TUTORIAL / ARTICLE DIDACTIQUE

Point interactions: boundary conditions or potentials with the Dirac delta function

Salvatore De Vincenzo and Carlet Sánchez

Abstract: We study the problem of a nonrelativistic quantum particle moving on a real line with an idealized and localized singular interaction with zero range at $x = 0$ (i.e., a point interaction there). This kind of system can be described in two ways: (*i*) by considering an alternative free system (i.e., without the singular potential) but excluding the point $x = 0$ (In this case, the point interaction is exclusively encoded in the boundary conditions.) and (*ii*) by explicitly considering the singular interaction by means of a local singular potential. In this paper we relate, compare, and discuss, in a simple and pedagogical way these two equivalent approaches. Our main goal in this paper is to introduce the essential ideas about point interactions in a very accesible form to advanced undergraduates.

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Résumé : Nous étudions le problème d'une particule quantique non relativiste sur la ligne réelle avec une interaction de portée nulle singulière, idéalisée et localisée à $x = 0$ (c.-à-d., une interaction ponctuelle en ce point). On peut décrire ce type de système de deux façons. (*i*) On peut étudier le système alternatif libre en excluant le point $x = 0$ (sans le potentiel singulier), auquel cas, le point d'interaction est exclusivement encodé dans la condition limite. (*ii*) On peut considérer l'interaction singulière comme étant un potentiel local singulier. Nous analysons, relions et comparons ici ces deux approches équivalentes de façon pédagogique simple. Notre objectif est de présenter de façon accessible les points essentiels de ce problèmes aux étudiants en fin de premier cycle.

[Traduit par la Rédaction]

1. Introduction

Many aspects of point interactions (sharply localized singular perturbations or simply called contact interactions) such as the common Dirac delta function (or rather distribution), are fascinating, such as their own derivatives, the boundary conditions arising from these potentials, and their bound states (which are few or non-existent). By a point interaction we mean an idealized localized singular interaction with zero range occurring at one point on the line $\mathbb{R}$. However, this kind of interaction can also be described by a free system on the line without the singular point, i.e., in the region $\mathbb{R} \setminus \{0\}$, in which case the interaction is encoded in boundary conditions rather than in a formal Hamiltonian operator. For a nonrelativistic free particle (i.e., under a constant or zero potential) moving on a line ($\mathbb{R}$) with origin ($x = 0$) excluded (a hole or a single defect), the Hamiltonian operator is (by setting $V(x) = 0$),

$$\widehat{h} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} \tag{1}$$

where $x \in \Omega = \mathbb{R} - \{0\} (= \mathbb{R} \setminus \{0\})$. This real and self-adjoint operator (the kinetic energy) is defined on a dense proper subset (its domain $D(\widehat{h})$) in the Hilbert space $\mathcal{H}$ for functions $u(x)$ such that $\|u\| < \infty$ in Ω (hence $(\widehat{h}f, g) = (f, \widehat{h}g)$, where $f, g \in D(\widehat{h})$, and the scalar product of the two functions is $(f, g) \equiv \int_\Omega \mathrm{d}x \bar{f} g$, where the bar means complex conjugation, with the usual definition of the norm $\| f \| \equiv \sqrt{(f, f)}$). Specifically, the domain of $\widehat{h}$ is all the functions belonging to $\mathcal{H}$ satisfying $\| \widehat{h}u \| < \infty$ (In addition, $u(x)$ and $du/dx \equiv u'(x)$ are absolutely continuous functions). Furthermore, $u(x)$ must satisfy some of the following (general) boundary conditions (see, for example, [1, 2]):

$$\begin{pmatrix} u(0+) - i\lambda u'(0+) \\ u(0-) + i\lambda u'(0-) \end{pmatrix} = \mathbf{U} \begin{pmatrix} u(0+) + i\lambda u'(0+) \\ u(0-) - i\lambda u'(0-) \end{pmatrix} \tag{2}$$

The parameter λ is inserted for dimensional reasons and the matrix $\mathbf{U}$ belongs to $U(2)$. We use the notation $u(0\pm) = \lim_{\varepsilon \to 0} u(\pm\varepsilon)$, and similarly for the derivative u'. The boundary conditions in (2) represent the whole family of nonrelativistic point interactions in one-dimensional quantum mechanics. The unitary matrix $\mathbf{U}$ in (2) can be written, for instance, as

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S. De Vincenzo[1] and C. Sánchez. Escuela de Física, Facultad de Ciencias, Universidad Central de Venezuela, A.P. 47145, Caracas 1041-A, Venezuela.

[1]Corresponding author (e-mail: salvatore.devincenzo@ucv.ve).

$$\mathbf{U} = \exp(i\phi)\begin{pmatrix} m_0 - im_3 & -m_2 - im_1 \\ m_2 - im_1 & m_0 + im_3 \end{pmatrix} \tag{3}$$

where $\phi \in [0, \pi]$, and quantities $m_\mu \in \mathbb{R}$ (μ = 0, 1, 2, 3) satisfy

$$(m_0)^2 + (m_1)^2 + (m_2)^2 + (m_3)^2 = 1$$

The matrix $\mathbf{U}$ is independent of the choice of function $u \in D(\widehat{h})$ in the sense that $\mathbf{U}$ is universal for $D(\widehat{h})$ [3], i.e., the boundary conditions (2) (also arising from Von Neumann's theory of self-adjoint extensions) is *for all* $u \in D(\widehat{h})$ [1, 3]. On the other hand, the same boundary conditions may be obtained using different parameters m_μ. However, there is a one-to-one correspondence between a physically distinct point interaction and a self-adjoint Hamiltonian whose domain (in general) depends on four (real) parameters [4, 5].

