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A delta well with a mass jump

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Abstract

In this paper, it is shown that a one-dimensional Hamiltonian with an attractive delta potential at the origin plus a mass jump at the same point cannot have a bound state, as is the case with the ordinary attractive delta potential with constant mass, unless another term is added into the potential in the form of a derivative of the Dirac delta at the origin. The consistency of this singular potential with two terms is guaranteed by choosing suitable matching conditions at the singular point for the wavefunctions. Furthermore, it is proved that the self-adjointness of the Hamiltonian with both singular interactions determines the coefficient of the derivative of the delta in a unique manner. Under these conditions, the bound state and its energy are obtained and it is checked that the correct results in the limit of equal masses are obtained.

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1. Introduction

The consideration of Hamiltonians with variable mass in non-relativistic quantum mechanics is an old problem that has recently attracted a lot of attention [1]. When the mass is not a constant, but depends on the position, $m(x)$, it has to be considered as a position-dependent operator not commuting with the momentum operator p. Therefore, the kinetic term K of the Hamiltonian cannot be written in the usual way, being the most generally accepted form of $H = K + V$ [2]:

$$H = K + V = \frac{1}{2} m^{\alpha}(x)\, p\, m^{\beta}(x)\, p\, m^{\alpha}(x) + V(x), \tag{1}$$

with $2\alpha + \beta = -1$. Note that the usual form of the kinetic energy is recovered for constant mass.

Physical systems with an abrupt discontinuity of the mass at one point are modeling the behavior of a quantum particle, i.e. an electron, moving in a media formed up by two different materials. On each of the materials the particle behaves as if it had a different mass. The discontinuity point represents the junction between these two materials. This situation is largely discussed in the literature, particularly in our references [1, 2].

The simplest model of such a situation is given by a one-dimensional system in which the mass is constant except for a finite jump at one point, which is taken to be the origin for simplicity. This is the situation we are going to consider along the present paper. In addition, we shall also consider the presence of a singular potential at the origin. This is a kind of situation that, up to our knowledge, has not been studied before. As in the case of point interactions with constant mass [3–5] or mass jump at the origin without singular interactions [6], the self-adjointness of the Hamiltonian is determined through matching conditions at the origin. The present study is a combination of both situations, which can be not only instructive but will also enrich our knowledge on solvable systems.

This is precisely the aim of the present paper, in which we study the behavior of a Dirac delta well centered at the origin, having a mass jump at the same point. This model is interesting as it combines a point interaction with a mass jump, it is exactly solvable, it has a unique bound state (as in the case of the delta well with constant mass) and provides an unexpected surprise: the bound state cannot survive without the existence of an additional $b\delta'(x)$ component in the potential. Furthermore, this coefficient b is not arbitrary, but it depends on the masses at one side and the other of the origin. The precise form of this coefficient b has its origin in deep mathematical reasons: the matching conditions that determine the self-adjointness of the total Hamiltonian. This latter fact is not trivial as it shows how a property that is often considered as a mathematical subtlety has physical consequences.

We will study the Hamiltonian given in equation (1) with

$$V(x) = -a\delta(x) + b\delta'(x), \qquad a > 0, \tag{2}$$

from two different points of view, both based on physical grounds. In both cases, we obtain different values for the energy of the bound state. This is because these two different treatments are based on two different versions of the kinetic energy term K. The former, studied in section 2, uses the K as given in equation (1). The second one is somewhat simpler and is considered in section 4. In the equal mass limit $m_1 = m_2 = m$, both cases give the same results, which coincide with those obtained for $H = p^2/2m - a\delta(x) + b\delta'(x)$ (see [7]).

It is important also to mention that, even in the constant mass case, the potential term $b\delta'(x)$ was a subject of controversy due the use of different matching conditions at the origin for the functions in the domain of the Hamiltonian. Here, we will use the matching conditions proposed by Kurasov [3] because

(i) they do not lead to unphysical results such transmission or reflections coefficients equal to zero [8, 9];
(ii) they allow us to combine properly the two distributions $\delta(x)$ and $\delta'(x)$;
(iii) they allow us to multiply both $\delta(x)$ and $\delta'(x)$ by functions discontinuous at the origin (note that, due to the mass jump, the functions in the domain of the Hamiltonian are expected to have a discontinuity at the origin).

This paper is organized as follows. In the next section, we study the Schrödinger equation associated to the Hamiltonian with a mass jump at the origin plus the mentioned delta interactions using our first approach. We shall find the bound state for this system and its energy. In section 3, we shall show how the condition of self-adjointness of the Hamiltonian determines the value of the coefficient of $\delta'(x)$ uniquely in terms of the values of the mass. In section 4, we analyze a second interpretation of the kinetic term with a mass jump and a singular potential of the form (2), and discuss results and properties. Finally, we end the paper with the most relevant conclusions.

