of square functions in $L^2(\mathbb{R})$ such that: i.) admit a first and second derivative which are square integrable (indeed it suffices that the derivative exists save for a null set, but we ignore here certain mathematical technicalities), ii.) so that all functions $\psi(x)$ in $\mathcal{D}_{0,\infty}$ satisfy $\psi(0) = \psi'(0) = 0$ at the origin and iii.) at the infinity we have $\psi(-\infty) = \psi(\infty) = \ref{footnote}$. Here, we want to remark that although a square integrable function may not have a limit at the infinite, if this limit exists it must be zero.

In this case, it is a simple exercise to see that the domain of the adjoint is the space of functions in $L^2(\mathbb{R})$ satisfying i.) and iii.), with ii.) replaced by the condition that both $\psi(x)$ and its derivative $\psi'(x)$ have a finite discontinuity or jump at the origin. On this domain, the adjoint acts exactly as $-d^2/dx^2$ does.

\[ \ref{footnote} \text{Or in more technical terms, the Sobolev space } W^2_2(\mathbb{R}). \]

\[ \ref{footnote} \text{This function may be even of class } C^\infty \text{ on the whole real line. See an example in the Appendix of } \ref{footnote}. \]

\[ \ref{footnote} \text{Here, we have avoided some technicalities. As a matter of fact this domain is the Sobolev space } W^2_2(\mathbb{R} \setminus \{0\}). \]
Now, let us assume that \( \varphi(x) \) and \( \psi(x) \) belong to the domain of the adjoint \((-d^2/dx^2)^{\dagger}\) of \(-d^2/dx^2\). Then, if we denote the left and right limits at the origin of a function \( \phi(x) \) by \( \phi(0-) \) and \( \phi(0+) \) respectively (as in (10)), we have by integration by parts:

\[
\left\langle \varphi \left( -\frac{d^2}{dx^2} \right)^{\dagger} \psi \right\rangle = - \int_{-\infty}^{\infty} \varphi(x) \psi''(x) \, dx = - \int_{-\infty}^{0} \varphi(x) \psi''(x) \, dx - \int_{0}^{\infty} \varphi(x) \psi''(x) \, dx =
\]

\[- \{\varphi(0-)\psi'(0-) - \varphi(-\infty)\psi'(-\infty)\} - \{\varphi(\infty)\psi'(\infty) - \varphi(0+)\psi'(0+)\} + \{\varphi'(0-)\psi(0+) - \varphi'(-\infty)\psi(-\infty)\} + \{\varphi'(\infty)\psi(\infty) - \varphi'(0+)\psi(0+)\} - \int_{-\infty}^{0} \varphi''(x) \psi(x) \, dx - \int_{0}^{\infty} \varphi''(x) \psi(x) \, dx.
\]

Taken into account that the functions in the domain of the adjoint vanish at the infinity, the above expression is equal to

\[- \{\varphi(0-)\psi'(0-) - \varphi(0+)\psi'(0+)\} + \{\varphi'(0-)\psi(0-) - \varphi'(0+)\psi(0+)\} - \int_{-\infty}^{\infty} \varphi''(x) \psi(x) \, dx = \left\langle \left( -\frac{d^2}{dx^2} \right)^{\dagger} \varphi \psi \right\rangle.
\]

As in the previous discussion about the operator \( K = -d^2/dx^2 \) on the infinite square well, in order to obtain the self adjoint extensions of this operator, we have to find the spaces of functions for which (12) vanishes identically, excluding the trivial possibility given by \( \mathbf{8} \). Then, these self adjoint extensions will be determined by \(-d^2/dx^2\) operating on each of these domains.

Each one of these self adjoint extensions is characterized by the fact that their functions \( \psi(x) \) satisfy relations of the type [2]:

\[
\begin{pmatrix}
\psi(0+) \\
\psi'(0+)
\end{pmatrix} = \begin{pmatrix}
\frac{(2+x_2)^2-x_1x_4+x_2^2}{(2-ix_3)^2+x_1x_4-x_2^2} & \frac{-4x_4}{(2-ix_3)^2+x_1x_4-x_2^2} \\
\frac{4x_1}{(2-ix_3)^2+x_1x_4-x_2^2} & \frac{(2-x_2)^2-x_1x_4+x_2^2}{(2-ix_3)^2+x_1x_4-x_2^2}
\end{pmatrix} \begin{pmatrix}
\psi(0-) \\
\psi'(0-)
\end{pmatrix}.
\]

Each set of values of the four real parameters, \( x_i, \ i = 1, 2, 3, 4 \), determines one self adjoint extension of \(-d^2/dx^2\) [2]. However, we are not interested here in all self adjoint extensions, which are anyway listed in [2].