It can be shown that for every function $u \in D(\widehat{h})$, the probability current density $j(x) = (\hbar/m) \times \mathrm{Im}(\bar{u}(x)u'(x))$ satisfies $j(0–) = j(0+)$, where the bar denotes complex conjugation. This condition is equivalent to the self-adjointness of the Hamiltonian (1). In fact, for each $f \in D(\widehat{h})$, on integrating by parts we obtain

$$0 = (\widehat{h}f, f) - (f, \widehat{h}f) = \mathrm{const} \times (j(0+) - j(0-))$$

Some of the boundary conditions verify $j(0–) = j(0+) = 0$, which is the impenetrability condition at $x = 0$, i.e., we have a (physically) real impenetrable barrier there. In relation to this important point, we can find an expression for the probability current density at $x = 0$,

$$j(0-) = j(0+) = -\frac{\hbar}{m}\frac{1}{\lambda}\left(\frac{1}{m_0 + \cos(\phi)}\right) \times \mathrm{Re}[(m_2 + im_1)u(0-)\bar{u}(0+)] \tag{4}$$

To obtain this result, one first writes $j(0-) = (\hbar/m) \times \mathrm{Im}(\bar{u}(0-)u'(0-))$, and then by using (8) one can write $u'(0–)$ in terms of $u(0+)$ and $u(0–)$. By substituting this last result in $j(0–)$ and by using the fact that the coefficients of the matrix $\mathbf{M}$, M_{11} and M_{12}, verify $(M_{11}/M_{12}) \in \mathbb{R}$ (plus the basic formula $\mathrm{Im}(iz) = \mathrm{Re}(z)$), the result (4) is obtained. Notice that by making $m_1 = m_2 = 0$, we obtain $j(0–) = j(0+) = 0$. The respective subfamily of boundary conditions could be written (from (2) and (3)) as

$$\begin{pmatrix} 1 & \cot\left(\dfrac{\phi-\theta}{2}\right) \\ 0 & 0 \end{pmatrix}\begin{pmatrix} u(0+) \\ \lambda u'(0+) \end{pmatrix} = \begin{pmatrix} 0 & 0 \\ 1 & -\cot\left(\dfrac{\phi+\theta}{2}\right) \end{pmatrix}\begin{pmatrix} u(0-) \\ \lambda u'(0-) \end{pmatrix} \tag{5}$$

where $\theta = \arctan(m_3/m_0)$ but $(m_0)^2 + (m_3)^2 = 1$. This subfamily of boundary conditions is similar to that studied and called "separated" by Kurasov and Albeverio et al. [6–8]. Note that (from (4)), if the functions u are real with $m_2 = 0$ and $m_1 \neq 0$, then we also have $j(0–) = j(0+) = 0$. In fact, if the Hamiltonian operator (1) is invariant under time-reversal, then $(\widehat{T}u)(x) \equiv (\bar{u})(x) \in D(\widehat{h})$. Thus, the matrix $\mathbf{U}$ must satisfy $\mathbf{U}^\dagger = \bar{\mathbf{U}}$, which implies $m_2 = 0$, and the eigenfunctions, or stationary states, for these $\widehat{T}$-invariant Hamiltonians can be real functions. Note that all of the boundary conditions included in (5) are $\widehat{T}$-invariant (in [9] we have a complete discussion of this theme for the apparently similar problem of a free particle in a box).

We mention here two boundary conditions imposed to both sides of the point $x = 0$ that are included in (5) (and the two half-spaces $x > 0$ and $x < 0$ are separated physically):

(a) The Dirichlet boundary condition

$$u(0+) = u(0-) = 0 \tag{6}$$

which is obtained by setting (for example) $m_0 = +1$, $m_3 = 0$ ($\Rightarrow \theta = 0$), and $\phi = \pi$ (which implies $\cot((\phi - \theta)/2) = 0$ and $\cot((\phi + \theta)/2) = 0$).

(b) The Neumann boundary condition

$$u'(0+) = u'(0-) = 0 \tag{7}$$

which is obtained by setting (for example) $m_0 = +1$, $m_3 = 0$ ($\Rightarrow \theta = 0$) and $\phi = 0$ (which implies $\cot((\phi - \theta)/2) = \infty$ and $\cot((\phi + \theta)/2) = \infty$).

When the probability current density is not null at $x = 0$, we may say that (physically) the wall at the singular point is transparent to the current. Therefore, we can write a second family of boundary conditions; this family may be called "nonseparated" because the two half-spaces cannot be separated (Note that the probability current is different than zero only if the respective functions, e.g., scattering functions, are complex functions, because real functions, e.g., bound states, lead to zero probability current at $x = 0$). Finally, this non-disjoint family together with the family (5) (as well as the general boundary condition (2)) represents the whole family of boundary conditions for the self-adjoint Hamiltonian for a particle on the real line with a point interaction at $x = 0$:

$$\begin{pmatrix} u(0+) \\ \lambda u'(0+) \end{pmatrix} = \mathbf{M}\begin{pmatrix} u(0-) \\ \lambda u'(0-) \end{pmatrix} \tag{8}$$

where the matrix $\mathbf{M}$ is

$$\mathbf{M} = \frac{i}{-m_2 + im_1}\begin{pmatrix} m_3 + \sin(\phi) & -m_0 - \cos(\phi) \\ -m_0 + \cos(\phi) & -m_3 + \sin(\phi) \end{pmatrix} \tag{9}$$

