

One-dimensional point interactions and bound states

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We analyze various representative examples of nonrelativistic (Schrödinger) point interactions in one dimension, with boundary conditions and with singular potentials, and study their corresponding bound states.

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1. Introduction

As is well known, the problem of a quantum particle moving on a real line with a point interaction (or a singular perturbation) at a single point, can be treated in two equivalent modes: (i) by considering an alternative free system without the singular potential (*i.e.*, $V(x) = 0$) and excluding the singular point, in which case the interaction is encoded in proper boundary conditions, and (ii) by explicitly considering the singular interaction by means of a local singular potential. See *e.g.* Ref. 1 and references therein.

The principal aim of this paper is to study and analyze some representative examples of nonrelativistic (Schrödinger) point interactions, *i.e.*, boundary conditions and singular potentials, and their corresponding bound states. In this introduction, we extract these examples from a general family of boundary conditions for the system described in the case (i), and from a general singular potential written in terms of the Dirac delta and derivatives d/dx for the system described in (ii). The introduction of the present paper is an abridged (and also complementary) version of Ref. 1, *i.e.*, it is a survey of point interactions with examples. In Sec. 2, we obtain and discuss the bound states for all these examples. The conclusions are given in Sec. 3. In the Appendix A we study some general aspects related with the eigenvalues and eigenvectors of the Hamiltonian operator corresponding to the case (i). Finally, in the Appendix B we explicitly solve the Schrödinger equation for a potential that is the first derivative of the Dirac delta, but we do not use the same definition of $\delta'(x)$ that was used throughout the article.

1.1. Case (i): point interactions as boundary conditions

In this case, one considers the line (\mathbb{R}) with the origin ($x = 0$) excluded (a hole or a single defect). The Hamiltonian operator is,

$$\hat{h} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}, \quad (1)$$

where $x = \mathbb{R} - \{0\} \equiv \Omega$. The operator \hat{h} is, essentially, self-adjoint on the domain $D(\hat{h})$ formed by functions ψ such that $\psi \in \mathcal{H} \equiv \mathcal{L}^2(\Omega)$ (*i.e.*, $\|\psi\| < \infty$ in Ω , with the usual definitions of the norm and the scalar product, $\|\psi\| \equiv \sqrt{\langle \psi, \psi \rangle}$ and $\langle \psi, \chi \rangle \equiv \int_{\Omega} dx \bar{\psi} \chi$, the bar meaning the complex conjugation). Moreover, $\hat{h}\psi$ also belongs to \mathcal{H} and ψ must satisfy some of the following general boundary conditions:

$$\begin{pmatrix} \psi(0+) - i\lambda\psi'(0+) \\ \psi(0-) + i\lambda\psi'(0-) \end{pmatrix} = \hat{U} \begin{pmatrix} \psi(0+) + i\lambda\psi'(0+) \\ \psi(0-) - i\lambda\psi'(0-) \end{pmatrix}. \quad (2)$$

The parameter λ is inserted for dimensional reasons and the 2×2 matrix \hat{U} is unitary (and therefore, Eq. (2) is a 4-parameter family of boundary conditions) [2]. We use the notation $\psi(0\pm) = \lim_{\epsilon \rightarrow 0} \psi(\pm\epsilon)$, and the same for the derivative ψ' . We write the matrix \hat{U} as follows:

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

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

Another 4-parameter family of boundary conditions can algebraically be obtained from Eq. (2) [1]:

$$\begin{pmatrix} \lambda\psi'(0+) - \lambda\psi'(0-) \\ \psi(0+) - \psi(0-) \end{pmatrix} = \hat{S} \begin{pmatrix} \psi(0+) + \psi(0-) \\ \lambda\psi'(0+) + \lambda\psi'(0-) \end{pmatrix}, \quad (4)$$

where the matrix \hat{S} is:

$$\hat{S} = \frac{1}{m_1 + \sin(\phi)} \begin{pmatrix} -m_0 + \cos(\phi) & -m_3 - im_2 \\ m_3 - im_2 & -m_0 - \cos(\phi) \end{pmatrix}. \quad (5)$$

Note that S_{11} and S_{22} are real, and $S_{21} = -\bar{S}_{12}$. This family of boundary conditions was also mentioned and related to others families in Ref. 3. It is worth mentioning that, in principle, we do not have within (4) all of the boundary conditions included in (2). For example, we do not have the cases where $m_1 + \sin(\phi) = 0$ in (4); nevertheless, if we have

a boundary condition where $m_1 = -\sin(\phi)$, the singularity in Eq. (5) could be conveniently avoided, and the respective boundary condition could thus emerge from Eq. (4) [1].

The following boundary conditions are included in Eqs. (2) and (4). Some of the names that identify these boundary conditions are obvious but others will be justified by studying their respective singular potentials:

(a) The Dirac delta interaction

$$\begin{pmatrix} \psi(0+) \\ \lambda\psi'(0+) \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ -2\frac{m_0}{m_1} & 1 \end{pmatrix} \begin{pmatrix} \psi(0-) \\ \lambda\psi'(0-) \end{pmatrix}, \quad (6)$$

which is obtained by setting: $m_0 = -\cos(\phi)$, $m_1 = \sin(\phi)$ and $m_2 = m_3 = 0$. Note that, by making $\phi = \pi/2$ ($\Rightarrow m_0/m_1 = 0$) in Eq. (6), we obtain the periodic boundary condition, $\psi(0+) = \psi(0-)$ and $\psi'(0+) = \psi'(0-)$.