The interesting point is that we can define point potentials of the type \( a\delta(x) + b\delta'(x) \) by means of these self adjoint extensions [2][3][10]. This can be achieved if we choose the following values for the parameters: \( x_1 = a, x_2 = b, x_3 = x_4 = 0 \) [2]. Note that the simplest choice, \( x_1 = x_2 = x_3 = x_4 = 0 \), produces the identity matrix in (13). It also determines a self adjoint extension of \(-d^2/dx^2\).

If we recover the arbitrary value for the mass (as we shall do consistently in the final section), we may write the Hamiltonian corresponding to this particular extension as \(-d^2/dx^2 + 2ma\delta(x) + 2mb\delta'(x)\). Then, \( x_1 = 2ma, x_2 = 2mb \) and \( x_3 = x_4 = 0 \). Thus, (13) takes the following form:

\[
\begin{pmatrix}
\psi(0+) \\
\psi'(0+)
\end{pmatrix} = \begin{pmatrix}
\frac{1+mb}{1-mb} & 0 \\
\frac{1-2ma}{1-mb} & \frac{1-mb}{1+mb}
\end{pmatrix} \begin{pmatrix}
\psi(0-) \\
\psi'(0-)
\end{pmatrix}.
\]
Relation (14) determines the domain of the self-adjoint extension of \(-\frac{d^2}{dx^2} \left(-\frac{1}{2m}\frac{d^2}{dx^2}\right)\) corresponding to the Hamiltonian given by \(-\frac{d^2}{dx^2} + 2ma\delta(x) + 2mb\delta'(x)\). Now let us go back to the case in which \(K = -\frac{d^2}{dx^2}\) is defined on the Hilbert space \(L^2[-c, c]\), i.e., is the operator relative to the infinite one dimensional square well studied in the previous version. In order to define a perturbation of the type \(a\delta(x) + b\delta'(x)\) on the infinite square well, we still need to define the self-adjoint extension of \(K\) using matching conditions (14). Now, the objective is to investigate how we can obtain this perturbation starting with conditions (9) and (10). This is the objective of the next section.

In a previous paper [11], we have discussed the effect on a one dimensional infinite square well of a perturbation of the free Hamiltonian of the type \(a\delta(x) + b\delta'(x)\). We have analyzed how the eigenvalues behave under changes of \(a\) and \(b\). We want to compare formulas (9) and (10) to (14) in order to identify which parameters in (10) correspond to this perturbation. This would permit us to compare the results for the energy levels obtained in [11] with those in [1]. This is the main objective of the present work and will be developed in the next section.

3. PARAMETERS OF THE SELF ADJOINT EXTENSION DEFINING THE PERTURBATION \(a\delta(x) + b\delta'(x)\) CENTERED ON THE INFINITE SQUARE WELL

This section contains the main objective of the present paper. As we have remarked, we want to discuss the relation between the determination of self-adjoint extensions of \(K = -\frac{d^2}{dx^2}\) given by the boundary conditions (9) and the matching conditions (14). However, this problem in its full generality seems too difficult and even untractable, so that we shall undergo a simpler task: the relation between (9) and (10). As we know, boundary conditions (14) determine the Hamiltonian with point potential (1). Therefore, our investigation consists in finding the values of the parameters in (9) that give the point potential \(a\delta(x) + b\delta'(x)\). As we shall see along the next lines, this is not a particularly simple task and the final result is not simple.