2. The formal Hamiltonian and its eigenvalue problem

The object of our study is the eigenvalue problem relative to a one-dimensional Hamiltonian with an attractive delta well and a mass jump at the origin. In principle, this Hamiltonian has the form

$$\widetilde{H} = \tfrac{1}{2}m^{\alpha}(x)\,p\,m^{\beta}(x)\,p\,m^{\alpha}(x) - a\delta(x), \tag{3}$$

with $2\alpha + \beta = -1$, $a > 0$ and

$$m(x) = m_1 H(-x) + m_2(x)H(x) = \begin{cases} m_1, & x < 0, \\ m_2, & x > 0, \end{cases} \tag{4}$$

where $H(x)$ is the Heaviside step function, whose derivative is the Dirac delta $\delta(x)$. Due to reasons that will become obvious later, we shall study instead a slightly more general situation in which an additional $\delta'(x)$ term is added to the Hamiltonian (3), which then takes the form

$$H = \tfrac{1}{2}\, m^{\alpha}(x)\,p\,m^{\beta}(x)\,p\,m^{\alpha}(x) - a\delta(x) + b\delta'(x)\,, \tag{5}$$

with $b \in \mathbb{R}$. The formal Hamiltonian (5) gives the following Schrödinger equation:

$$\tfrac{1}{2}m^{\alpha}(x)pm^{\beta}(x)pm^{\alpha}(x)\psi(x) - a\delta(x)\psi(x) + b\delta'(x)\psi(x) = E\psi(x). \tag{6}$$

Expression (6) is an equation in ordinary distributions. However, we note that the solution $\psi(x)$ should have a discontinuity at the origin due to the mass jump [6]. Then, we adopt the following definitions for the product of a function and a Dirac delta:

$$\psi(x)\delta(x) = \frac{\psi(0+) + \psi(0-)}{2}\,\delta(x), \tag{7}$$

$$\psi(x)\delta'(x) = \frac{\psi(0+) + \psi(0-)}{2}\,\delta'(x) - \frac{\psi'(0+) + \psi'(0-)}{2}\,\delta(x), \tag{8}$$

where $\psi(0+)$ and $\psi(0-)$ denote the right and left limits, respectively, of $\psi(x)$ at the origin. Same notation is used for the derivative. These definitions have been given already in [3]. However, we should note that in our case (7) and (8) can be looked as ordinary distributions (with test space of continuous smooth functions) and not as distributions on a test space of discontinuous functions at the origin as in [3]. Then, we can look at the Schrödinger equation (6) as an equation on ordinary distributions.

Since the solution of (6) should have a discontinuity at the origin, it must have the following form:

$$\psi(x) = f_1(x)H(-x) + f_2(x)H(x), \tag{9}$$

where, without loss of generality, we can assume that $f_i(x)$, $i = 1, 2$, are continuous functions.

The kinetic term in (6) can be written as

$$K\psi(x) = -\frac{\hbar^2}{2}\left[m^{\alpha}(x)\,\frac{\mathrm{d}}{\mathrm{d}x}\,m^{\beta}(x)\frac{\mathrm{d}}{\mathrm{d}x}\,m^{\alpha}(x)\psi(x)\right]. \tag{10}$$

If we define

$$f(x) := m^{\alpha}(x)\psi(x) = m_1^{\alpha} f_1(x)H(-x) + m_2^{\alpha} f_2(x)H(x)\,, \tag{11}$$

and we apply (7), we get

$$\frac{\mathrm{d}}{\mathrm{d}x}\,f(x) = m_1^{\alpha} f_1'(x)H(-x) + m_2^{\alpha} f_2'(x)H(x) + \big(m_2^{\alpha} f_2(0) - m_1^{\alpha} f_1(0)\big)\delta(x). \tag{12}$$

If we multiply (12) by $m^\beta(x) = m_1^\beta H(-x) + m_2^\beta H(x)$ and use again (7), we get

$$m^\beta(x)\frac{\mathrm{d}f}{\mathrm{d}x} = m_1^{\alpha+\beta} f_1'(x)H(-x) + m_2^{\alpha+\beta} f_2'(x)H(x) + \left[m_2^\alpha f_2(0) - m_1^\alpha f_1(0)\right]\frac{m_1^\beta + m_2^\beta}{2}\delta(x).$$

If we derive this expression and multiply the result by $m^\alpha(x)$, we obtain

$$\begin{aligned} m^\alpha(x)\frac{\mathrm{d}}{\mathrm{d}x} m^\beta(x)\frac{\mathrm{d}}{\mathrm{d}x} f(x) &= m_1^{2\alpha+\beta} f_1''(x)H(-x) + m_2^{2\alpha+\beta} f_2''(x)H(x) \\ &\quad + \left(m_2^{\alpha+\beta} f_2'(x) - m_1^{\alpha+\beta} f_1'(x)\right) m^\alpha(x)\,\delta(x) \\ &\quad + \left[m_2^\alpha f_2(0) - m_1^\alpha f_1(0)\right]\frac{m_1^\beta + m_2^\beta}{2} m^\alpha(x)\,\delta'(x). \end{aligned} \tag{13}$$

