Impenetrable barriers in quantum mechanics

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We derive the expression $V(x)\,u(x) = c\,\delta(x-a) + v(x)\,u(x)$ (where $V(x)$ is the potential, $u(x)$ the wave function, c a constant and $v(x)$ a finite potential function for $x \leq a$), which is present in the one-dimensional Schrödinger equation on the whole real line when we have an impenetrable barrier at $x \geq a$, that is, an infinite step potential there. By studying the solution of this equation, we identify, connect and discuss three different Hamiltonian operators that describe the barrier. We extend these results by constructing an infinite square-well potential from two impenetrable barriers.

Keywords: Quantum mechanics; Schrödinger equation; impenetrable barriers.

Derivamos la expresión $V(x)\,u(x) = c\,\delta(x-a) + v(x)\,u(x)$ (donde $V(x)$ es el potencial, $u(x)$ la función de onda, c una constante y $v(x)$ una función potencial finita para $x \leq a$), la cual se presenta en la ecuación de Schrödinger unidimensional sobre toda la línea real cuando se tiene una barrera impenetrable en $x \geq a$, es decir, un potencial salto infinito allí. Estudiando la solución de esta ecuación, identificamos, conectamos y discutimos tres diferentes operadores hamiltonianos que describen la barrera. Extendemos estos resultados al construir un potencial de pozo cuadrado infinito a partir de dos barreras impenetrables.

Descriptores: Mecánica cuántica; ecuación de Schrödinger; barreras impenetrables.

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1. Introduction

The topic of this paper is the concept of impenetrable barriers and non-equivalent Hamiltonian operators that attemp to describe these walls. Physically, an impenetrable barrier is a place where an infinite potential barrier exists; thus, we have a singular perturbation there. Mathematically, one usually (and naturally) considers and studies the problem only in the allowed region, and tries to find a (self-adjoint) Hamiltonian. For this operator, one must find adequate boundary conditions for which the probability current on the impenetrable wall vanishes. The Dirichlet boundary condition can be one of these, at least, in non-relativistic quantum mechanics.

In this paper, we are particularly interested in describing a barrier in other ways. First, we need to know the following result, which is used to introduce the subject: Some time ago, Seki examined the elementary problem of a particle in the spherical infinite square-well (or shell) potential: $V(r) = \infty$, $r \geq a$, and $V(r) = 0$, $0 \leq r < a$ (see Ref. 1). It was noted therein that when the radial Schrödinger equation for the S wave

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}u(r) + V(r)\,u(r) = E\,u(r) \tag{1}$$

was integrated from $r = a-\varepsilon$ to $r = a+\varepsilon$, while $\varepsilon \to 0$, the following expression could be written:

$$\lim_{\varepsilon\to 0}\frac{\hbar^2}{2m}u'(a-\varepsilon) + \lim_{\varepsilon\to 0}\int_{a-\varepsilon}^{a+\varepsilon} dr\,V(r)\,u(r) = 0 \tag{2}$$

(since $u'(a+\varepsilon) = 0$, because $u(r \geq a) = 0$ and the integral

$$\int_{a-\varepsilon}^{a+\varepsilon} dr\,u(r)$$

vanishes at the limit). In order to satisfy Eq. (2), it was shown by Seki that the product $V(r)\,u(r)$ should be expressed as

$$V(r)\,u(r) = -\frac{\hbar^2}{2m}u'(a-)\,\delta(r-a). \tag{3}$$

As a result, $V(r)\,u(r)$ must be zero everywhere except at the barrier ($r = a$), where it becomes infinite. This result appears to be consistent with the fact that the solution $u(r)$ must go to zero only in the region $r \geq a$, but $V(r)$ is zero everywhere up to the wall and infinite at the extensive impenetrable barrier ($r \geq a$). Earlier, a boundary potential term such as $V(r)\,u(r) \propto \delta(r-a) + w(r)$ ($w(r) \neq 0$ being finite in $r < a$) was also indicated by Bethe and Goldstone in association with a treatment of hard core potentials in nuclear matter calculations (see Ref. 2 and also Ref. 3 for a succinct repetition of some of the original Bethe and Goldstone calculations). On the other hand, the result expressed in Eq. (3) was specifically demonstrated in Ref. 1 by considering the big impenetrable barrier at $r \geq a$ to be the limit of a (finite) step potential (as the height of the step becomes extremely large).