To see this, note first that (2) can be written as

$$(\mathbf{U} + \mathbf{1})\begin{pmatrix} -i\lambda u'(0+) \\ +i\lambda u'(0-) \end{pmatrix} = (\mathbf{U} - \mathbf{1})\begin{pmatrix} u(0+) \\ u(0-) \end{pmatrix}$$

where $\mathbf{1}$ is the 2×2 unit matrix. Then from this pair of linear relations ($u'(0+)$ and also $u'(0–)$ in terms of $u(0+)$ and $u(0–)$), one easily deduces the result (8). The matrix $\mathbf{M}$ can also be written as,

$$\mathbf{M} = \frac{\exp\left\{i\left[\tan^{-1}\left(\frac{m_1}{m_2}\right) + \frac{\pi}{2}\right]\right\}}{\sqrt{(m_1)^2 + (m_2)^2}} \times \begin{pmatrix} m_3 + \sin(\phi) & -m_0 - \cos(\phi) \\ -m_0 + \cos(\phi) & -m_3 + \sin(\phi) \end{pmatrix} \tag{10}$$

which confirms, due to the relation

$$(m_0)^2 + (m_1)^2 + (m_2)^2 + (m_3)^2 = 1$$

that $\mathbf{M}$ does belong to the group $U(1) \times SL(2, \mathbb{R})$. Moreover, the elements in the matrix $\mathbf{M}$ should take only finite values, i.e., $m_1 \neq 0$ and $m_2 \neq 0$. In fact, the subfamily of boundary conditions (8) is similar to what is called "connected" by Kurasov and Albeverio et al. [6–8]. Note that the matrix $\mathbf{M}$ is real for $\widehat{T}$-invariant boundary conditions (because $m_2 = 0$). This result was noted in [10]. As examples of boundary conditions that are included in (8) we have:

(c) The Dirac delta interaction

$$\begin{pmatrix} u(0+) \\ \lambda u'(0+) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -2\dfrac{m_0}{m_1} & 1 \end{pmatrix} \begin{pmatrix} u(0-) \\ \lambda u'(0-) \end{pmatrix} \tag{11}$$

which is obtained by setting $m_0 = -\cos(\phi)$, $m_1 = \sin(\phi)$, and $m_2 = m_3 = 0$.

(d) The first derivative of the Dirac delta interaction

$$\begin{pmatrix} u(0+) \\ \lambda u'(0+) \end{pmatrix} = \begin{pmatrix} \dfrac{1+m_3}{m_1} & 0 \\ 0 & \dfrac{1-m_3}{m_1} \end{pmatrix} \begin{pmatrix} u(0-) \\ \lambda u'(0-) \end{pmatrix} \tag{12}$$

which is obtained by setting $m_0 = m_2 = 0 \Rightarrow [(1-m_3)/m_1] = m_1/(1+m_3)$, $\cos(\phi) = 0$, and $\sin(\phi) = 1 \Rightarrow \phi = \pi/2$.

(e) The quasi-periodic interaction

$$\begin{pmatrix} u(0+) \\ \lambda u'(0+) \end{pmatrix} = \begin{pmatrix} m_1 - im_2 & 0 \\ 0 & m_1 - im_2 \end{pmatrix} \begin{pmatrix} u(0-) \\ \lambda u'(0-) \end{pmatrix} \tag{13}$$

which is obtained by setting $m_0 = m_3 = 0 \Rightarrow (m_1)^2 + (m_2)^2 = 1$, $\cos(\phi) = 0$, and $\sin(\phi) = 1 \Rightarrow \phi = \pi/2$. Note that (if $m_2 \neq 0$) this boundary condition is not $\widehat{T}$-invariant and therefore it is complex.

(f) The delta-prime interaction

$$\begin{pmatrix} u(0+) \\ \lambda u'(0+) \end{pmatrix} = \begin{pmatrix} 1 & -2\dfrac{m_0}{m_1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} u(0-) \\ \lambda u'(0-) \end{pmatrix} \tag{14}$$

which is obtained by setting $m_0 = \cos(\phi)$, $m_1 = \sin(\phi)$, and $m_2 = m_3 = 0$.

It is worth noting that if we (conveniently) impose $m_1 = m_2 = 0$ on the "nonseparated" family of boundary conditions (8) (or (10)), then we could obtain the boundary conditions included in the "separated" family in (5). For example, the Dirichlet boundary condition is obtained from boundary condition (11) (the latter is included in (8)) by noticing that $-2m_0/m_1 = +2\cot(\phi) = -\infty$ (because $\phi = \pi$), thus, $u(0+) = u(0-)$ and

$$u'(0+) = -\infty \times u(0-) + u'(0-) \Rightarrow u(0-) = 0$$

therefore $u(0+) = u(0-) = 0$. Likewise, the Neumann boundary condition is obtained from boundary condition (14) (the latter is also included in (8)) by noticing that $-2m_0/m_1 = -2\cot(\phi) = -\infty$ (because $\phi = 0$), so $u'(0+) = u'(0-)$ and

$$u(0+) = u(0-) - \infty \times u'(0-) \Rightarrow u'(0-) = 0$$

therefore $u'(0+) = u'(0-) = 0$.