To begin with, the solutions of the Schrödinger equation on the infinite square well

\[-\psi''(x) + 2ma\delta(x)\psi(x) + 2mb\delta'(x) = 2mE\psi(x)\]

are given by the following plane waves:

\[
\psi_1(x) = De^{ikx} + Ce^{-ikx}, \quad -c < x < 0 \tag{15}
\]

\[
\psi_2(x) = Ae^{ikx} + Be^{-ikx}, \quad 0 > x > c \tag{16}
\]

Note that \(\psi_1(x)\) and \(\psi_2(x)\) are the solutions to the left and to the right respectively of the origin. At the origin, we assume that \(t[15]\) and \(t[10]\) satisfy (14). Let us use these results in equations (9) and (10). We obtain:

\[
\begin{pmatrix}
D\beta e^{-ikc} - C\alpha e^{ikc} \\
A\alpha e^{ikc} - B\beta e^{-ikc}
\end{pmatrix}
=
\begin{pmatrix}
U_{11} & U_{12} \\
U_{21} & U_{22}
\end{pmatrix}
\begin{pmatrix}
D\alpha e^{-ikc} - C\beta e^{ikc} \\
A\beta e^{ikc} - B\alpha e^{-ikc}
\end{pmatrix},
\]

where \(\alpha = 2ck + 1\) and \(\beta = 2ck - 1\) and \(U_{ij}\) are the entries of matrix \(U\) given in (10). We write \(U\) in this form just for convenience in our presentation and also in order to simplify our calculations as much as possible. It is straightforward that we can write (17) as

\[
\begin{pmatrix}
A\beta U_{22} e^{ikc} - B\alpha U_{12} e^{-ikc} \\
A(\alpha - U_{22}\beta) e^{ikc} - B(\beta - U_{22}\alpha) e^{-ikc}
\end{pmatrix}
=
\begin{pmatrix}
D(\beta - U_{11}\alpha) e^{-ikc} - C(\alpha - U_{11}\beta) e^{ikc} \\
DU_{21}\alpha e^{-ikc} - CU_{21}\beta e^{ikc}
\end{pmatrix}.
\]

Equation (18) can obviously be rewritten in abridged form as:
\[ R \begin{pmatrix} A \\ B \end{pmatrix} = V \begin{pmatrix} D \\ C \end{pmatrix}, \]

where

\[
R = \begin{pmatrix} U_{12} \beta e^{ikc} & -U_{12} \alpha e^{-ikc} \\ (\alpha - U_{22} \beta) e^{ikc} & - (\beta - U_{22} \alpha) e^{-ikc} \end{pmatrix}
\]

\[
V = \begin{pmatrix} (\beta - U_{11} \alpha) e^{-ikc} & - (\alpha - U_{11} \beta) e^{ikc} \\ U_{21} \alpha e^{-ikc} & -U_{21} \beta e^{ikc} \end{pmatrix}.
\]

Equation (19) can be obviously rewritten as:

\[ \begin{pmatrix} A \\ B \end{pmatrix} = R^{-1} V \begin{pmatrix} D \\ C \end{pmatrix}, \]

with

\[
R^{-1} = \frac{1}{\Delta} \begin{pmatrix} - (\beta - U_{22} \alpha) e^{-ikc} & U_{12} \alpha e^{-ikc} \\ - (\alpha - U_{22} \beta) e^{ikc} & U_{12} \beta e^{ikc} \end{pmatrix}
\]

and

\[
\Delta = U_{12} (\alpha^2 - \beta^2) = -8ck (im_1 + m_2) e^{i\phi}.
\]

Now, we are going to obtain a similar result by another method and then, compare this result with the already obtained. First of all, let us write \((14)\) in accordance with the notation used in \((15-16)\), in the following form:

\[ \begin{pmatrix} \psi_2(0+) \\ \psi_2'(0+) \end{pmatrix} = \begin{pmatrix} t_1 & 0 \\ t_2 & \frac{1}{t_1} \end{pmatrix} \begin{pmatrix} \psi_1(0-) \\ \psi_1'(0-) \end{pmatrix}, \]

with

\[
T = \begin{pmatrix} t_1 & 0 \\ t_2 & \frac{1}{t_1} \end{pmatrix} = \begin{pmatrix} \frac{1+mb}{1-mb} & 0 \\ -\frac{2ma}{1-m^2} & \frac{1-mb}{1+mb} \end{pmatrix}.
\]

We write the matrix \(T\) in the form \((24)\) in order to simplify the subsequent calculations. Then, if we use \((15,16)\) in \((26)\), we obtain

\[
\begin{pmatrix} A + B \\ ik(A - B) \end{pmatrix} = \begin{pmatrix} \frac{1+mb}{1-mb} & 0 \\ -\frac{2ma}{1-m^2} & \frac{1-mb}{1+mb} \end{pmatrix} \begin{pmatrix} D + C \\ ik(D - C) \end{pmatrix}.
\]