The paper is planned as follows: In Sec. 2, we present a straightforward and simple derivation of the property $V(x)\,u(x) \propto \delta(x-a)$ (the impenetrable barrier being at the point $x = a = 0$). By considering issues surrounding the well-known problem of a particle in an infinite step potential

($V(x<0)=0$ and $V(x\geq 0)=\infty$), we show that this result can be directly obtained, without using a limiting process (as Seki used). We complement the result obtained in Ref. 1 but in its simplest form (by using only some ordinary properties of the Dirac delta distribution). In Sec. 3, we also present a very simple extension of this procedure with a well potential in the allowed region $x\leq 0$ ($V(x<0)\equiv v(x)\neq 0$). In the course of this demonstration, the two most reasonable but mathematically different Hamiltonian operators associated with the existence of an impenetrable barrier at $x=0$ appear:

(i) the operator $\hat{H}$ (with a singular potential, *i.e.*, infinite, in a huge region) acting on suitable functions $u(x)$ on the interval $-\infty<x<+\infty$ but verifying $u(x\geq 0)=0$ and

(ii) the operator $\hat{h}$ acting on functions $f(x)$ on the interval $-\infty<x\leq 0$ and obeying the Dirichlet boundary condition $f(0)=0$. In Sec. 4, we present another operator:

(iii) the operator $\hat{H}_\delta$ (with a distributional potential satisfying $V(x)\,u(x)\propto u'(0-)\,\delta(x)$) acting on functions $u(x)$ on the interval $-\infty<x<+\infty$ and obeying $u(0)=0$.

We connect these Hamiltonian operators and discuss their differences. In what follows (Sec. 5), we also consider the representative problem of a particle in an infinite square-well potential ($V(0<x<L)=0$ and $V(x\leq 0)=V(x\geq L)=\infty$) and merely use some of the results presented at the beginning to study this system. Finally in Sec. 6, we summarize and discuss the results obtained. We believe that the discussion followed here may complement the standard textbook discussion about one-dimensional potentials and impenetrable barriers as well as some results recently examined about "related confined and global observables" (see Ref. 4 and other references therein).

2. A usual infinite step potential giving a boundary potential term

We start our discussion with the examination of a very common system: a particle of mass m in the one-dimensional step potential, $V(x)=V_0\,\Theta(x)$, where $x\in(-\infty,+\infty)$ and $\Theta(x)$ is the Heaviside function. We look for positive energy solutions to the Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x)+V(x)\,u(x)=E\,u(x). \tag{4}$$

If we write $k\equiv\sqrt{2mE}/\hbar$ and $\alpha\equiv\sqrt{2m(V_0-E)}/\hbar$, the most general solution to this equation is

$$u(x)=a\,\Theta(-x)\,\left(\exp(ikx)+\frac{ik+\alpha}{ik-\alpha}\exp(-ikx)\right)+a\,\Theta(x)\,\frac{2ik}{ik-\alpha}\exp(-\alpha x), \tag{5}$$

which satisfies $u(0-)=u(0+)$ and $u'(0-)=u'(0+)$ for energies $0<E<V_0$, with a a complex constant. Taking the limit of $V_0\to\infty$, we easily obtain

$$u(x)=a\,2i\,\Theta(-x)\,\sin(kx), \tag{6}$$

this expression being a solution to Eq. (4) with the new potential $V(x)=\lim_{V_0\to\infty}V_0\,\Theta(x)$. With this procedure, we have obtained an impenetrable barrier at $x=0$ because $\bar{u}(x)u'(x)$ is real and, as a result, the probability current vanishes at that wall. The solution in (6) is continuous over the real line ($u(0-)=u(0+)=u(0)=0$), but its derivative is discontinuous at $x=0$ ($u'(0-)\neq u'(0+)=0$). As is well known, for a discontinuous function, a term proportional to the Dirac delta function is added to the ordinary derivative. We now write explicitly the two first derivatives of the solution (6):

$$u'(x)=a\,2ik\,\Theta(-x)\,\cos(kx), \tag{7}$$

$$u''(x)=-a\,2ik^2\,\Theta(-x)\,\sin(kx)-a\,2ik\,\delta(x)=-k^2u(x)-a\,2ik\,\delta(x). \tag{8}$$

Note that $u''(x)$ does have a δ-term owing to the discontinuity in $u'(x)$. We made use of the relation $\Theta'(x)=\delta(x)$ and also of one common property of the Dirac delta function $\sin(kx)\delta(x)=\sin(0)\delta(x)=0$ and

$$\cos(kx)\delta(x)=\cos(0)\delta(x)=\delta(x).$$

We used Eq. (6) to finally write (8) as well.