Now, we apply (7) and (8), respectively, in the second and third line of (13), and therefore the Schrödinger equation (6) reads

$$\begin{aligned} -\frac{\hbar^2}{2}\Bigg[\frac{1}{m_1} f_1''(x)H(-x) &+ \frac{1}{m_2} f_2''(x)H(x) + \left[m_2^{\alpha+\beta} f_2'(0) - m_1^{\alpha+\beta} f_1'(0)\right]\frac{m_1^\alpha + m_2^\alpha}{2}\delta(x) \\ &+ \left[m_2^\alpha f_2(0) - m_1^\alpha f_1(0)\right]\frac{m_1^\beta + m_2^\beta}{2}\frac{m_1^\alpha + m_2^\alpha}{2}\delta'(x)\Bigg] - a\frac{f_1(0) + f_2(0)}{2}\delta(x) \\ &+ b\frac{f_1(0) + f_2(0)}{2}\delta'(x) - b\frac{f_1'(0) + f_2'(0)}{2}\delta(x) \\ &= E[f_1(x)H(-x) + f_2(x)H(x)]. \end{aligned} \tag{14}$$

From here, and taking into account that we are looking for the bound states ($E < 0$), we obtain the following set of equations:

$$-\frac{\hbar^2}{2m_1} f_1''(x) = Ef_1(x) \Longrightarrow f_1(x) = \gamma\,\mathrm{e}^{k_1 x} \tag{15}$$

$$-\frac{\hbar^2}{2m_2} f_2''(x) = Ef_2(x) \Longrightarrow f_2(x) = \gamma\sigma\,\mathrm{e}^{-k_2 x} \tag{16}$$

$$-\frac{\hbar^2}{2}\left[m_2^{\alpha+\beta} f_2'(0) - m_1^{\alpha+\beta} f_1'(0)\right]\frac{m_1^\alpha + m_2^\alpha}{2} - \frac{a}{2}(f_1(0) + f_2(0)) - \frac{b}{2}(f_1'(0) + f_2'(0)) = 0 \tag{17}$$

$$-\frac{\hbar^2}{2}\left[m_2^\alpha f_2(0) - m_1^\alpha f_1(0)\right]\frac{m_1^\alpha + m_2^\alpha}{2}\frac{m_1^\beta + m_2^\beta}{2} + \frac{b}{2}(f_1(0) + f_2(0)) = 0, \tag{18}$$

where $\gamma \neq 0$ is the normalization constant of the wavefunction (9), σ is another constant that will be determined immediately and $k_i = \sqrt{-2m_i E/\hbar^2}$, $i = 1, 2$. From (15) and (16), we see that (6) has square integrable solutions and therefore bound states that we are going to determine in the sequel. In addition, we have

$$f_1(0) = \gamma, \qquad f_2(0) = \gamma\sigma, \qquad f_1'(0) = \gamma k_1, \qquad f_2'(0) = -\gamma\sigma k_2. \tag{19}$$

As a consequence of (19), (18) can be written as

$$-\frac{\hbar^2}{4}\left[m_2^\alpha\sigma - m_1^\alpha\right]\left(m_1^\alpha + m_2^\alpha\right)\left(m_1^\beta + m_2^\beta\right) + b(1+\sigma) = 0. \tag{20}$$

After (20), we can fix uniquely the value of σ in terms of the initial parameters of the problem to be

$$\sigma = -\frac{4b + \hbar^2 m_1^\alpha\left(m_1^\alpha + m_2^\alpha\right)\left(m_1^\beta + m_2^\beta\right)}{4b - \hbar^2 m_2^\alpha\left(m_1^\alpha + m_2^\alpha\right)\left(m_1^\beta + m_2^\beta\right)}. \tag{21}$$

If $m_1 = m_2 = m$, and taking into account that $2\alpha + \beta = -1$, we have that

$$\sigma_0 = \frac{\hbar^2 + mb}{\hbar^2 - mb}, \tag{22}$$

which is the result we obtain if we had operated directly without the mass jump.

On the other hand, from (19) and (17), one obtains

$$\frac{\hbar^2}{2}\left[m_2^{\alpha+\beta}\sigma k_2 + m_1^{\alpha+\beta}k_1\right]\left(m_1^\alpha + m_2^\alpha\right) - a(1+\sigma) - b(k_1 - \sigma k_2) = 0. \tag{23}$$

If we call $\mu = \sqrt{-2E/\hbar^2}$, $k_i = \mu\sqrt{m_i}$, and then from equation (23)

$$\mu = \frac{2a(1+\sigma)}{\sigma m_2^{1/2}\left[2b + \hbar^2 m_2^{\alpha+\beta}\left(m_1^\alpha + m_2^\alpha\right)\right] - m_1^{1/2}\left[2b - \hbar^2 m_1^{\alpha+\beta}\left(m_1^\alpha + m_2^\alpha\right)\right]}. \tag{24}$$

This expression readily gives the value of the energy $E = -\hbar^2\mu^2/2$ for the unique possible bound state coming from the solution of the equations (15)–(18). However, as we shall see later, the condition for the self-adjointness of the Hamiltonian (5) determines that b, that in principle can be considered as a free parameter or as an initial datum of the problem, can have only one value (up to a sign). In the limit $m_1 = m_2 = m$, one readily obtains from (24) and (22)

$$E_0 = -\frac{\hbar^2\mu_0^2}{2} = -\frac{1}{2}\,\frac{ma^2\hbar^6}{(\hbar^4 + b^2m^2)^2}, \tag{25}$$

which is the expression one obtains through a direct calculation (see [7] taking $\hbar = 1$).