(b) The first derivative of the Dirac delta interaction

$$\begin{pmatrix} \psi(0+) \\ \lambda\psi'(0+) \end{pmatrix} = \begin{pmatrix} \frac{1+m_3}{m_1} & 0 \\ 0 & \frac{1-m_3}{m_1} \end{pmatrix} \begin{pmatrix} \psi(0-) \\ \lambda\psi'(0-) \end{pmatrix}, \quad (7)$$

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 $\sin(\phi) = 1 \Rightarrow \phi = \pi/2$.

(c) The quasi-periodic interaction

$$\begin{pmatrix} \psi(0+) \\ \lambda\psi'(0+) \end{pmatrix} = \begin{pmatrix} m_1 - im_2 & 0 \\ 0 & m_1 - im_2 \end{pmatrix} \begin{pmatrix} \psi(0-) \\ \lambda\psi'(0-) \end{pmatrix}, \quad (8)$$

which is obtained by making: $m_0 = m_3 = 0 \Rightarrow (m_1)^2 + (m_2)^2 = 1$, $\cos(\phi) = 0$ and $\sin(\phi) = 1 \Rightarrow \phi = \pi/2$. Note that, by making $m_1 = +1$ and $m_2 = 0$ in Eq. (8), we obtain the periodic boundary condition ($\psi(0+) = \psi(0-)$ and $\psi'(0+) = \psi'(0-)$). Likewise, by making $m_1 = -1$ and $m_2 = 0$, we obtain the antiperiodic boundary condition, $\psi(0+) = -\psi(0-)$ and $\psi'(0+) = -\psi'(0-)$.

(d) The so-called ‘‘delta-prime’’ interaction

$$\begin{pmatrix} \psi(0+) \\ \lambda\psi'(0+) \end{pmatrix} = \begin{pmatrix} 1 & -2\frac{m_0}{m_1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \psi(0-) \\ \lambda\psi'(0-) \end{pmatrix}, \quad (9)$$

which is obtained by setting: $m_0 = \cos(\phi)$, $m_1 = \sin(\phi)$ and $m_2 = m_3 = 0$. As in the example of the boundary condition (a), the case $\phi = \pi/2$ ($\Rightarrow m_0/m_1 = 0$) leads to the periodic boundary condition.

(e) The Dirichlet boundary condition

$$\psi(0+) = \psi(0-) = 0, \quad (10)$$

which is obtained by setting: $m_0 = +1$, $m_2 = m_3 = 0$ ($\Rightarrow m_1 = 0$) and $\phi = \pi$.

(f) The Neumann boundary condition

$$\psi'(0+) = \psi'(0-) = 0, \quad (11)$$

which is obtained by setting: $m_0 = +1$, $m_2 = m_3 = 0$ ($\Rightarrow m_1 = 0$) and $\phi = 0$.

It is worth mentioning that, boundary condition (e) is obtained from boundary condition (a) by noticing that

$-2m_0/m_1 = +2 \cot(\phi) = -\infty$ (because $\phi \rightarrow \pi^-$), thus, $\psi(0+) = \psi(0-)$ and $\psi'(0+) = ((-\infty) \times \psi(0-)) + \psi'(0-) \Rightarrow \psi(0-) = 0$, and therefore $\psi(0+) = \psi(0-) = 0$. Likewise, boundary condition (f) is obtained from boundary condition (d) by noticing that $-2m_0/m_1 = -2 \cot(\phi) = -\infty$ (because $\phi \rightarrow 0+$), so $\psi'(0+) = \psi'(0-)$ and $\psi(0+) = \psi(0-) + ((-\infty) \times \psi'(0-)) \Rightarrow \psi'(0-) = 0$, and therefore $\psi'(0+) = \psi'(0-) = 0$.

1.2. Case (ii): point interactions as singular potentials

In this case, one considers the line (\mathbb{R}) with a singular potential at the origin ($x = 0$). The Hamiltonian operator is,

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \hat{V}(x), \quad (12)$$

where $x \in \mathbb{R}$. A plausible formal expression for a general singular potential $\hat{V}(x)$ in terms of the Dirac delta and derivatives d/dx is the following:

$$\begin{aligned} \hat{V}(x) = & g_1 \delta(x) - (g_2 - ig_3) \delta(x) \frac{d}{dx} \\ & + (g_2 + ig_3) \frac{d}{dx} \delta(x) - g_4 \frac{d}{dx} \left(\delta(x) \frac{d}{dx} \right), \end{aligned} \quad (13)$$

where $g_B \in \mathbb{R}$ ($B = 1, 2, 3, 4$) [1, 4]. In this paper, the derivative of the Dirac delta is written as $\delta'(x) \equiv d\delta/dx$, that is, with the prime on the delta. The operator \hat{H} is formally self-adjoint and depends on four real parameters [1]. It has also been proved that every \hat{H} with the singular potential (13) coincides with a certain self-adjoint extension of \hat{h} ; see Ref. 5 and references therein. In other words, any point interaction encoded in the general boundary condition given by Eq. (2) can be described by an operator with a singular potential.