Another particular family of boundary conditions can easily be obtained from (8),

$$\begin{pmatrix} \lambda u'(0+) - \lambda u'(0-) \\ u(0+) - u(0-) \end{pmatrix} = \mathbf{S} \begin{pmatrix} u(0+) + u(0-) \\ \lambda u'(0+) + \lambda u'(0-) \end{pmatrix} \tag{15}$$

where the matrix $\mathbf{S}$ can be written in terms of $\mathbf{M}$ as follows:

$$\mathbf{S} = \sigma_x(\mathbf{M} - \mathbf{1})(\mathbf{M} + \mathbf{1})^{-1} \tag{16}$$

where σ_x is one of the Pauli matrices. Notice that by using (8), the relation (15) can be written as,

$$\sigma_x(\mathbf{M} - \mathbf{1}) \begin{pmatrix} u(0-) \\ \lambda u'(0-) \end{pmatrix} = \mathbf{S}(\mathbf{M} + \mathbf{1}) \begin{pmatrix} u(0-) \\ \lambda u'(0-) \end{pmatrix}$$

and thus we obtain (16). Explicitly, the matrix $\mathbf{S}$ is

$$\mathbf{S} = \frac{1}{m_1 + \sin(\phi)} \begin{pmatrix} -m_0 + \cos(\phi) & -m_3 - im_2 \\ m_3 - im_2 & -m_0 - \cos(\phi) \end{pmatrix} \tag{17}$$

where the coefficients $\{S_{pq}\}$ (obviously) verify $S_{11}, S_{22} \in \mathbb{R}$, $S_{21} = -\bar{S}_{12}$, and $\det(\mathbf{S}) = (-m_1 + \sin(\phi))/(m_1 + \sin(\phi)))$. Likewise, $(m_0)^2 + (m_1)^2 + (m_2)^2 (m_3)^2 = 1$. Moreover, if the matrix $\mathbf{S}$ takes only finite values, we have $m_1 \neq -\sin(\phi)$. Within the subfamily (15), we have the boundary conditions (c), (d), (e), and (f). This family of boundary conditions was mentioned and related to other families in [11]. Because (15) was obtained from (8), it appears that we do not have within (15) all of the boundary conditions included in $D(\widehat{h})$. In fact, we do not have the cases where $m_1 + \sin(\phi) = 0$ in (15); nevertheless, if we have a boundary condition where $m_1 = -\sin(\phi)$, the singularity in (17) could be (conveniently) avoided, and the respective boundary condition could thus emerge from (15). For example, the boundary conditions (a) and (b) emerge in this way (First, the term $m_1 + \sin(\phi)$ in (17) must be placed on the left-hand side in (15), then the rest of the parameters on the right-hand side in (15) must be evaluated and simplified where possible. Finally, ϕ and m_1 can be evaluated).

In this introduction, we have presented the most important results for the Hamiltonian for a nonrelativistic free particle moving on the real line with a hole at the origin. With this Hamiltonian (without any singular potential), whose domain depends on four (real) parameters, the point interactions are modeled exclusively through boundary conditions. In conclusion, every (physically) possible boundary condition encodes a different kind of wall at $x = 0$.

The rest of the paper is organized as follows. In Sect. 2, we present a Hamiltonian with a singular potential in terms of the Dirac delta and (conveniently positioned) derivatives d/dx, which depends on four (real) parameters to describe a nonrelativistic particle moving on the real line with a point interaction at $x = 0$. This local singular potential can be written in various ways, particularly as a sum of four (specific) singular potentials that are certainly four representative point interactions. Here, for example, we encounter the Dirac delta interaction and the so-called delta-prime interaction. In this section, we also discuss and relate the different expressions that could be written for a local general singular potential (here, and in the following section, we make full use of various properties related to the Dirac delta and its derivative). In Sect. 3, we integrate (in two different ways) the eigenvalue equation for the Hamiltonian with the general singular potential, and as a result we obtain a four-parameter family of boundary conditions. This result allows us to connect any boundary condition for the free Hamiltonian on the real line with the origin excluded, with a specific Hamiltonian with a singular potential at $x = 0$. To conclude, a summary is given in the last section.

2. Singular potentials at $x = 0$

As we commented earlier, a point interaction is a singular interaction (with zero range) at one point, say $x = 0$, on the real line. Therefore, a nonrelativistic particle moving on a line ($\mathbb{R}$) with a point interaction at $x = 0$ may also be described by a general (formally) self-adjoint Hamiltonian operator of the type,

$$\widehat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \widehat{V}(x) \tag{18}$$

where $x \in \mathbb{R}$ (then, one consistently has $(\widehat{H}f, g) = (f, \widehat{H}g)$, where f and g belong to the respective domains for $\widehat{H}$). In the literature [6–8, 12–14], different expressions for the (most general) local singular potential $\widehat{V}(x)$ have been given. In this section, we want to relate, compare, and explain, in a simple and accessible way, the results obtained by all these authors.

In fact, a plausible (formal) expression for the operator $\widehat{V}(x)$ in terms of the Dirac delta and derivatives d/dx could be [13] (in our paper, the derivatives of the Dirac delta will always be written as $\delta'(x) \equiv \mathrm{d}\delta/\mathrm{d}x$ and $\delta''(x) \equiv \mathrm{d}^2\delta/\mathrm{d}x^2$, that is, with the prime or primes on the delta),

$$\widehat{V}(x) = g_1\delta(x) - (g_2 - ig_3)\delta(x)\frac{\mathrm{d}}{\mathrm{d}x} + (g_2 + ig_3)\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - g_4\frac{\mathrm{d}}{\mathrm{d}x}\left(\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) \tag{19}$$