Obviously, since μ in (24) is real and $E = -\hbar^2\mu^2/2$, the energy of the unique bound state is always negative (except if $a = 0$, a case in which no bound state is present). From (9), (15) and (16), the eigenfunction of the bound state is precisely

$$\psi(x) = \gamma[\mathrm{e}^{k_1x}H(-x) + \sigma\,\mathrm{e}^{-k_2x}H(x)], \tag{26}$$

where σ is given in (21) and γ is the normalization constant, whose precise value is not relevant for the rest of this work.

Note that if we make the substitution $m_1 \leftrightarrow m_2$ and change b by $-b$, then σ is changed into $1/\sigma$. A simple calculation shows that μ remains invariant under these operations. This shows that our model is symmetric with respect to the interchange of the notions of left and right, for which we have to interchange the value of the masses plus the sign of b (note that $\delta'(x)$ is an odd distribution).

In the next section, we shall study the constraints coming out after imposing the self-adjointness of the Hamiltonian (5) we are working with.

3. Self adjointness of the Hamiltonian and its consequences

In a recent work [6], we have characterized the set of all the self-adjoint extensions of a type of Hamiltonian with non-constant mass as in equation (42) below. It is well known that singular interactions can be obtained from self-adjoint extensions of symmetric operators with equal non-zero deficiency indices [3–5]. This is exactly what happens in the present case, where we have the symmetric operator associated with the kinetic energy, $K = \frac{1}{2}m^\alpha(x)pm^\beta(x)pm^\alpha(x)$, with domain

$$\mathcal{D}_0 := \left\{\psi(x) \in W_2^2(\mathbb{R}) \big/ \psi(0) = \psi'(0) = 0\right\}. \tag{27}$$

Here, $W_2^2(\mathbb{R})$ is the space of continuous functions from $\mathbb{R}$ into $\mathbb{C}$ such that

(i) any $f(x) \in W_2^2$ admits a first continuous derivative;

(ii) the second derivative exists almost everywhere (a.e.);

(iii) both $f(x) \in W_2^2$ and its second derivative a.e. are square integrable, so that

$$\int_{-\infty}^{\infty} \{|f(x)|^2 + |f''(x)|^2\}\, dx < \infty.$$

The adjoint of K, $K^\dagger$, has domain $\mathcal{D}^* \equiv W_2^2(\mathbb{R}/\{0\})$. The functions in $W_2^2(\mathbb{R}/\{0\})$ satisfy the same properties of the functions in W_2^2 except that they and their derivatives may admit a finite jump at the origin.

It is straightforward that K has deficiency indices $(2, 2)$ and therefore it has an infinite number of self-adjoint extensions. These self-adjoint extensions are restrictions of $K^\dagger$ to certain subdomains, which are determined by the matching conditions at the origin.

Let $\psi, \varphi \in \mathcal{D}^*$. A simple calculation shows that

$$\langle\psi|K^\dagger\varphi\rangle = \mathcal{G} + \langle K^\dagger\psi|\varphi\rangle, \tag{28}$$

with

$$\mathcal{G} = -\frac{\hbar^2}{2m_1}[\psi^*(0-)\varphi'(0-) - \psi'^*(0-)\varphi(0-)] + \frac{\hbar^2}{2m_2}[\psi^*(0+)\varphi'(0+) - \psi'^*(0+)\varphi(0+)].$$

We recall that $\psi(0+)$ and $\psi(0-)$ are the right and left limits of $\psi(x)$ at the origin. This expression for $\mathcal{G}$ can be written in the matrix form as

$$\mathcal{G} = -(\psi^*(0-), \psi'^*(0-))M_1\begin{pmatrix}\varphi(0-)\\ \varphi'(0-)\end{pmatrix} + (\psi^*(0+), \psi'^*(0+))M_2\begin{pmatrix}\varphi(0+)\\ \varphi'(0+)\end{pmatrix}, \tag{29}$$

with

$$M_i := \frac{\hbar^2}{2m_i}\begin{pmatrix}0 & 1\\ -1 & 0\end{pmatrix}, \qquad i = 1, 2. \tag{30}$$

The matching conditions at the origin, for an arbitrary function $\psi(x)$, are given by a 2×2 matrix as

$$\begin{pmatrix}\psi(0+)\\ \psi'(0+)\end{pmatrix} = T\begin{pmatrix}\psi(0-)\\ \psi'(0-)\end{pmatrix}, \qquad T \equiv \begin{pmatrix}A & D\\ B & C\end{pmatrix}, \tag{31}$$

where A, B, C and D are complex numbers, not yet known.