The singular potential $\hat{V}(x)$ can be written in a more symmetric way. For this, one uses the formulas $\psi(0) = \langle \delta, \psi \rangle$ and $\psi'(0) = -\langle \delta', \psi \rangle$. In essence, the latter formulas can be obtained by using the (symbolic) sifting property for the Dirac delta:

$$\delta(x)\psi(x) = \delta(x)\psi(0) = \delta(x)\langle \delta, \psi \rangle \quad (14)$$

$$\left[\Rightarrow \int_{-\infty}^{+\infty} dx \delta(x)\psi(x) = \psi(0) \int_{-\infty}^{+\infty} dx \delta(x) = \psi(0) = \langle \delta, \psi \rangle \right],$$

and

$$\delta(x)\psi'(x) = \delta(x)\psi'(0) = -\delta(x)\langle \delta', \psi \rangle \quad (15)$$

$$\begin{aligned} & \left[\Rightarrow \int_{-\infty}^{+\infty} dx \delta(x)\psi'(x) = \psi'(0) \right. \\ & \left. \times \int_{-\infty}^{+\infty} dx \delta(x) = \psi'(0) = -\langle \delta', \psi \rangle, \right. \end{aligned}$$

because $\delta'(x)\psi(x) = (d/dx)(\delta(x)\psi(x)) - \delta(x)\psi'(x) = \delta'(x)\psi(0) - \delta(x)\psi'(0)$

$$\Rightarrow \left[\int_{-\infty}^{+\infty} dx \delta'(x)\psi(x) = \psi(0) \int_{-\infty}^{+\infty} dx \delta'(x) - \psi'(0) \int_{-\infty}^{+\infty} dx \delta(x) = -\psi'(0) \right]$$

(the common delta function properties

$$\int_{-\infty}^{+\infty} dx \delta(x) = 1$$

and

$$\int_{-\infty}^{+\infty} dx \delta'(x) = 0$$

were also used above). Because functions $\psi(x)$ and $\psi'(x)$ are not generally continuous at $x = 0$, $\psi(0)$ and $\psi'(0)$ may be written as the average at the discontinuity (this is certainly one a plausible choice for discontinuous test functions):

$$\begin{aligned} \psi(0) &\equiv \frac{\psi(0+) + \psi(0-)}{2}, \\ \psi'(0) &\equiv \frac{\psi'(0+) + \psi'(0-)}{2} \end{aligned} \quad (16)$$

(see Ref. 6 for a discussion about situations in which the latter definitions do not hold). Thus, one can also write expression (13) as follows:

$$\begin{aligned} \hat{V}(x) &= g_1 \langle \delta, \cdot \rangle \delta(x) + (g_2 - ig_3) \langle \delta', \cdot \rangle \delta(x) \\ &+ (g_2 + ig_3) \langle \delta, \cdot \rangle \delta'(x) + g_4 \langle \delta', \cdot \rangle \delta'(x), \end{aligned} \quad (17)$$

where $\langle F, \psi \rangle$ (with $F = \delta$ or δ') also denotes the action $F[\psi]$ of the distribution (or linear functional) F on the test function ψ . Note that, if one defines the quantities $t_{00} \equiv g_1$, $t_{01} \equiv g_2 - ig_3$, $t_{10} \equiv g_2 + ig_3 = \bar{t}_{01}$ and $t_{11} \equiv g_4$, then these coefficients $\{t_{pq}\}$ define a 2×2 hermitian matrix [5].

Due to the presence of $\delta(x)$ and $\delta'(x)$ in $\hat{V}(x)$, the Schrödinger equation can yield boundary conditions. In effect, one can use a procedure introduced earlier by Griffiths for the n -th derivative of a delta function potential in the following way [7]: integrating $\hat{H}\psi = E\psi$ from $-\epsilon$ to $+\epsilon$ and taking the limit $\epsilon \rightarrow 0$ gives the following first boundary condition:

$$\begin{aligned} \lambda\psi'(0+) - \lambda\psi'(0-) &= \frac{1}{2}\lambda\alpha g_1 (\psi(0+) + \psi(0-)) \\ &- \frac{1}{2}\alpha(g_2 - ig_3) (\lambda\psi'(0+) + \lambda\psi'(0-)), \end{aligned} \quad (18)$$

where $\alpha \equiv 2m/\hbar^2$. Similarly, integrating $\hat{H}\psi = E\psi$ first from $x = -L$ (with $L > 0$) to x , then once more from $-\epsilon$

to $+\epsilon$ and taking the limit $\epsilon \rightarrow 0$ again, one obtains a second boundary condition:

$$\begin{aligned} \psi(0+) - \psi(0-) &= \frac{1}{2}\alpha(g_2 + ig_3) (\psi(0+) + \psi(0-)) \\ &- \frac{1}{2}\frac{\alpha g_4}{\lambda} (\lambda\psi'(0+) + \lambda\psi'(0-)), \end{aligned} \quad (19)$$

where the relations

$$\int_{-L}^x dy \delta(y) = \Theta(x)$$

($\Theta(x)$ is the Heaviside function: $\Theta(x < 0) = 0$ and $\Theta(x > 0) = 1$) and

$$\int_{-L}^x dy \delta'(y) = \delta(x)$$

should be used. Note that Eqs. (18) and (19) precisely constitute the family of boundary conditions (4), where, in this case, the matrix \hat{S} is

$$\hat{S} = \frac{1}{2}\alpha \begin{pmatrix} \lambda g_1 & -(g_2 - ig_3) \\ g_2 + ig_3 & -\frac{g_4}{\lambda} \end{pmatrix}. \quad (20)$$

By comparing the matrix \hat{S} in Eq. (5) with the matrix \hat{S} in Eq. (20), one obtains the following relations:

$$\frac{1}{2}\alpha\lambda g_1 = \frac{-m_0 + \cos(\phi)}{m_1 + \sin(\phi)}, \quad (21)$$

$$\frac{1}{2}\alpha g_2 = \frac{m_3}{m_1 + \sin(\phi)}, \quad (22)$$

$$\frac{1}{2}\alpha g_3 = \frac{-m_2}{m_1 + \sin(\phi)}, \quad (23)$$

$$\frac{1}{2}\alpha \frac{g_4}{\lambda} = \frac{m_0 + \cos(\phi)}{m_1 + \sin(\phi)}. \quad (24)$$

Thus, if we use Eqs. (21)-(24), we can relate boundary conditions included in (4) with potentials dependent of deltas included in (13) (or (17)). The following potentials correspond respectively to the examples of boundary conditions that were introduced above:

(a) The Dirac delta potential

$$\hat{V}(x) = g_1\delta(x), \quad (25)$$

which is obtained by setting: $m_0 = -\cos(\phi)$, $m_1 = \sin(\phi)$ and $m_2 = m_3 = 0$, thus, (from relations (21)-(24)) $g_1 = 2 \cot(\phi)/\alpha\lambda$ and $g_2 = g_3 = g_4 = 0$. Therefore, (from Eq. (13)) we obtain the result given in Eq. (25). Note that, by making $\phi = \pi/2$, we obtain $g_1 = 0$, and therefore $\hat{V}(x) = 0$.