where $g_k \in \mathbb{R}$, $(k = 1, 2, 3, 4)$. There are many things to explain about this "momentum-dependent" expression (remember that $\widehat{p} = -i\hbar\mathrm{d}/\mathrm{d}x$ [13, 15]). First, the operator $\widehat{V}(x)$ is (formally) self-adjoint, i.e., $\widehat{V}(x) = \widehat{V}^{\dagger}(x)$. Although we will only check that the Hamiltonian (18) with the singular potential $\widehat{V}(x)$ in (19) is formally self-adjoint, it has been shown that this formal differential operator has a corresponding self-adjoint operator (see the discussion that follows (35)). In fact, this extension for $\widehat{H}$ (in a generalized sense) was determined by resorting to a theory of distributions where the test functions $u(x)$ and $u'(x)$ are discontinuous at the origin, but they also must have equal weights on the left and the right side at $x = 0$, i.e., $(\delta, u) = u(0) \equiv (u(0+) + u(0-))/2$ and similarly for the function $u'(x)$, as well as $(\delta', u) = -u'(0) \equiv -(u'(0+) + u'(0-))/2$ [6–8]. Finally, it was also proved that every formal self-adjoint operator with the singular potential (19) coincides with a certain self-adjoint extension of the second derivative operator given in (1) [6–8]. In other words, any point interaction at the origin, for instance, those belonging to the family of separated boundary conditions in (5) or those belonging to the nonseparated boundary conditions in (8), can be described by an operator with a singular interaction. This result is clearly illustrated in Sect. 3.

To demonstrate the important property $\widehat{V}(x) = \widehat{V}^{\dagger}(x)$ from (19), we first write another convenient expression for $\widehat{V}(x)$,

$$\widehat{V}(x) = g_1\delta(x) - g_2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) + g_2\delta'(x) + ig_3\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - ig_3\delta'(x) + g_2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) + ig_3\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - g_4\frac{\mathrm{d}}{\mathrm{d}x}\left(\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\right)$$

where we have used the (elementary) relation

$$\delta(x)\frac{\mathrm{d}}{\mathrm{d}x} = \frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - \delta'(x) \tag{20}$$

As usual, this expression, as well as all those used here, is understood in a distributional sense. We can write immediately (after a trivial simplification) the operator potential $\widehat{V}(x)$ in a suitable form,

$$\widehat{V}(x) = g_1\delta(x) + g_2\delta'(x) + ig_3\left(2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - \delta'(x)\right) - g_4\frac{\mathrm{d}}{\mathrm{d}x}\left(\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) \tag{21}$$

and we can now introduce four local potentials, each with its proper particularity. Note that $\widehat{V}(x)$ is precisely the sum of these four potentials, and each one of these potentials will lead to the boundary conditions (c), (d), (e), and (f), which were introduced in the introduction.

(c) The usual (and well-known) Dirac delta potential:

$$\widehat{V}_{\delta}(x) = g_1\delta(x) \tag{22}$$

It is evidently (formally) self-adjoint because g_1 is real (and obviously the even-parity function $\delta(x)$ is real as well).

(d) The pure derivative of the Dirac delta potential:

$$\widehat{V}_{\delta'}(x) = g_2\delta'(x) \tag{23}$$

It is also (formally) self-adjoint because the strength g_2 and the odd-parity function $\delta'(x)$ are real.

(e) We may call this (not so familiar) operator a quasi-free potential:

$$\widehat{V}_0(x) = ig_3\left(2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - \delta'(x)\right) \tag{24}$$

This operator is (formally) self-adjoint; in fact

$$\begin{aligned}\left(\widehat{V}_0(x)\right)^{\dagger} &= \left(ig_3 2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x)\right)^{\dagger} + ig_3\delta'(x)\\ &= -ig_3 2\delta(x)\left(-\frac{\mathrm{d}}{\mathrm{d}x}\right) + ig_3\delta'(x)\\ &= ig_3 2\delta(x)\frac{\mathrm{d}}{\mathrm{d}x} + ig_3\delta'(x)\\ &= ig_3 2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - ig_3 2\delta'(x) + ig_3\delta'(x)\\ &= ig_3\left(2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - \delta'(x)\right) = \widehat{V}_0(x)\end{aligned}$$

where we have used the relation (20), the adjoint property $(\widehat{f}\widehat{g})^{\dagger} = \widehat{g}^{\dagger}\widehat{f}^{\dagger}$, and also $(\mathrm{d}/\mathrm{d}x)^{\dagger} = -\mathrm{d}/\mathrm{d}x$. The Schrödinger operator with this uncommon potential has been studied in the literature [6–8, 16]. The authors of these papers claim that $\widehat{H}_0 \equiv -\mathrm{d}^2/\mathrm{d}x^2 + \widehat{V}_0(x)$ (with $\hbar^2 = 2m = 1$) is equivalent to a Schrödinger operator with a singular gauge field at $x = 0$. Certainly, we obtain the following result:

$$\begin{aligned}\widehat{H}_0 &= -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + ig_3\left(2\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) - \delta'(x)\right)\\ &= \left(-i\frac{\mathrm{d}}{\mathrm{d}x} - g_3\delta(x)\right)^2 - g_3^2\Big(\delta(x)\Big)^2 \end{aligned}\tag{25}$$

because the right-hand side of this expression can be written as

$$\begin{aligned}&\left(-i\frac{\mathrm{d}}{\mathrm{d}x} - g_3\delta(x)\right)\left(-i\frac{\mathrm{d}}{\mathrm{d}x} - g_3\delta(x)\right) - g_3^2\Big(\delta(x)\Big)^2 = \\ &\quad -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + ig_3\frac{\mathrm{d}}{\mathrm{d}x}\delta(x) + ig_3\delta(x)\frac{\mathrm{d}}{\mathrm{d}x} + g_3^2\Big(\delta(x)\Big)^2 - g_3^2\Big(\delta(x)\Big)^2\end{aligned}$$

Finally, by using the relation (20), the result (25) is easily obtained.