This equation can be written in a similar form as in \((19)\). A rather straightforward calculation gives:
\[
\begin{pmatrix}
A \\
B
\end{pmatrix} = M^{-1} TM \begin{pmatrix}
D  \\
C
\end{pmatrix},
\]

with
\[
M = \begin{pmatrix}
1 & 1 \\
\text{i}k & -\text{i}k
\end{pmatrix} \quad \text{and} \quad M^{-1} = \frac{1}{2\text{i}k} \begin{pmatrix}
\text{i}k & 1 \\
\text{i}k & -1
\end{pmatrix}.
\]

Comparing (21) and (27), we have:
\[
R^{-1} V = M^{-1} TM.
\]

The next step is to identify matrix elements in the right and left hand sides of (29) in order to write a system of four equations in the four undeterminates \(U_{ij}\). This system is:
\[
\begin{align*}
-(\beta - U_{22}\alpha) (\beta - U_{11}\alpha) + U_{12} U_{21} \alpha^2 &= \frac{ik(t_1 + \frac{1}{t_1}) + t_2}{2ik} e^{2\text{i}ck} \Delta, \\
(\beta - U_{22}\alpha) (\alpha - U_{11}\beta) - U_{12} U_{21} \alpha \beta &= \frac{ik(t_1 - \frac{1}{t_1}) + t_2}{2ik} \Delta, \\
-(\alpha - U_{22}\beta) (\beta - U_{11}\alpha) + U_{12} U_{21} \beta \alpha &= \frac{ik(t_1 - \frac{1}{t_1}) - t_2}{2ik} \Delta, \\
(\alpha - U_{22}\beta) (\alpha - U_{11}\beta) - \beta^2 U_{12} U_{21} &= \frac{ik(t_1 + \frac{1}{t_1}) - t_2}{2ik} e^{-2\text{i}ck} \Delta.
\end{align*}
\]

Although the calculations that we shall introduce here in the sequel are rather straightforward, their complexity makes it advisable to give them with some detail. Otherwise the regular reader may have unnecessary difficulties to reproduce the whole procedure.

Next, we write the matrix elements \(U_{ij}\) in terms of \(\Phi\) and the \(m_i\), for which we use (10). We shall also use the explicit form for \(\alpha\) and \(\beta\), which have been defined after equation (17). Then, (30–33) are transformed into, respectively:
\[
\begin{align*}
-(2ck - 1)^2 + 2(4c^2 k^2 - 1)m_0 e^{i\phi} - (2ck + 1)^2 e^{2i\phi} &= -8c k(1 + m^2 b^2) + im_1 e^{i\phi} (m_2 + im_1)e^{2i\phi}, \\
(4c^2 k^2 - 1) - 2(4c^2 k^2 + 1)m_0 e^{i\phi} - im_3 8c k e^{i\phi} + (4c^2 k^2 - 1) e^{2i\phi} &= -8c \frac{2kmb + im_1}{1 - m^2 b^2} e^{i\phi} (m_2 + im_1),
\end{align*}
\]
\(9\) \(\frac{2kmb - ima}{1 - m^2b^2}\) e^{i\Phi} (m_2 + im_1),

Then, we divide all these equations by \(e^{i\Phi}\) and use trigonometric relations to obtain:

\(38\) \(4c^2k^2 + 1) \cos \Phi + i4ck \sin \Phi - (4c^2k^2 - 1)m_0 = 4c \frac{1 + m^2b^2}{1 - m^2b^2} (m_2 + im_1) e^\Phi\),

\(39\) \((4c^2k^2 - 1) \cos \Phi - (4c^2k^2 + 1)m_0 - im_34ck = -4c \frac{2kmb + ima}{1 - m^2b^2} (m_2 + im_1),

\(40\) \((4c^2k^2 - 1) \cos \Phi - (4c^2k^2 + 1)m_0 + im_34ck = 4c \frac{2kmb - ima}{1 - m^2b^2} (m_2 + im_1),

\(41\) \((4c^2k^2 + 1) \cos \Phi - i4ck \sin \Phi - (4c^2k^2 - 1)m_0 = -4c \frac{k(1 + m^2b^2) - ima}{1 - m^2b^2} (m_2 + im_1)e^{-2ikel}.

Then, subtract \(39\) from \(40\). It gives:

\(42\) \(im_3 = \frac{2mb}{1 - m^2b^2} (m_2 + im_1)\).