Also, by making $\phi \rightarrow \pi-$, we obtain $g_1 \rightarrow -\infty$ (this is the case (e), which is presented below).

(b) The first derivative of the Dirac delta potential

$$\hat{V}(x) = g_2 \delta'(x), \quad (26)$$

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 $\sin(\phi) = 1 \Rightarrow \phi = \pi/2$, thus, (from relations (21)-(24)) $g_2 = 2m_3/\alpha(1 + m_1)$ and $g_1 = g_3 = g_4 = 0$. Therefore, (from Eq. (13)) we obtain the result given in Eq. (26). Note that, by making $m_3 = 0 \Rightarrow m_1^2 = 1$, and taking the solution $m_1 = 1$, we obtain $g_2 = 0$, and therefore $\hat{V}(x) = 0$.

(c) The quasi-periodic (or quasi-free) potential

$$\hat{V}(x) = ig_3 \left(2 \frac{d}{dx} \delta(x) - \delta'(x) \right), \quad (27)$$

which is obtained by setting: $m_0 = m_3 = 0 \Rightarrow (m_1)^2 + (m_2)^2 = 1$, $\cos(\phi) = 0$ and $\sin(\phi) = 1 \Rightarrow \phi = \pi/2$, thus, (from relations (21)-(24)) $g_3 = -2m_2/\alpha(1 + m_1)$ and $g_1 = g_2 = g_4 = 0$. Therefore, (from Eq. (13)) we obtain the result given in Eq. (27). It is worth noting that, by making $m_1 = -1$ and $m_2 = 0$, we obtain $g_3 = 0/0$. However, in this case we can write $m_1 = -\sqrt{1 - (m_2)^2}$, and therefore $g_3 = -(2/\alpha) [(2/m_2) - (m_2/2) + O((m_2)^3)]$, which implies that $g_3 \rightarrow -\infty$ when $m_2 \rightarrow 0$ ($\Rightarrow m_1 \rightarrow -1$). Precisely, the latter case corresponds to the antiperiodic boundary condition (see the paragraph that follows Eq. (8)). Likewise, if $m_1 = +1$ and $m_2 = 0$, we obtain $\hat{V}(x) = 0$ (because $g_3 = 0$). Incidentally, the Hamiltonian operator (12) with the potential (27) can also be written as $\hat{H} = (-i(d/dx) - g_3\delta(x))^2 - g_3^2(\delta(x))^2$ ($\hbar^2 = 2m = 1$) [5, 8].

(d) The so-called “delta-prime” interaction potential

$$\hat{V}(x) = -g_4 \frac{d}{dx} \left(\delta(x) \frac{d}{dx} \right), \quad (28)$$

which is obtained by setting: $m_0 = \cos(\phi)$, $m_1 = \sin(\phi)$ and $m_2 = m_3 = 0$, thus, (from relations (21)-(24)) $g_4 = 2\lambda \cot(\phi)/\alpha$ and $g_1 = g_2 = g_3 = 0$. Hence, (from Eq. (13)) we obtain the result given in Eq. (28). Note that, by making $\phi = \pi/2$, we obtain $g_4 = 0$, and therefore $\hat{V}(x) = 0$. Moreover, by making $\phi \rightarrow 0+$, we obtain $g_4 \rightarrow +\infty$ (this is the case (f), which is presented below). It is worth noting that, the general singular potential $\hat{V}(x)$ in Eq. (13) is exactly the sum of the four potentials (25)-(28) [1].

(e) The Dirichlet potential

$$\hat{V}(x) = \lim_{g_1 \rightarrow -\infty} g_1 \delta(x), \quad (29)$$

which is obtained by making: $m_0 = +1$, $m_2 = m_3 = 0$ and $\phi = \pi$, thus, (from relations (21)-(24)) $g_1 = -4/\alpha\lambda m_1$ and $g_2 = g_3 = g_4 = 0$. Also, $m_1 = 0$ and therefore $g_1 = -\infty$ (in fact, $m_1 \rightarrow 0+ \Rightarrow g_1 \rightarrow -\infty$, and $m_1 \rightarrow 0- \Rightarrow g_1 \rightarrow +\infty$). Therefore, (from Eq. (13)) we obtain the result given in Eq. (29). Note that the Dirichlet potential is the Dirac

delta potential with infinite strength, and it can (heuristically) be written in the form $\hat{V}(x) = -\delta(0)\delta(x) = -(\delta(x))^2$.

(f) The Neumann potential

$$\hat{V}(x) = \lim_{g_4 \rightarrow \infty} -g_4 \frac{d}{dx} \left(\delta(x) \frac{d}{dx} \right), \quad (30)$$

which is obtained by setting: $m_0 = +1$, $m_2 = m_3 = 0$ and $\phi = 0$, thus, (from relations (21)-(24)) $g_4 = 4\lambda/\alpha m_1$ and $g_1 = g_2 = g_3 = 0$. Also, $m_1 = 0$ and therefore $g_4 = +\infty$ (in fact, $m_1 \rightarrow 0+ \Rightarrow g_4 \rightarrow +\infty$, and $m_1 \rightarrow 0- \Rightarrow g_4 \rightarrow -\infty$). Therefore, (from Eq. (13)) we obtain the result given in Eq. (30). Note that the Neumann potential is the “delta-prime” interaction potential with infinite strength.