If we substitute $u''(x)$ into the Schrödinger equation: $u''(x)+k^2u(x)=(2m/\hbar^2)\,V(x)\,u(x)$, we obtain the relation

$$V(x)\,u(x)=-\frac{\hbar^2}{2m}a\,2ik\,\delta(x), \tag{9}$$

being precisely $u'(0-)=a\,2ik$ (Note that for a stationary state with energy E, the delta strength is energy dependent, *i.e.*, $u'(0-)\propto\sqrt{E}$). With this simple procedure, the same type of "boundary potential" obtained for Seki's system ($V(r)\,u(r)$ at $r=a$) is also obtained in our system ($V(x)\,u(x)$ at $x=0$).

3. Two Hamiltonian operators describing an impenetrable barrier

First, let us generalize the result given by Eq. (9) by considering the potential

$$V(x)=v(x)\,\Theta(-x)+\lim_{V_0\to\infty}V_0\,\Theta(x), \tag{10}$$

where $v(x<0)<0$, $v(x\to-\infty)\to 0$ and $v(0)=0$, that is, $v(x)$ is a well potential. In this new situation, the solution $u(x)$ to the Schrödinger equation (on the real line)

$$(\hat{H}u)(x)\equiv-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x)+V(x)\,u(x)=E\,u(x) \tag{11}$$

once again vanishes at the origin ($x = 0$) and for $x > 0$ as well. Thus, $u(x)$ has the form

$$u(x) = F(x)\,\Theta(-x). \tag{12}$$

We suppose at this point that the function $F(x)$ and the potential $v(x)$ also have values in the region $x > 0$. However, in the region $x \le 0$, the function $F(x)$ is: $F(x) \equiv f(x)$, which satisfies the equation

$$(\hat{h}\,f)(x) \equiv -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}f(x) + v(x)\,f(x) = E\,f(x) \tag{13}$$

and must fulfill $f(0-) = f(0) = 0$, whereas $u(x)$ satisfies $u(0+) = u(0-) = u(0) = 0$. The energy values satisfy $E_{\min} < E < +\infty$, since $v(x)$ is bounded from below and the allowed energies must exceed a $v_{\min}$ value.

As usual, one must assume that the operator $\hat{H}$ introduced in (11) (and describing a particle on the whole real line $-\infty < x < +\infty$ but permanently living in the region $x \le 0$) acts on functions $u(x)$ belonging to the Hilbert space of square-integrable functions $L^2(\Re)$, that is, $\|\,u\,\| < \infty$ (with the usual definition of the norm $\|\,u\,\| = \sqrt{\langle\,u,u\,\rangle}$, where the scalar product of two functions is

$$\langle\, f,g\,\rangle = \int\limits_{\Re} dx\,\bar{f}g \quad).$$

The function $(\hat{H}u)(x)$ is also normalizable, that is, $\left\|\hat{H}u\right\| < \infty$. Moreover, $u(x)$ has a continuous derivative and $u'(x)$ is not only continuous but also is absolutely continuous (roughly speaking, a function is absolutely continuous if it is the integral of its derivative), $i.e.$, we say that $u(x)$ belongs to $AC^2(\Re)$ and, moreover, $u(x \ge 0) = 0$. The space of functions $u(x)$ satisfying all these requirements is a "natural" domain for $\hat{H}$: $D(\hat{H})$. With the potential given by Eq. (10), we automatically have $u(x \ge 0) = 0$; but supposing that there is no an infinite potential at the region $x \ge 0$, the boundary condition $u(x) = 0$ for all $x \ge 0$ mathematically characterizes an impenetrable barrier there. In Appendix A we gathered some (technical) results about this non self-adjoint Hamiltonian operator (specifically, with the domain that we have written above).

On the other hand, the operator $\hat{h}$ in Eq. (13) describes a particle living on the half line $x \le 0$ and acts on functions $f(x)$ belonging to the Hilbert space $L^2(\Omega)$ with $\Omega = (-\infty, 0] \subset \Re$, thus, $\|\,f\,\| < \infty$, in the same way, we must add to $D(\hat{h})$ the conditions $\left\|\hat{h}f\right\| < \infty$, with $f(x)$ belonging to $AC^2(\Omega)$ and obeying the Dirichlet boundary condition $f(0) = 0$ (in this last case, the scalar product in the definition of the norm is obtained by integrating on the new interval Ω).