Sum \(39\) and \(40\):

\(43\) \(4c^2k^2 - 1) \cos \Phi - (4c^2k^2 + 1)m_0 = -4c \frac{ima}{1 - m^2b^2} (m_2 + im_1)\).

Sum \(38\) and \(41\):

\(44\) \((4c^2k^2 + 1) \cos \Phi - (4c^2k^2 - 1)m_0 = i8c \frac{k(1 + m^2b^2)\sin 2ck + ma\cos 2ck}{1 - m^2b^2} (m_2 + im_1).

Subtract \(41\) from \(38\):

\(45\) \(i4ck \sin \Phi = 8c \frac{k(1 + m^2b^2)\cos 2ck - ma\sin 2ck}{1 - m^2b^2} (m_2 + im_1)\).

The system of transcendental equations equations \(42\)–\(45\) should give us the values of the parameters \(\Phi\) and \(m_i\) in terms of \(a\) and \(b\). It is important to note that these equations are complex as they have real and imaginary parts. Therefore, each one splits into two equations, one corresponding to the identity of its real parts and the other to the imaginary part. On the other hand, we look for bound states, so that the solutions in \(k\) must be real. Then, the final result is a system of eight equations given by:
\begin{align}
\tag{46} & \frac{2mb}{1-m^2b^2} m_2 = 0, \\
\tag{47} & \frac{2mb}{1-m^2b^2} m_1 = m_3, \\
\tag{48} & 4c \frac{ma}{1-m^2b^2} m_2 = 0, \\
\tag{49} & (4c^2k^2 - 1) \cos \Phi - (4c^2k^2 + 1)m_0 = 4c \frac{ma}{1-m^2b^2} m_1, \\
\tag{50} & (4c^2k^2 + 1) \cos \Phi - (4c^2k^2 - 1)m_0 = -8c \frac{k(1+m^2b^2) \sin 2ck+ma \cos 2ck}{1-m^2b^2} m_1, \\
\tag{51} & 8c \frac{k(1+m^2b^2) \sin 2ck+ma \cos 2ck}{1-m^2b^2} m_2 = 0, \\
\tag{52} & 8c \frac{k(1+m^2b^2) \cos 2ck-ma \sin 2ck}{1-m^2b^2} m_2 = 0, \\
\tag{53} & 4ck \sin \Phi = 8c \frac{k(1+m^2b^2) \cos 2ck-ma \sin 2ck}{1-m^2b^2} m_1.
\end{align}

Since we are looking for a relation between the two independent parameters \(a\) and \(b\) with \(\Phi\) and the \(m_i\), these equations cannot be independent. This system looks to be hopeless, but it can be solved with a little effort. Let us see how. First of all, it is obvious that (46) and (48) give

\begin{equation}
\tag{54} m_2 = 0.
\end{equation}

From equations (49) and (50), we manage the elimination of \(m_0\). If we multiply (50) by \(4ck^2 + 1\), by \(4ck^2 - 1\) subtract and divide by \(4ck\), we obtain:

\begin{equation}
\tag{55} 4ck \cos \Phi = - \frac{(4c^2k^2 - 1)ma + 2(4c^2k^2 + 1)[k(1+m^2b^2) \sin 2ck+ma \cos 2ck]}{k(1-m^2b^2)} m_1.
\end{equation}

Now, take (55) and (53), find their squares and sum. We obtain an expression from where it is simple to write \(m_1\) in terms of \(a\), \(b\) and \(k\). This gives:

\begin{equation}
\tag{56} m_1 = \frac{4ck(1-m^2b^2)}{\sqrt{A}},
\end{equation}

with

\begin{equation}
\tag{57} A = 16c^2 \Bigl[k(1+m^2b^2) \cos 2ck-ma \sin 2ck\Bigr]^2 + \\
\quad + \frac{1}{k^2} \Bigl[(4c^2k^2 - 1)ma + 2(4c^2k^2 + 1)[k(1+m^2b^2) \sin 2ck+ma \cos 2ck]\Bigr]^2.
\end{equation}