2. Bound States

In this section, we present the (normalized) bound state eigenfunctions and their respective energy eigenvalues corresponding to the examples of point interactions that were introduced above.

(a) For the Hamiltonian with the Dirac delta potential (25), $\hat{V}(x) = g_1\delta(x)$, there exists a single bound state with energy $E < 0$:

$$\psi(x) = \sqrt{-\frac{1}{2}\alpha g_1} \exp\left(\frac{1}{2}\alpha g_1 |x|\right),$$

$$E = -\frac{1}{4}\alpha(g_1)^2, \quad (31)$$

where $g_1 < 0$. This eigenfunction satisfies the boundary condition (6): $\psi(0+) = \psi(0-) \equiv \psi(0)$ and $\lambda\psi'(0+) - \lambda\psi'(0-) = 2 \cot(\phi)\psi(0)$, where $g_1 = 2 \cot(\phi)/\alpha\lambda$. A nice discussion of the Dirac delta potential, which includes the scattering states, can be found in the book by Griffiths [9]. For studies on the completeness of the eigenfunctions in this problem, see Refs. 10 and 11.

(b) For the Hamiltonian with the potential first derivative of the Dirac delta (26), $\hat{V}(x) = g_2\delta'(x)$, there exists the trivial bound state solution ($\psi(x) = 0$) with zero energy $E = 0$, *i.e.*, there is no a non-trivial square integrable solution that satisfies the boundary condition (7): $\psi(0+) = ((1 + m_3)/m_1)\psi(0-)$ and $\psi'(0+) = (m_1/(1 + m_3))\psi'(0-)$, where $g_2 = 2m_3/\alpha(1 + m_1)$ and $(m_1)^2 + (m_3)^2 = 1$. For a concise discussion of this potential, which includes the scattering states, we recommend Ref. 12. For a study that considers the potential $-a\delta(x) + b\delta'(x)$, see Ref. 13. It should be noted that different definitions of the derivative of the delta interaction exist in the literature; see *e.g.* Refs. 6 and 14 and other references quoted therein. Finally, another article that presents a very particular study that involves the same potential $\delta'(x)$ used by us throughout the article can be found in Ref. 15. In the Appendix B, we treat precisely with a different but very natural definition of this potential. However, we do not get a nontrivial bound state in this case either.

(c) For the Hamiltonian with the quasi-periodic potential (27), $\hat{V}(x) = ig_3(2(d/dx)\delta(x) - \delta'(x))$, there also exists the trivial bound state solution with zero energy $E = 0$, where $\psi(0+) = (m_1 - im_2)\psi(0-)$ along with $\psi'(0+) = (m_1 - im_2)\psi'(0-)$ is the corresponding boundary condition (formula (8)), and $g_3 = -2m_2/\alpha(1 + m_1)$ with $(m_1)^2 + (m_2)^2 = 1$. We have not found a complete discussion of the scattering states for this potential (with $m_1 \neq 0$ and $m_2 \neq 0$) in the literature. However, see Refs. 5 and 8 where various aspects related to the boundary condition associated with this potential are discussed.

(d) For the Hamiltonian with the “delta-prime” interaction potential (28), $\hat{V}(x) = -g_4(d/dx)(\delta(x)(d/dx))$, there exists a single odd-parity bound state with energy $E < 0$:

$$\psi(x) = \sqrt{\frac{2}{\alpha g_4}} \operatorname{sgn}(x) \exp\left(-\frac{2}{\alpha g_4} |x|\right),$$

$$E = -\frac{4}{\alpha^3 (g_4)^2}, \tag{32}$$

where $g_4 > 0$ and $\operatorname{sgn}(x)$ is the sign function ($\operatorname{sgn}(x > 0) = +1$ and $\operatorname{sgn}(x < 0) = -1$). This eigenfunction satisfies the boundary condition (9): $\psi(0+) - \psi(0-) = -2 \cot(\phi) \lambda \psi'(0)$ and $\psi'(0+) = \psi'(0-) \equiv \psi'(0)$, where $g_4 = 2\lambda \cot(\phi)/\alpha$. Scattering states arising from this boundary condition were obtained, for example, in Ref. 16 and the most important spectral properties associated with the free Hamiltonian for this boundary condition (as well as with others) were analyzed in [3]. In Ref. 17, it was shown that the boundary condition defining this interaction arises precisely from the potential (28).

(e) Because the Dirichlet potential (29) is obtained from the Dirac delta potential (25) by setting the limit to $g_1 \rightarrow -\infty$, the eigenfunction and the respective energy eigenvalue for the Hamiltonian with the Dirichlet potential can be obtained from (31) by taking the same limit. Thus, we obtain the following formal results:

$$\psi(x) = \lim_{g_1 \rightarrow -\infty} \sqrt{-\frac{1}{2}\alpha g_1} \exp\left(\frac{1}{2}\alpha g_1 |x|\right)$$

$$\equiv \lim_{g_1 \rightarrow -\infty} \psi(g_1, x) \Rightarrow |\psi(x)|^2 = \delta(x),$$

$$E = -\infty, \tag{33}$$

where we have used the following representation of the Dirac delta [18]: $\delta(x) = \lim_{n \rightarrow \infty} (n/2) \exp(-n|x|)$. Clearly, $\psi(x)$ looks like a highly localized state with infinite energy, in fact, it is essentially the square root of the Dirac delta. Despite these results, it is easy to show that the scalar product of $\psi(x)$ with a square integrable function, $f \in \mathcal{H} \equiv \mathcal{L}^2(\mathbb{R})$, vanishes. The latter result implies that the distribution (or linear functional) associated with $\psi(x)$,