(f) We may call this operator a delta-prime interaction potential:

$$\widehat{V}_{\tilde{\delta}'}(x) = -g_4\frac{\mathrm{d}}{\mathrm{d}x}\left(\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\right)\tag{26}$$

This operator is also (formally) self-adjoint,

$$\begin{aligned}\Big(\widehat{V}_{\tilde{\delta}'}(x)\Big)^{\dagger} &= \left(-g_4\delta'(x)\frac{\mathrm{d}}{\mathrm{d}x} - g_4\delta(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)^{\dagger} = \\ &\quad - g_4\left(-\frac{\mathrm{d}}{\mathrm{d}x}\right)\delta'(x) - g_4\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\delta(x)\end{aligned}$$

where we have used the trivial property about the adjoint of a product of operators, and also $(\mathrm{d}/\mathrm{d}x)^{\dagger} = -\mathrm{d}/\mathrm{d}x$ and $(\mathrm{d}^2/\mathrm{d}x^2)^{\dagger} = \mathrm{d}^2/\mathrm{d}x^2$. Finally, if we substitute the following two (elementary) relations into the preceding expression,

$$\frac{\mathrm{d}^2}{\mathrm{d}x^2}\delta(x) = \delta''(x) + 2\delta'(x)\frac{\mathrm{d}}{\mathrm{d}x} + \delta(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\tag{27}$$

$$\frac{\mathrm{d}}{\mathrm{d}x}\delta'(x) = \delta''(x) + \delta'(x)\frac{\mathrm{d}}{\mathrm{d}x}\tag{28}$$

we can prove the (formal) self-adjointness of the $\widehat{V}_{\tilde{\delta}'}(x)$:

$$\begin{aligned}\Big(\widehat{V}_{\tilde{\delta}'}(x)\Big)^{\dagger} &= g_4\frac{\mathrm{d}}{\mathrm{d}x}\delta'(x) - g_4\frac{\mathrm{d}^2}{\mathrm{d}x^2}\delta(x)\\ &= g_4\left(\delta''(x) + \delta'(x)\frac{\mathrm{d}}{\mathrm{d}x}\right)\\ &\quad - g_4\left(\delta''(x) + 2\delta'(x)\frac{\mathrm{d}}{\mathrm{d}x} + \delta(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2}\right)\\ &= -g_4\delta'(x)\frac{\mathrm{d}}{\mathrm{d}x} - g_4\delta(x)\frac{\mathrm{d}^2}{\mathrm{d}x^2} = \widehat{V}_{\tilde{\delta}'}(x)\end{aligned}$$

It is now clear that the first plausible expression for the operator $\widehat{V}(x)$ given by (19) (and specifically introduced in that way in [13]) or the equivalent expression for $\widehat{V}(x)$ in (21) (which was essentially introduced in [6–8]), is formally self-adjoint and depends on four real parameters. Our parameters g_k (k = 1, 2, 3, 4) are the four parameters x_k used in [6–8]. Likewise, our parameters are related to those used in [13] (c, γ, η, and $\tilde{\lambda}$) by means of the relations ($\hbar = 2m = 1$): $g_1 = c$, $g_2 = 2\gamma$, $g_3 = 2\eta$, and $g_4 = -4\tilde{\lambda}$. Note that we write here $\tilde{\lambda}$ instead of λ because we already used λ as a parameter in (2).

Let us consider again the expression (19) for the operator $\widehat{V}(x)$. The action of this operator on a function $u(x)$ (with $x \in \mathbb{R}$) has the form,

$$\begin{aligned}\widehat{V}(x)u(x) &= g_1u(x)\delta(x) - (g_2 - ig_3)u'(x)\delta(x)\\ &\quad + (g_2 + ig_3)\frac{\mathrm{d}}{\mathrm{d}x}[u(x)\delta(x)] - g_4\frac{\mathrm{d}}{\mathrm{d}x}[u'(x)\delta(x)]\end{aligned}\tag{29}$$

Now, we need to use the (symbolic) sifting property for the Dirac delta,

$$u(x)\delta(x) = u(0)\delta(x)\tag{30}$$

$$\begin{aligned}&\Rightarrow \int_{-\infty}^{+\infty}\mathrm{d}x\, u(x)\delta(x) \equiv (\delta, u)\\ &\quad = u(0)\int_{-\infty}^{+\infty}\mathrm{d}x\,\delta(x) = u(0) \equiv \frac{1}{2}[u(0+) + u(0-)]\end{aligned}$$

(where the common delta function property $\int_{-\infty}^{+\infty}\mathrm{d}x\,\delta(x) = 1$ was also used above). Because the function $u(x)$ (and its derivative) is not generally continuous at $x = 0$ (i.e., $u(x)$ and (or) $u'(x)$ have a possible discontinuity at the origin), $u(0)$ is written as the average at the discontinuity (clearly this is a plausible choice for discontinuous test functions). Thus, we can also write,

$$u'(x)\delta(x) = u'(0)\delta(x)\tag{31}$$

where $u'(0) \equiv (u'(0+) + u'(0-))/2$. By using the relations (30) and (31), the term $\widehat{V}(x)u(x)$ in (29) takes the form,

$$\begin{aligned}\widehat{V}(x)u(x) &= g_1u(0)\delta(x) - (g_2 - ig_3)u'(0)\delta(x)\\ &\quad + (g_2 + ig_3)u(0)\delta'(x) - g_4u'(0)\delta'(x)\end{aligned}\tag{32}$$