Once we have obtained \(m_1\), we can get the value of \(m_3\) through (51). Also, dividing (53) and (55), we find:

\begin{equation}
\tag{58} \tan \Phi = -8ck \frac{k(1+m^2b^2) \cos 2ck-ma \sin 2ck}{(4c^2k^2 - 1)ma + 2(4c^2k^2 + 1)[k(1+m^2b^2) \sin 2ck+ma \cos 2ck]}.
\end{equation}
It is noteworthy to say that, as we have eliminated \( m_0 \) from (49) and (50), we could also have eliminated \( \Phi \). We can do it by multiplying (50) by \( 4ck^2 + 1 \) subtracting the result of multiplying (49) by \( 4ck^2 - 1 \) and then dividing this result by \( 4ck \). We obtain:

\[
4ckm_0 = -\frac{(4c^2k^2 + 1)ma + 2(4c^2k^2 - 1)[k(1 + m^2b^2) \sin 2ck + ma \cos 2ck]}{k(1 - m^2b^2)}m_1 ,
\]

thus relating \( m_0 \) to \( m_1 \). As we have already commented, relations \( m_i \) are not independent but fulfil the relation \( m_0^2 + m_1^2 + m_2^2 + m_3^2 = 1 \). If we write \( m_0 \) and \( m_3 \) in terms of \( m_1 \), we obtain:

\[
\left( \frac{(4c^2k^2 + 1)ma + 2(4c^2k^2 - 1)[k(1 + m^2b^2) \sin 2ck + ma \cos 2ck]}{4ck^2(1 - m^2b^2)} \right)^2 + \left( \frac{2mb}{1 - m^2b^2} \right)^2 + 1 \right) m_1^2 = 1 .
\]

Next, we use (56) in (60). After some manipulations, we obtain a simple transcendent equation for \( k \):

\[
k(1 + m^2b^2) \sin 2ck + ma \cos 2ck = 0 .
\]

This equation can give us the energy values for given determinations of the parameters \( a \) and \( b \). The variation of each of the first three energy levels with \( a \) and \( b \) for \( m \) fixed is given in the Figure 1. Note that the parameters \( b \), \( c \) and \( m \) are always positive and we have taken \( a \) positive. The use of the Mathematica tool called manipulate can give us the energy levels for different values of \( a \), \( b \) and \( m \). In Figure 1, we have chosen the values given for the parameters, although the figure is quite similar for another choices.

The use of (61) greatly simplifies some of the above expressions. Now, we can write the parameters \( m_1 \) and \( \Phi \) in terms of \( a \) and \( b \):
\[ m_1 = \frac{4ck(1 - m^2b^2)}{\sqrt{16c^2[k(1 + m^2b^2) \cos 2ck - ma \sin 2ck]^2 + \frac{1}{16c^2}(4c^2k^2 - 1)ma^2}} \]

and

\[ \tan \Phi = \frac{-8ck\cos 2ck}{k(1 + m^2b^2) - ma \sin 2ck}. \]

Then, we have to analyze formulas (62) and (63). One would have expected that the relation between the parameters \( m_1 \) and \( \Phi \) be one to one. Then, take one self adjoint extension of \( K \) characterized by the values of \( a \) and \( b \), i.e., take specific values of these parameters in (1). We would have expected that these values give a unique pair of numbers for \( m_1 \) and \( \Phi \). However, (62) and (63) depend also on \( k \) and therefore on the energy levels.

The conclusion is that the relation between parameters is not one to one, contrarily to what we may have expected.

We have an apparent difficulty with formula (63). If we use (61) in (63), \( ma \) is simplified and we have an expression like:

\[ \tan \Phi = \frac{8ck}{\sin 2ck} \frac{\cos 2ck - \sin^2 2ck}{4c^2k^2 - 1}. \]

For \( \Phi \) being fixed, this is a transcendental equation on \( k \). According to the inverse function theorem, one may at least locally, obtain a relation of the form \( k = h(\Phi) \). If we use this relation in (62), we finally obtain something like \( m_1 = F(\Phi, a, b) \), which is not a desired relation.

Nevertheless, we have a cure for this problem and here is the correct treatment: From (61) and using the inverse function theorem, we can obtain local expressions of the type \( k = \psi_n(a, b) \). We can use this in (62) and (63) so as to obtain local relations of the type:

\[ m_1 = F_n(a, b), \quad \Phi = G_n(a, b). \]

This result is somehow unexpected as it shows that the relation between two different parameterizations of the self adjoint extensions of the kinetic operator on the infinite square well is not given by a unique function, but instead by a sequence of functions depending on the energy levels. This means that for each energy level, there is a distinct function that relates the values of \( a \) and \( b \) with those of \( m_1 \) and \( \Phi \) giving the same self adjoint extension and therefore the same set of energy values.