$$\psi[f] = \langle \psi, f \rangle = \int_{-\infty}^{+\infty} dx \psi(x) f(x)$$

$$= \lim_{g_1 \rightarrow -\infty} \int_{-\infty}^{+\infty} dx \psi(g_1, x) f(x),$$

is precisely zero. In fact,

$$\psi[f] = \lim_{g_1 \rightarrow -\infty} 2 \sqrt{-\frac{2}{\alpha g_1}} \int_{-\infty}^{+\infty} dx \frac{1}{2} \left(-\frac{1}{2}\alpha g_1\right)$$

$$\times \exp\left(\frac{1}{2}\alpha g_1 |x|\right) f(x)$$

$$= \lim_{g_1 \rightarrow -\infty} 2 \sqrt{-\frac{2}{\alpha g_1}} f(0) = 0. \tag{34}$$

In the last step we used the representation of the Dirac delta that was used to derive Eq. (33), and also the property

$$\int_{-\infty}^{+\infty} dx \delta(x) f(x) = f(0).$$

Thus, we conclude that the eigenfunction is really trivial, *i.e.*, $\psi(x) = 0$ everywhere on \mathbb{R} , and it satisfies the boundary condition (10): $\psi(0+) = \psi(0-) = 0$ (of course, to the system corresponding to the case (i) where the origin is excluded). A similar result to that given in Eq. (34) emerges in the problem of the one-dimensional hydrogen atom. In that case the state $\psi(x)$ corresponds to the (nonexistent) ground state of infinite binding energy [19, 20].

(f) Because the Neumann potential (30) is obtained from the “delta-prime” interaction potential (28) by setting the limit to $g_4 \rightarrow \infty$, the eigenfunction and the respective energy eigenvalue for the Hamiltonian with the Neumann potential can be obtained from (32) by taking the same limit. Thus, we obtain the following results:

$$\psi(x) = 0, \quad E = 0. \tag{35}$$

This is the trivial bound state with zero energy, and it obviously satisfies the boundary condition (11): $\psi'(0+) = \psi'(0-) = 0$.

3. Conclusion

We have presented and examined the bound states for a number of representative examples of (Schrödinger) point interactions, *i.e.*, boundary conditions and singular potentials, that were introduced, related and also discussed, throughout the article. As we have seen, the (attractive) Dirac delta function potential provides an even-parity bound state; this is a well-known fact. If this potential has infinite strength it becomes the Dirichlet potential, and therefore the state must satisfy the Dirichlet boundary condition. Thus, the bound state becomes

trivial in this latter case. Likewise, the labelled as “delta-prime” interaction potential (this is not the first derivative of the Dirac delta potential) also provides a bound state (an odd-parity state). If this potential has infinite strength it becomes the Neumann potential, *i.e.*, the state must satisfy the Neumann boundary condition. However, this state is equal to zero. On the other hand, in our model, the potential first derivative of the Dirac delta function does not provide a non-trivial bound state. If we change the definition of $\delta'(x)$ for a more natural, we do not obtain a nontrivial bound state either. It is worth mentioning that this new potential is also a legitimate point interaction because it corresponds to a boundary condition included in the domain of the (self-adjoint) Hamiltonian \hat{h} (in fact, it is the Dirichlet boundary condition).

Appendix A

In this appendix we study some general aspects that have to do with the eigenvalues and eigenvectors of the Hamiltonian operator given by Eq. (1). More technical details can be found, for example, in Ref. 21.

The Schrödinger equation for the eigenvalues with negative energy $E \equiv -\hbar^2\kappa^2/2m < 0$ and eigenfunctions $\psi(x)$ is: $\hat{h}\psi(x) - E\psi(x) = 0 \Rightarrow \psi''(x) - \kappa^2\psi(x) = 0$, in the region $\Omega \equiv \mathbb{R} - \{0\}$. The solution of this equation has the general form

$$\psi(x) = A \exp(\kappa x) \Theta(-x) + B \exp(-\kappa x) \Theta(x), \quad (A1)$$

where $\kappa = \sqrt{2m(-E)}/\hbar$, $\Theta(x)$ is the Heaviside function, and the constants A and B are related by imposing boundary conditions. We will consider the following four parameters (general) family of boundary conditions, which was obtained from Eq. (2) in Ref. 1:

$$\begin{pmatrix} \psi(0+) \\ \lambda\psi'(0+) \end{pmatrix} = \exp(i\varphi) \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} \psi(0-) \\ \lambda\psi'(0-) \end{pmatrix}, \quad (A2)$$

where

$$a \equiv \frac{m_3 + \sin(\phi)}{\sqrt{(m_1)^2 + (m_2)^2}}, \quad (A3)$$

$$b \equiv \frac{-m_0 - \cos(\phi)}{\sqrt{(m_1)^2 + (m_2)^2}}, \quad (A4)$$

$$c \equiv \frac{-m_0 + \cos(\phi)}{\sqrt{(m_1)^2 + (m_2)^2}}, \quad (A5)$$

$$d \equiv \frac{-m_3 + \sin(\phi)}{\sqrt{(m_1)^2 + (m_2)^2}}, \quad (A6)$$

and

$$\varphi \equiv \tan^{-1} \left(\frac{m_1}{m_2} \right) - \frac{\pi}{2}, \quad (A7)$$

with $(m_0)^2 + (m_1)^2 + (m_2)^2 + (m_3)^2 = 1$ (because $ad - bc = 1$). By imposing on the solution (A1) the boundary conditions

given in Eq. (A2), we find the following homogeneous system of equations (for the constants A and B):

$$\begin{aligned} B &= (a + \lambda\kappa b) \exp(i\varphi) A, \\ \lambda\kappa B &= -(c + \lambda\kappa d) \exp(i\varphi) A. \end{aligned} \quad (A8)$$