In order to find the self-adjoint extensions of K, we need to find subspaces of $\mathcal{D}^*$ for which $\mathcal{G} \equiv 0$ nontrivially. This can be done by giving suitable matching conditions at the origin. From (29) and (31), one obtains that $\mathcal{G} \equiv 0$ if and only if

$$(\psi^*(0-), \psi'^*(0-))[-M_1 + T^\dagger M_2 T]\begin{pmatrix}\varphi(0-)\\ \varphi'(0-)\end{pmatrix} = 0. \tag{32}$$

Note that $T^\dagger$ is the adjoint matrix of T, i.e. its transpose and complex conjugate. Since $\psi(x)$ and $\varphi(x)$ are arbitrary functions, so are their boundary values. Then (32) holds if and only if

$$M_1 = T^\dagger M_2 T. \tag{33}$$

From (33) and (30) one readily obtains

$$|\det T| = \frac{m_2}{m_1}, \tag{34}$$

which is a necessary condition for the matching conditions given by T to determine a self-adjoint extension of K. The matrix T give the matching conditions at the origin and determines a dense subspace $\mathcal{D}$ of $L^2(\mathbb{R})$ of continuous functions except at the origin. The discontinuities of the functions and their first derivative at the origin are given by T through (31). The restriction of $K^\dagger$ into $\mathcal{D}$ determines a self-adjoint extension of K if and only if T satisfies (33).

3.1. Matching conditions

In order to determine the explicit form of T in our case, let us go back to (9) and note that

$$\psi(0+) = f_2(0), \qquad \psi'(0+) = f_2'(0), \qquad \psi(0-) = f_1(0), \qquad \psi'(0-) = f_1'(0). \tag{35}$$

We already know from (15)–(16) that $\psi(0+) = \sigma\psi(0-)$, so that in the matrix T in (31) we have that $A = \sigma$ and $D = 0$. Entries B and C are then easily calculated from (17) so that

$$B = -\frac{2a(1+\sigma)}{2b + \hbar^2 m_2^{\alpha+\beta}\left(m_1^\alpha + m_2^\alpha\right)} \tag{36}$$

and

$$C = -\frac{2b - \hbar^2 m_1^{\alpha+\beta}\left(m_1^\alpha + m_2^\alpha\right)}{2b + \hbar^2 m_2^{\alpha+\beta}\left(m_1^\alpha + m_2^\alpha\right)}. \tag{37}$$

In the limit of equal masses, $m_1 = m_2 = m$, we obtain this known result [7]:

$$T_0 = \begin{pmatrix} \dfrac{\hbar^2 + mb}{\hbar^2 - mb} & 0 \\ \dfrac{-2am\hbar^2}{\hbar^4 - m^2b^2} & \dfrac{\hbar^2 - mb}{\hbar^2 + mb} \end{pmatrix}. \tag{38}$$

This matrix T_0 in (38) gives the boundary conditions that define the domain of self-adjointness of the operator $H = p^2/2m - a\delta(x) + b\delta'(x)$, $a > 0$, as given in [3].

As we have anticipated, not all values of b are compatible with the self-adjointness of the Hamiltonian. The coefficients of the matrix T in (31) are: $A = \sigma$ is given in (21), B and C are given in (36) and (37), respectively, and $D = 0$. Since the coefficients are all real numbers, we can write equation (33) as

$$\frac{m_2}{m_1}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} A & B \\ 0 & C \end{pmatrix}\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}\begin{pmatrix} A & 0 \\ B & C \end{pmatrix} = \begin{pmatrix} 0 & AC \\ -AC & 0 \end{pmatrix}, \tag{39}$$

from where

$$AC = \frac{m_2}{m_1}. \tag{40}$$

Using the values of A and C given in equations (21) and (37), equation (40) turns out to be a constraint that gives only two possible values for b:

$$b = 0, \qquad b = \hbar^2\,\frac{m_1^\alpha + m_2^\alpha}{2}\,\frac{m_1^\beta - m_2^\beta}{2}\,\frac{m_1^{\alpha+1} - m_2^{\alpha+1}}{m_1 - m_2}. \tag{41}$$

The well-known solution with $b = 0$ (delta well) appears directly from our study, but we see that a new option with $b \neq 0$ as in (41) also arises in a natural way, which is a very interesting and novel result coming from our study. In the limit of equal masses, $m_1 = m_2 = m$, the equation that results after (40) is satisfied identically, and no restriction on the possible values of b is obtained. Conversely, from the second identity in equation (41), we see that $b = 0$ implies $m_1 = m_2$. Therefore, the mass jump cannot exist with the term $-a\delta(x)$ only, unless the term $b\delta'(x)$ is present.