4. Concluding remarks

Being giving two specific values of \( a \) and \( b \) in (1), the number of energy levels for the Hamiltonian \( H \) is infinite. This is a fact shared by any self adjoint extension of \( K \). Numerical estimations show that the largest deviations of the values for the energy values given \( E_n = \frac{k_n^2}{2}, k_n = \frac{n\pi}{2c} \) happens for the lowest levels, being negligible for high values of \( n \). Then, for any value of \( a \) and \( b \), we give an infinite series of values for \( k \), say \( k_n \). For any value of \( k_n \), the function that relates \( a \) and \( b \) to \( m_1 \) and \( \Phi \) is different. The somehow surprising conclusion of the present paper is that the relations between different parameterizations of the self adjoint extensions of \( K \) are not simple as they are not given by a unique equation as stated in the last section.

Acknowledgements

Financial support is acknowledged to the Ministry of Economy and Innovation of Spain through the Grant MTM2009-10751.
REFERENCES

[1] Bonneau G, Faraut J and Valent G, Self adjoint extensions of operators and the teaching of quantum mechanics, American Journal of Physics, 69, 322-331 (2001)
[2] Kurasov P, Distribution theory for discontinuous test functions and differential operators with generalized coefficients, J. Math. Appl. 201 297-323 (1996)
[3] Golovaty Y, Schrödinger operators with ($\alpha e' + \beta e$)-like potentials: norm resolvent convergence and solvable models, Methods of Functional Analysis and Topology, 18, 243-255 (2012).
[4] Zolotaryuk A V, Boundary conditions for the states with resonant tunnelling across the $e'$-potential, Phys. Lett. A, 374, 1636-1641 (2010)
[5] Seba P, Some remarks on the $e'$ interaction in one dimension, Rep. Math. Phys., 24 111-120 (1986)
[6] Toyama F M and Nagami Y, Transmission-reflection problem with a potential of the form of the derivative of the delta function, Journal of Physics A: Mathematical and Theoretical, 40 F685-F690 (2007)
[7] Zolotaryuk A V and Zolotaryuk Y, Controlling a resonant transmission across the delta'-potential: the inverse problem, Journal of Physics A: Mathematical and Theoretical, 45 375305 (2011); Corrigendum, Journal of Physics A: Mathematical and Theoretical, 45 119501 (2012)
[8] Gadella M, Negro J and Nieto L M, Bound states and scattering coefficients of the $-a\delta(x) + b\delta'(x)$ potential, Phys. Lett. A, 373 1310-1313 (2009)
[9] Bohm A, Gadella M, Wickramasekara W, Some little things about rigged Hilbert spaces and quantum mechanics and all that. Generalized Functions, Operator Theory and Dynamical Systems. I. Antoniou and E. Lumer, Eds. CRC Press (1999), pp. 202-250.
[10] Alveberio S, Gesztesy F, Høeg-Krohn R and Holden H, Solvable Models in Quantum Mechanics, AMS Chelsea Publishing, vol 350.H (2005)
[11] Gadella M, Glasser M L and Nieto L M, The Infinite Square Well with a Singular Perturbation, Int. J. Theor. Phys., 50 2191-2200 (2011)

DEPARTMENT OF THEORETICAL, ATOMIC PHYSICS AND OPTICS. FACULTAD DE CIENCIAS. UNIVERSITY OF VALLADOLID,
47011 VALLADOLID, SPAIN
E-mail address: manuelgadella1@gmail.com

DEPARTMENT OF THEORETICAL, ATOMIC PHYSICS AND OPTICS. FACULTAD DE CIENCIAS. UNIVERSITY OF VALLADOLID,
47011 VALLADOLID, SPAIN
E-mail address: mariangelesferrero@gmail.com

DEPARTMENT OF THEORETICAL, ATOMIC PHYSICS AND OPTICS. FACULTAD DE CIENCIAS. UNIVERSITY OF VALLADOLID,
47011 VALLADOLID, SPAIN
E-mail address: sergio.gonzalez.martin@csic.es

DEPARTAMENTO DE FÍSICA. CENTRO DE INVESTIGACIÓN Y ESTUDIOS AVANZADOS DEL IPN. 07360, MÉXICO DF.
MÉXICO
E-mail address: felixmaldonado@gmail.com