Note that, it follows from the equation that is on the left in (A8) (for instance) that the eigenfunctions may be written as

$$\begin{aligned} \psi(x) &= A \left[\exp(\kappa x) \Theta(-x) \right. \\ &\quad \left. + (a + \lambda\kappa b) \exp(i\varphi) \exp(-\kappa x) \Theta(x) \right]. \end{aligned} \quad (A9)$$

Moreover, from Eq. (A8) we obtain the equation for the energy eigenvalues:

$$b(\lambda\kappa)^2 + (a + d)\lambda\kappa + c = 0, \quad (A10)$$

which has the following solutions:

$$\begin{aligned} \lambda\kappa &= -\frac{c}{a + d}, \quad (b = 0); \\ \lambda\kappa &= -\frac{(a + d)}{2b} \pm \frac{\sqrt{(a + d)^2 - 4bc}}{2b}, \quad (b \neq 0). \end{aligned} \quad (A11)$$

Let us suppose that the eigenfunctions have definite parity, *i.e.*, (i) if ψ is an even function, then $\psi(0+) = \psi(0-)$ and also $\psi'(0+) = -\psi'(0-)$; (ii) if ψ is an odd function, then $\psi(0+) = -\psi(0-)$ and also $\psi'(0+) = \psi'(0-)$. These two conditions imply the following relations:

$$a = d, \quad \exp(i\varphi) = 1, \quad (A12)$$

which allow us to rewrite the results given in (A11) as follows:

$$\begin{aligned} \lambda\kappa &= -\frac{c}{2a}, \quad (b = 0); \\ \lambda\kappa &= -\frac{a}{b} \pm \frac{1}{b}, \quad (b \neq 0) \end{aligned} \quad (A13)$$

(in the last expression we also use the fact that $bc = ad - 1$). Note that, by taking the limit $\kappa \rightarrow 0$ in the latter results, we obtain the relation $c = 0$ (see Eq. (A10)). The latter is the necessary condition for the existence of the eigenvalue zero; however, in the case at hand the eigenfunction is trivial (or it is not square integrable).

For example, for the Dirac delta interaction (a) (see Eq. (6)), we have that $a = d = 1$, $b = 0$ and $c = -2m_0/m_1 = \alpha\lambda g_1$ (and also $\varphi = 0$); therefore (from Eq. (A9) and Eq. (A13) with $b = 0$) we obtain the results given by Eq. (31) (we also have to normalize the eigenfunction). Likewise, for the “delta-prime” interaction (d) (see Eq. (9)), we have that $a = d = 1$, $b = -2m_0/m_1 = -\alpha g_4/\lambda$, $c = 0$ (and also $\varphi = 0$); hence (from Eq. (A9) and Eq. (A13) with $b \neq 0$) we obtain the results given by Eq. (32) (again, we also have to normalize the eigenfunction).

Appendix B

In this appendix we explicitly solve the Schrödinger equation for the eigenvalues with negative energy $E \equiv -\hbar^2 \kappa^2 / 2m < 0$ and eigenfunctions $\psi(x)$ in the potential $\hat{V}(x) = g_2 \delta'(x)$, where

$$\delta'(x) = \lim_{N \rightarrow 0} \frac{\delta(x + N) - \delta(x - N)}{2N}, \tag{B1}$$

in the region $\Omega \equiv \mathbb{R}$. That is to say,

$$\begin{aligned} \hat{H}\psi(x) - E\psi(x) &= 0 \Rightarrow \psi''(x) \\ &- \kappa^2\psi(x) = \alpha \hat{V}(x)\psi(x) \tag{36} \\ \Rightarrow \psi''(x) - \kappa^2\psi(x) &= \lim_{N \rightarrow 0} \frac{\alpha g_2}{2N} \\ &\times [\delta(x + N) - \delta(x - N)]\psi(x), \tag{B2} \end{aligned}$$

where $\alpha \equiv 2m/\hbar^2$ (\hat{H} is given by Eq. (12)). As discussed below, the potential $\hat{V}(x)$ defined in this appendix is not exactly the same as that used throughout the article (see potential (b) in Eq. (26)).

Due to the presence of two Dirac deltas in Eq. (B2), $\psi(x)$ must satisfy the following boundary conditions at $x = -N$ and $x = N$, letting $N \rightarrow 0$ at the end:

$$\begin{aligned} \psi((-N)+) &= \psi((-N)-) \equiv \psi(-N), \\ \psi'((-N)+) - \psi'((-N)-) &= \frac{\alpha g_2}{2N} \psi(-N) \tag{B3} \end{aligned}$$

and

$$\begin{aligned} \psi(N+) &= \psi(N-) \equiv \psi(N), \\ \psi'(N+) - \psi'(N-) &= -\frac{\alpha g_2}{2N} \psi(N), \tag{B4} \end{aligned}$$

where $\psi(x \pm) = \lim_{\epsilon \rightarrow 0} \psi(x \pm \epsilon)$ (and the same definition for the derivative ψ'). Notice that boundary conditions (B3) and (B4) tend to the Dirichlet boundary condition, $\psi(0+) = \psi(0-) \equiv \psi(0) = 0$, when $N \rightarrow 0$. Thus, this confirms that we are using a different definition of the first derivative of the Dirac delta interaction to that presented in Sec. I (compare the Dirichlet boundary condition with boundary condition (b) given in Eq. (7)).