4. Another self-adjoint extension of the Hamiltonian

The approach for the solution of the eigenvalue problem for mass jump Hamiltonian given in section 2 seems to be the most logical one although is not the only possible. Indeed, the mass jump of equation (4), in combination with the usual form of the kinetic term $\frac{1}{2m}p^2$, suggests that we could express the kinetic term in the following form:

$$\hat{K} = -\frac{\hbar^2}{2m(x)}\frac{\mathrm{d}^2}{\mathrm{d}x^2} = \begin{cases} -\dfrac{1}{2m_1}\dfrac{\mathrm{d}^2}{\mathrm{d}x^2} & \text{if} \quad x < 0, \\ -\dfrac{1}{2m_2}\dfrac{\mathrm{d}^2}{\mathrm{d}x^2} & \text{if} \quad x > 0, \end{cases} \tag{42}$$

which is obviously independent of the the order parameters α and β. The analysis of self-adjoint extensions for (42) does not differ of the study given in section 3. In particular, functions in the domain of its self-adjoint extension have to fulfill matching conditions (31), where the matrix T fulfills (33). A complete discussion about these extensions is given in [6]. Then, if we use the form (42) for the kinetic operator, the Schrödinger equation for the potential (2) can be written as

$$\hat{H}\psi(x) = \left[-\frac{\hbar^2}{2m(x)}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - a\delta(x) + b\delta'(x)\right]\psi(x) = \hat{E}\psi(x) \tag{43}$$

or

$$\hbar^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) = -2m(x)\,a\,\delta(x)\psi(x) + 2m(x)\,b\,\delta'(x)\psi(x) - 2m(x)\hat{E}\psi(x), \tag{44}$$

where we have denoted as $\hat{E}$ the eigenvalue of the energy for the present choice. Our goal is to solve this Schrödinger equation. Should it have a square integrable solution (bound state), it must have the form $\psi(x) = f_1(x)H(-x) + f_2(x)H(x)$, given in equation (9) of section 2. Equation (44) should be again an equation of distributions (as was (6)) in which the product of discontinuous functions at the origin by deltas is defined as in (7)–(8). If we derive (9) twice, insert the result into (44), recall (35) and use (8), we obtain

$$\begin{aligned} \psi''(x) &= f_1''(x)H(-x) + f_2''(x)H(x) + [\psi'(0+) - \psi'(0-)]\delta(x) + [\psi(0+) - \psi(0-)]\delta'(x) \\ &= -\frac{2\hat{E}}{\hbar^2}[m_1 f_1(x)H(-x) + m_2 f_2(x)H(x)] - \frac{a}{\hbar^2}[m_1\psi(0-) + m_2\psi(0+)]\delta(x) \\ &\quad + \frac{b}{\hbar^2}[[m_1\psi(0-) + m_2\psi(0+)]\delta'(x) - [m_1\psi'(0-) + m_2\psi'(0+)]\delta(x)]. \end{aligned} \tag{45}$$

Then, we equalize the coefficients of $H(-x)$, $H(x)$, $\delta(x)$ and $\delta'(x)$. As in section 2, this gives a system of four equations:

$$-f_1''(x) = \frac{2m_1\hat{E}}{\hbar^2}f_1(x) \Longrightarrow f_1(x) = \rho\,\mathrm{e}^{\hat{k}_1 x}, \qquad \hat{k}_1 = \sqrt{-2\hat{E}m_1/\hbar^2}, \tag{46}$$

$$-f_2''(x) = \frac{2m_2\hat{E}}{\hbar^2}f_2(x) \Longrightarrow f_2(x) = \tau\,\mathrm{e}^{-\hat{k}_2 x}, \qquad \hat{k}_2 = \sqrt{-2\hat{E}m_2/\hbar^2}, \tag{47}$$

$$-\hbar^2[\psi'(0+) - \psi'(0-)] = a(m_1\psi(0-) + m_2\psi(0+)) + b[m_1\psi'(0-) + m_2\psi'(0+)], \tag{48}$$

$$\hbar^2[\psi(0+) - \psi(0-)] = b[m_1\psi(0-) + m_2\psi(0+)], \tag{49}$$

where ρ and τ are constants. The first two equations of the previous system, (46)–(47), are similar to (15)–(16), but we have used different integration constants for giving their square integrable solutions. Note that (49) can be written as

$$\psi(0+) = \frac{\hbar^2 + m_1 b}{\hbar^2 - m_2 b}\,\psi(0-), \tag{50}$$

or equivalently

$$b = \frac{\psi(0+) - \psi(0-)}{m_2\psi(0+) + m_1\psi(0-)}\hbar^2. \tag{51}$$

Equation (50) gives the jump at the origin of any possible square integrable solution of the Schrödinger equation (44). To obtain the jump of the first derivative, we use (48) to get

$$\psi'(0+) = -\frac{a\hbar^2(m_1+m_2)}{\hbar^4 - m_2^2 b^2}\,\psi(0-) + \frac{\hbar^2 - m_1 b}{\hbar^2 + m_2 b}\,\psi'(0-). \tag{52}$$

Equations (50) and (52) can be written together in matrix form as

$$\begin{pmatrix}\psi(0+)\\ \psi'(0+)\end{pmatrix} = \begin{pmatrix}\hat{A} & 0\\ \hat{B} & \hat{C}\end{pmatrix}\begin{pmatrix}\psi(0-)\\ \psi'(0-)\end{pmatrix} = \begin{pmatrix}\dfrac{\hbar^2+m_1 b}{\hbar^2 - m_2 b} & 0\\ \dfrac{-a\hbar^2(m_1+m_2)}{\hbar^4 - m_2^2 b^2} & \dfrac{\hbar^2 - m_1 b}{\hbar^2 + m_2 b}\end{pmatrix}\begin{pmatrix}\psi(0-)\\ \psi'(0-)\end{pmatrix}. \tag{53}$$

The matching conditions given by (53) are not only satisfied by the bound state of $\hat{H}$ but also characterize the domain of a self-adjoint extension of $\hat{K}$ that can be written as $\hat{H} = \hat{K} + V(x)$, where $V(x)$ is the singular potential with support at the origin given in equation (2). However, b cannot be arbitrary, as we shall see later.