This last expression could be still written in a different and interesting way. For this, we use the preceding formula, (i) $u(0) = (\delta, u)$ (but not its "partner" (ii) $u'(0) = (\delta, u')$). Likewise, by considering the following important property (which is obtained by applying to a function $u(x)$ the relation (20) and using (30) and (31)),

$$u(x)\delta'(x) = u(0)\delta'(x) - u'(0)\delta(x)\tag{33}$$

$$\begin{aligned}&\Rightarrow \int_{-\infty}^{+\infty}\mathrm{d}x\, u(x)\delta'(x) \equiv (\delta', u)\\ &\quad = u(0)\int_{-\infty}^{+\infty}\mathrm{d}x\,\delta'(x) - u'(0)\int_{-\infty}^{+\infty}\mathrm{d}x\,\delta(x)\\ &\quad = -u'(0) \equiv -\frac{1}{2}[u'(0+) + u'(0-)]\end{aligned}$$

(where the delta function properties $\int_{-\infty}^{+\infty} \mathrm{d}x\, \delta(x) = 1$ and $\int_{-\infty}^{+\infty} \mathrm{d}x\, \delta'(x) = 0$ were also used above). In this way, we also use: (*iii*) $u'(0) = -(\delta', u)$. Thus, expression (32) (in fact, by using only (*i*) and (*iii*)) can be "symmetrically" written as,

$$\widehat{V}(x)u(x) = g_1(\delta, u)\delta(x) + (g_2 - ig_3)(\delta', u)\delta(x) + (g_2 + ig_3)(\delta, u)\delta'(x) + g_4(\delta', u)\delta'(x) \quad (34)$$

That is, the local potential $\widehat{V}(x)$ can have the following appearance (compare with similar expressions given, for example, in [7, 14]),

$$\widehat{V}(x) = g_1(\delta, \cdot)\delta(x) + (g_2 - ig_3)(\delta', \cdot)\delta(x) + (g_2 + ig_3)(\delta, \cdot)\delta'(x) + g_4(\delta', \cdot)\delta'(x) \quad (35)$$

Note that if one defines the quantities $t_{00} \equiv g_1$, $t_{01} \equiv g_2 - ig_3$, $t_{10} \equiv g_2 + ig_3$, and $t_{11} \equiv g_4$, then these coefficients $\{t_{pq}\}$ define a 2×2 Hermitian matrix (i.e., t_{00}, $t_{11} \in \mathbb{R}$, and $t_{10} = \bar{t}_{01}$). More precisely, the formal Hamiltonian (18) with $\widehat{V}(x)$ given by expresion (35) is self-adjoint on the domain

$$D(\widehat{H}) = \{u(x) : u(x) \in W_2^2(\mathbb{R} \setminus \{0\}); (\widehat{H}u)(x) \in L^2(\mathbb{R})\}$$

where $W_2^2(\mathbb{R} \setminus \{0\})$ is the Sobolev space of continuous functions with continuous bounded first derivative, except for a finite jump at $x = 0$. This result has been sufficiently discussed previously [7, 12]. In summary, if one writes the general expression,

$$\widehat{V}(x) = a(\delta, \cdot)\delta(x) + b(\delta', \cdot)\delta(x) + c(\delta, \cdot)\delta'(x) + d(\delta', \cdot)\delta'(x) \quad (36)$$

where a, b, c, d are complex numbers, the condition on the singular potential $\widehat{V}(x) = (\widehat{V}(x))^\dagger$ implies that its parameters satisfy the conditions $a, d \in \mathbb{R}$, and $c = \bar{b}$ (clearly the potential (35) satisfies these conditions). If the potential is not (formally) self-adjoint but satisfies the condition of $\widehat{P}$-symmetry, $(\widehat{P}\widehat{V}^\dagger)(x) = (\widehat{V}\widehat{P})(x)$, where $\widehat{P}$ is the space parity operator $(\widehat{P}f)(x) = f(-x)$, and $\widehat{V}^\dagger$ is defined by the usual relation $(\widehat{V}f, g) = (f, \widehat{V}^\dagger g)$, then one obtains the following restrictions on the parameters of $\widehat{V}(x)$: $a, d \in \mathbb{R}$, but $c = -\bar{b}$ [14].

3. Boundary conditions for a general singular potential at *x* = 0

The eigenvalue equation for the Hamiltonian (18) with the general singular potential $\widehat{V}(x)$ is

$$\widehat{H}u(x) = -\alpha^{-1}\frac{\mathrm{d}^2}{\mathrm{d}x^2}u(x) + \widehat{V}(x)u(x) = Eu(x) \quad (37)$$

where $\widehat{V}(x)u(x)$ is given in (32) and $\alpha \equiv 2m/\hbar^2$. Because of the delta function and its first derivative in (32), (37) can provide boundary conditions. We follow a routine introduced by Griffiths for the nth derivative of a delta function potential [17]. In fact, integrating it from $-\varepsilon$ to $+\varepsilon$ and taking the limit $\varepsilon \to 0$ yields the following first boundary condition:

$$\lambda u'(0+) - \lambda u'(0-) = \lambda\alpha g_1 \frac{1}{2}\Big(u(0+) + u(0-)\Big) - \alpha(g_2 - ig_3)\frac{1}{2}\Big(\lambda u'(0+) + \lambda u'(0-)\Big) \quad (38)$$