The solution of Eq. (B2) has the general form

$$\begin{aligned} \psi(x) &= A \exp(\kappa x) \Theta(-N-x) + B \exp(-\kappa x) \Theta(x - N) \\ &+ [C \exp(\kappa x) + D \exp(-\kappa x)] \\ &\times [\Theta(x + N) - \Theta(x - N)], \tag{B5} \end{aligned}$$

where $\kappa = \sqrt{2m(-E)}/\hbar$, $\Theta(x)$ is the Heaviside function. The following homogeneous system of equations to the constant A, B, C and D is obtained after imposing the boundary conditions (B3) and (B4) on solution (B5), with $N \rightarrow 0$:

$$\begin{pmatrix} \exp(-\kappa N) & 0 & -\exp(-\kappa N) & -\exp(\kappa N) \\ (\kappa N + \frac{\alpha g_2}{2}) \exp(-\kappa N) & 0 & -\kappa N \exp(-\kappa N) & \kappa N \exp(\kappa N) \\ 0 & \exp(-\kappa N) & -\exp(\kappa N) & -\exp(-\kappa N) \\ 0 & (\frac{\alpha g_2}{2} - \kappa N) \exp(-\kappa N) & -\kappa N \exp(\kappa N) & \kappa N \exp(-\kappa N) \end{pmatrix} \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix} = 0. \tag{B6}$$

The cancellation of the determinant of the square matrix in (B6) provides the following equation for the energy eigenvalues:

$$(\kappa N)^2 + \frac{1}{4} \left(\frac{\alpha g_2}{2} \right)^2 [\exp(-4\kappa N) - 1] = 0, \tag{B7}$$

where $N \rightarrow 0$ is understood. Therefore,

$$\begin{aligned} 4\kappa N &= -\ln \left[1 - 4 \left(\frac{2}{\alpha g_2} \right)^2 (\kappa N)^2 \right] \\ &= - \left[-4 \left(\frac{2}{\alpha g_2} \right)^2 (\kappa N)^2 + O(\kappa N)^4 \right], \\ \Rightarrow \kappa \xrightarrow{N \rightarrow 0} \frac{1}{N} \left(\frac{\alpha g_2}{2} \right)^2 &= \infty. \tag{B8} \end{aligned}$$

Finally, the energy corresponding to the bound state is

$$E = \lim_{N \rightarrow 0} -\frac{\kappa^2}{\alpha} = \lim_{N \rightarrow 0} -\frac{1}{\alpha N^2} \left(\frac{\alpha g_2}{2} \right)^4 = -\infty. \tag{B9}$$

Using the two equations in (B6) that are independent of $\alpha g_2/2$, we obtain the constants C and D in terms of A and B ,

$$\begin{aligned} C &= \frac{A - B \exp(2\kappa N)}{1 - \exp(4\kappa N)}, \\ D &= \frac{B - A \exp(2\kappa N)}{1 - \exp(4\kappa N)}. \tag{B10} \end{aligned}$$

For example, substituting these relations into the second equation of (B6), the following relation is obtained:

$$\begin{aligned} B &= A \left[1 + \frac{1 - \exp(-4\kappa N)}{2\sqrt{\kappa N}} \right] \\ &= A \left[1 + 2\sqrt{\kappa N} + 2\kappa N + O(\kappa N)^2 \right], \\ \Rightarrow B \xrightarrow{N \rightarrow 0} A. \tag{B11} \end{aligned}$$

Therefore, the eigenfunction that corresponds to the eigenvalue of infinite energy has the form:

$$\psi(x) = \lim_{\kappa \rightarrow \infty} A \exp(\kappa x), \quad \text{for } x \leq 0; \quad (\text{B12})$$

$$\psi(x) = \lim_{\kappa \rightarrow \infty} A \exp(-\kappa x), \quad \text{for } x \geq 0; \quad (\text{B13})$$

$$\begin{aligned} \psi(x) &= \lim_{\kappa \rightarrow \infty} \lim_{N \rightarrow 0} \lim_{x \rightarrow 0} A \left[\frac{-4 \exp(\kappa N) \sinh(\kappa N)}{1 - \exp(4\kappa N)} \right] \\ &\quad \times \cosh(\kappa x) = \lim_{\kappa \rightarrow \infty} \lim_{N \rightarrow 0} A \left[1 - \kappa N + \frac{1}{3}(\kappa N)^3 \right. \\ &\quad \left. + O(\kappa N)^5 \right] = \lim_{\kappa \rightarrow \infty} A, \quad \text{for } x = 0. \quad (\text{B14}) \end{aligned}$$

That is to say,

$$\begin{aligned} \psi(x) &= \lim_{\kappa \rightarrow \infty} A \exp(-\kappa |x|), \\ &\text{for } -\infty < x < \infty; \quad (\text{B15}) \end{aligned}$$

where $A = \sqrt{\kappa}$ if $\psi(x)$ is normalized. Also note that, because $\delta(x) = \lim_{\kappa \rightarrow \infty} \kappa \exp(-2\kappa |x|)$ [18], then $|\psi(x)|^2 = \delta(x)$. However, $\langle \psi, f \rangle = 0$ for all square integrable function f , therefore $\psi = 0$ in \mathbb{R} . These results are not unexpected since the potential $\hat{V}(x) = g_2 \delta'(x)$, with $\delta'(x)$ given by Eq. (B1), leads to the Dirichlet boundary condition (e). That is, these results are consistent with those for the Dirichlet potential (e). The procedure made in this appendix is close to that made in Ref. 22. Likewise, a very nice and also recent study that discusses the difficulties surrounding the definition of the delta prime potential can be seen in Ref. 23.

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