4.1. The value of the energy for the bound state

Our next goal is to obtain the explicit expression for the energy $\hat{E}$ of the bound state. Taking into account that from equations (46)–(47)

$$\psi(0-) = \rho, \qquad \psi'(0-) = \rho\hat{k}_1, \qquad \psi(0+) = \tau, \qquad \psi'(0+) = -\tau\hat{k}_2, \tag{54}$$

equation (53) yields

$$\hat{k}_2\hat{A} + \hat{B} + \hat{k}_1\hat{C} = 0. \tag{55}$$

Then, we use in (55) the relations between $\hat{k}_i$ and $\hat{E}$ given in (46)–(47) and the values of $\hat{A}$, $\hat{B}$ and $\hat{C}$ given in (53), we finally get the following expression for the eigenvalue $\hat{E}$:

$$\hat{E} = -\frac{\hbar^2}{2}\,\frac{(m_1+m_2)^2 a^2\hbar^4}{[(\hbar^2 - m_1 b)(\hbar^2 - m_2 b)\sqrt{m_1} + (\hbar^2 + m_1 b)(\hbar^2 + m_2 b)\sqrt{m_2}]^2}. \tag{56}$$

Thus, the eigenvalue problem is solved for the chosen self-adjoint extension $\hat{H}$ of $\hat{K}$. We have found that $\hat{H}$ has a unique non-degenerate eigenvalue. The corresponding eigenvector is given by (46) and (47) as

$$\psi(x) \propto [(\hbar^2 - m_2 b)\,\mathrm{e}^{\hat{k}_1 x}\,H(-x) + (\hbar^2 + m_1 b)\,\mathrm{e}^{\hat{k}_2 x}\,H(x)]. \tag{57}$$

Finally, let us enumerate some properties that follow straightforwardly from the discussion above.

(i) Formula (56) is not symmetric with respect to the interchange of m_1 and m_2, but is symmetric with respect to the interchange of the notions of left and right for which we have to interchange the value of the masses as well as the sign of b. This is the same behavior as the energy (24) in the previous case discussed in section 2.

(ii) In the equal masses limit, $m_1 = m_2 = m$, equation (56) gives exactly the same equal masses limit obtained in section 2, see equation (25), which is the only eigenvalue of the Hamiltonian $H = \frac{p^2}{2m} - a\delta(x) + b\delta'(x)$ with $a > 0$, $b \in \mathbb{R}$, with fixed mass $m > 0$, as defined in [3].

(iii) In the present case, formula (40) takes the form

$$\hat{A}\hat{C} = \frac{\hbar^4 - m_1^2 b^2}{\hbar^4 - m_2^2 b^2} = \frac{m_2}{m_1}. \tag{58}$$

This gives

$$b^2 = \frac{\hbar^4}{m_1^2 + m_2^2 + m_1 m_2}. \tag{59}$$

If $m_1 = m_2$, (58) is an identity and (59) makes no sense. If $m_1 \neq m_2$, this result shows that (53) does not determine a self-adjoint extension of $\hat{K}$ unless b is given by (59).

(iv) From (58), we see that if $b = 0$ then $m_1 = m_2$. Thus, without the presence of the $b\delta'(x)$ term, the problem of the existence of a bound state for a delta well with a mass jump at the same point does not make sense. Note that, in any case, b must be of the form (59).

(v) Let us consider the equal limit mass of the matrix T in (53):

$$T_0 = \begin{pmatrix} \dfrac{\hbar^2 + mb}{\hbar^2 - mb} & 0 \\ -\dfrac{2am\hbar^2}{\hbar^4 - m^2 b^2} & \dfrac{\hbar^2 - mb}{\hbar^2 + mb} \end{pmatrix}. \tag{60}$$

These are the boundary conditions that determine the domain of self-adjointness of $\hat{H}$ in (53) having *constant mass*, $m_1 = m_2 = m$. Restriction (59) for b is not valid in this case, although b cannot be either $\hbar^2/m$ or $-\hbar^2/m$. Although the result in [3] is presented into a more general setting, formula (60) follows straightforwardly.