Likewise, integrating (37) first from $x = -L$ (with $L > 0$) to x, then once more from $-\varepsilon$ to $+\varepsilon$ and taking the limit $\varepsilon \to 0$ again, we obtain a second boundary condition,

$$u(0+) - u(0-) = \alpha(g_2 + ig_3)\frac{1}{2}\Big(u(0+) + u(0-)\Big) - \frac{\alpha g_4}{\lambda}\frac{1}{2}\Big(\lambda u'(0+) + \lambda u'(0-)\Big) \quad (39)$$

where the relations $\int_{-L}^{x} \mathrm{d}y\, \delta(y) = \Theta(x)$ (where $\Theta(x)$ is the Heaviside function: $\Theta(x < 0) = 0$ and $\Theta(x > 0) = 1$) and $\int_{-L}^{x} \mathrm{d}y\delta'(y) = \delta(x)$ were used. Note that expressions (38) and (39) precisely constitute the family of boundary conditions (15), where in this case, the matrix **S** is

$$\mathbf{S} = \frac{\alpha}{2}\begin{pmatrix} \lambda g_1 & -(g_2 - ig_3) \\ (g_2 + ig_3) & -\dfrac{g_4}{\lambda} \end{pmatrix} \quad (40)$$

Our parameters g_k (k = 1, 2, 3, 4) are really related to those used in [13] by the relations $g_1 = c/\alpha$, $g_2 = 2\gamma/\alpha$, $g_3 = 2\eta/\alpha$, and $g_4 = -4\tilde{\lambda}/\alpha$.

Now, the following remark is in order. Although the definitions $(\delta, u) = u(0) \equiv (u(0+) + u(0-))/2$ and $(\delta', u) = -u'(0) \equiv -(u'(0+) + u'(0-))/2$ (used to obtain (38) and (39)) look inoffensive, there are certain situations in which they do not hold. For example, if $u(x)$ is defined by a differential equation in which $\delta(x)$ is involved, the relation $(\delta, u) = u(0+) + u(0-))/2$ does not hold [18, 19]. For a complete discussion about this subject, we recommend reference [19].

By comparing the matrix **S** in (17) with the matrix **S** in (40), we can immediately establish the four real parameters g_k (k = 1, 2, 3, 4), included in the general operator potential $\widehat{V}(x)$ in (19) or (21), as a function of the five real parameters, ϕ and m_μ (μ = 0, 1, 2, 3), included in the general boundary condition (15). We must not forget the "constraint" $(m_0)^2 + (m_1)^2 + (m_2)^2 + (m_3)^2 = 1$. The following are precisely these relations:

$$\frac{\alpha}{2}\lambda g_1 = \frac{-m_0 + \cos(\phi)}{m_1 + \sin(\phi)} \quad (41)$$

$$\frac{\alpha}{2}g_2 = \frac{m_3}{m_1 + \sin(\phi)} \quad (42)$$

$$\frac{\alpha}{2}g_3 = \frac{-m_2}{m_1 + \sin(\phi)} \quad (43)$$

$$\frac{\alpha}{2}\frac{g_4}{\lambda} = \frac{m_0 + \cos(\phi)}{m_1 + \sin(\phi)} \quad (44)$$

It is worth noting that it is not only the boundary conditions included in (15) with the condition $m_1 \neq -\sin(\phi)$ that may be associated with a local potential dependent of the Dirac delta and the derivative operator d/dx; in fact, as explained after (17), we can extract boundary conditions from the family (15) for which $m_1 \neq -\sin(\phi)$. Thus, if we use the relations (41)–(44), we can also find their respective local potentials. For example, for the Dirichlet boundary condition, we impose on the relations (41)–(44): $m_0 = 1$,

$m_2 = m_3 = 0$, and $\phi = \pi$, thus, $g_1 = -4/\alpha\lambda m_1$ and $g_2 = g_3 = g_4 = 0$. Moreover, because $m_1 = 0$, then $g_1 = -\infty$, and (from (21)) the associated local potential is therefore:

(a) The Dirichlet potential,

$$\widehat{V}_{\mathrm{D}}(x) = \lim_{g_1 \to -\infty} g_1 \delta(x) \tag{45}$$

This potential is the Dirac delta potential $\widehat{V}_{\delta}(x)$ with infinite strength.

Likewise, for the Neumann boundary condition we impose on the relations (41)–(44): $m_0 = 1$, $m_2 = m_3 = 0$, and $\phi = \cancel{\pi}$; thus, $g_1 = g_2 = g_3 = 0$ and $g_4 = 4\lambda/\alpha m_1$. Moreover, because $m_1 = 0$, then $g_4 = \infty$ and therefore, the associated local potential is:

(b) The Neumann potential,

$$\widehat{V}_{\mathrm{N}}(x) = \lim_{g_4 \to \infty} -g_4 \frac{\mathrm{d}}{\mathrm{d}x}\left(\delta(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) \tag{46}$$

This potential is the delta-prime interaction potential $\widehat{V}_{\tilde{\delta}'}(x)$ with infinite strength.

Clearly, the relations (41)–(44) illustrate the fact that any point interaction at $x = 0$, characterized by a boundary condition, can also be characterized by an operator with a singular interaction at $x = 0$.

4. Discussion

To summarize, we have discussed how point interactions can be modeled through boundary conditions only; in this case the Hamiltonian does not have a singular potential, but its domain depends on four (real) parameters [1–5]. On the other hand, point interactions can also be modeled with a Hamiltonian that has a singular potential (written in terms of the Dirac delta function and its derivatives d/dx positioned properly) dependent on four (real) parameters [6–8, 12–15]. We have also shown that these two sets of parameters can be related, and a Hamiltonian with a singular potential at $x = 0$ thus corresponds (formally) to any boundary condition for the free Hamiltonian on the real line with the origin excluded. To obtain this result, we made extensive use of various properties principally related to the Dirac delta and its derivatives in a very accessible form to advanced undergraduates (this is a pedagogical aspect that deserves to be highlighted). We sincerely hope that our article can serve as a stimulating introduction to the subject of point interactions.

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