5. Concluding remarks

We have initiated the study of one-dimensional quantum systems with a mass jump at one point plus a singular potential at the same point. This singularity has been formerly proposed to be a Dirac delta well. The idea was that if a Dirac delta well had a unique bound state in the case of constant mass, this property should be kept when the mass is constant at each side of the origin and having a discontinuity at this point. This is essentially true, although some surprises arise in this study. First of all, twice derivation in the distributional sense of functions with a discontinuity at the origin, like $\psi(x)$ in (8), gives a $\delta'(x)$ term. This term *per se* is quite innocent as it would show that $\psi(0+) = \psi(0-)$ when $b = 0$, as it should be. However, as we have seen, $b = 0$ necessarily implies that $m_1 = m_2$, and therefore, the discussion of the delta well with a mass jump necessarily includes the presence of the $b\delta'(x)$ term in the potential. The existence of a discontinuity in the wavefunctions solutions of the Schrödinger equation is due to the mass jump itself. The need of a distributional derivation in the Schrödinger equation comes after the presence of a singular potential.

The presence of a $\delta'(x)$ has to be tackled with care, as no unique definition for a singular potential with such a term exists in the literature, even in the constant mass case. In any case, we believe that the best way of defining singular potentials is through matching conditions at the origin for wavefunctions. These matching conditions determine self-adjoint extensions of the symmetric non-self-adjoint kinetic operator in either the constant or variable mass cases. These self-adjoint extensions define different Hamiltonians with the same kinetic part and with singular potentials.

In the case of variable mass, we are faced with the additional difficulty that well-justified different forms of operating may give quite different results. In this paper, we give two examples. We have used two different choices for the free Hamiltonian with a mass jump at the origin: $K = \frac{1}{2}m^\alpha(x)pm^\beta(x)pm^\alpha(x)$, $2\alpha+\beta=-1$ or $\hat{K} = \frac{1}{2m(x)}p^2$, where $m(x)$ is the function giving the mass in terms of the position (here we use (4) only). Both provide one self-adjoint extension that could be in each case a good candidate for the one-dimensional Hamiltonian with a mass jump at the origin and a potential $V(x) = -a\delta(x) + b\delta'(x)$. This can be seen from the manipulations carried over all the discussion and by the fact that both give the same results in the equal masses limit $m_1 = m_2 = m$. These results coincide with the results obtained for $H = p^2/2m - a\delta(x) + b\delta'(x)$. Since we have used different choices for the kinetic term, both approaches give different results and in particular different energies for the (unique) bound state.

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References

[1] Wannier G H 1937 *Phys. Rev.* **52** 191
Slater J C 1949 *Phys. Rev.* **76** 1592
BenDaniel D J and Duke C B 1966 *Phys. Rev.* **152** 683
Bastard G 1981 *Phys. Rev.* B **24** 5693
Von Roos O 1983 *Phys. Rev.* B **27** 7547
Morrow R A and Brownstein K R 1984 *Phys. Rev.* B **30** 678
Morrow R A 1987 *Phys. Rev.* B **35** 8074
Lévy-Leblond J-M 1995 *Phys. Rev.* A **52** 1845
Moiseyev N and Lefebvre R 2001 *Phys. Rev.* A **64** 052711
Ganguly A, Kuru Ş, Negro J and Nieto L M 2006 *Phys. Lett.* A **360** 228
Ganguly A, Ioffe M V and Nieto L M 2006 *J. Phys. A: Math. Gen.* **39** 14659
Cruz S, Negro J and Nieto L M 2007 *Phys. Lett.* A **369** 400
Ganguly A and Nieto L M 2007 *J. Phys. A: Math. Theor.* **40** 7265
Cruz S, Negro J and Nieto L M 2008 *J. Phys.: Conf. Ser.* **128** 012053
[2] Zhu Q and Kroemer H 1983 *Phys. Rev.* B **27** 3519
Balian R, Bessis D and Mezincescu G A 1995 *Phys. Rev.* B **51** 17624
Pistol M E 1999 *Phys. Rev.* B **60** 14269
Tokatly I V, Tsibizov A G and Gorbatsevich A A 2002 *Phys. Rev.* B **65** 165328
Thomsen J, Einevoll G T and Hemmer P C 1989 *Phys. Rev.* B **39** 12783
Einevoll G T, Hemmer P C and Thomsen J 1990 *Phys. Rev.* B **42** 3485
Koç R, Koca M and Şahinoğlu G 2005 *Eur. Phys . J.* B **48** 583
[3] Kurasov P 1996 *J. Math. Anal. Appl.* **201** 297
[4] Albeverio S, Gesztesy F, Hoegh-Krohn R and Holden H 1988 *Solvable Models in Quantum Mechanics* (Berlin: Springer)
[5] Albeverio S and Kurasov P 2000 *Singular Perturbations of Differential Operators. Solvable Schrödinger Type Operators* (*London Mathematical Society Lecture Notes* vol 271) (Cambridge, UK: Cambridge University Press)
[6] Gadella M, Kuru Ş and Negro J 2007 *Phys. Lett.* A **362** 265
[7] Gadella M, Negro J and Nieto L M 2009 *Phys. Lett.* A **373** 1310
[8] Seba P 1986 *Rep. Math. Phys.* **24** 111
[9] Coutinho FAB, Nogami Y and Perez J F 1997 *J. Phys. A: Math. Gen.* **30** 3937