From expression (12), we can easily write $u''(x)$ (but first $u'(x) = F'(x)\,\Theta(-x)$, since $\Theta'(-x) = -\delta(x)$ and $F(x)\,\delta(x) = F(0)\,\delta(x) = 0$):

$$\begin{aligned} u''(x) &= F''(x)\,\Theta(-x) + F'(x)\,\Theta'(-x) \\ &= -\frac{2m}{\hbar^2}(E - v(x))\,F(x)\,\Theta(-x) - F'(x)\,\delta(x), \end{aligned} \tag{14}$$

where we have used Eq. (13) and $\Theta'(-x) = -\delta(x)$ again. We can go further with $u''(x)$ by using Eq. (12), $F'(x)\,\delta(x) = F'(0)\,\delta(x)$. At this point, $F'(x)$ must be considered as a continuous function at $x = 0$, and $u'(0-) = F'(0-) = F'(0)$. Note that, $F'(x)$ is in fact only relevant in the region $x \le 0$, that is, $u'(0+) = 0$; on the other hand, $u'(0) = F'(0)\,\Theta(0)$ cannot be defined since $\Theta(-x)$ is not defined at $x = 0$. Eq. (14) becomes

$$u''(x) - \frac{2m}{\hbar^2}v(x)\,u(x) + u'(0-)\,\delta(x) = -\frac{2m}{\hbar^2}E\,u(x). \tag{15}$$

By comparing this expression with the Schrödinger equation (11) (in the potential given by Eq. (10)), we finally obtain

$$V(x)\,u(x) = v(x)\,u(x) - \frac{\hbar^2}{2m}u'(0-)\,\delta(x), \tag{16}$$

which is a generalization of the result obtained in Eq. (9).

4. Another Hamiltonian operator for an impenetrable barrier

Let us consider the Schrödinger equation on the whole real line:

$$(\hat{H}_\delta\,u)(x) \equiv -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) + V(x)\,u(x) = E\,u(x) \tag{17}$$

with the potential term given by Eq. (16). Clearly, Eq. (17) is precisely the differential equation (15), however, with its solution $u(x)$ satisfying the Dirichlet boundary condition $u(0+) = u(0-) = u(0) = 0$. Since the wall is placed at $x = 0$, we impose preliminarily only this condition on the solutions to Eq. (17). As is well known, due to the delta interaction in Eq. (17), this equation can be turned into boundary conditions. In fact, integrating it from $-\varepsilon$ to $+\varepsilon$ yields

$$\begin{aligned} -\frac{\hbar^2}{2m}(u'(+\varepsilon) - u'(-\varepsilon)) + \int\limits_{-\varepsilon}^{+\varepsilon} dx\,v(x)\,u(x) - \frac{\hbar^2}{2m}u'(0-) \\ = E\int\limits_{-\varepsilon}^{+\varepsilon} dx\,u(x), \end{aligned} \tag{18}$$

where we also used the delta function property

$$\int\limits_{-\varepsilon}^{+\varepsilon} dx\,\delta(x) = 1.$$

Taking the limit $\varepsilon \to 0$, we get the following boundary condition:

$$u'(0+) = 0. \tag{19}$$

Likewise, integrating Eq. (17) first from $x = -L$ (with $L > 0$) to x and then once more from $-\varepsilon$ to $+\varepsilon$ gives

$$-\frac{\hbar^2}{2m}(u(+\varepsilon) - u(-\varepsilon)) + \frac{\hbar^2}{2m}u'(-L)\int_{-\varepsilon}^{+\varepsilon} dx + \int_{-\varepsilon}^{+\varepsilon} dx \int_{-L}^{x} dy\, v(y)\, u(y) - \frac{\hbar^2}{2m}u'(0-)\int_{-\varepsilon}^{+\varepsilon} dx\Theta(x) = E\int_{-\varepsilon}^{+\varepsilon} dx \int_{-L}^{x} dy\, u(y). \tag{20}$$

In the limit $\varepsilon \to 0$, we obtain

$$u(0+) = u(0-), \tag{21}$$

which is not an unexpected boundary condition. What can be obtained from all this? If we impose on a general solution $u(x)$ (but with $x \geq 0$) the starting Dirichlet boundary condition ($u(0+) = 0$) together with Eq. (19) ($u'(0+)$=0), we necessarily get $u(x \geq 0) = 0$. In fact, the solution in the region $x > 0$ could be written in the form $u(x) = a\, u_1(x) + b\, u_2(x)$, where a and b are complex constants. The solutions $u_1(x)$ and $u_2(x)$ are linearly independent and satisfy the following Wronskian relation in that region: $u_1(x)\, u_2'(x) - u_2(x)\, u_1'(x) \neq 0$. By imposing the two boundary conditions we have mentioned in this regard, one obtains a homogeneous system: $a\, u_1(0+) + b\, u_2(0+) = 0$, $a\, u_1'(0+) + b\, u_2'(0+) = 0$, the determinant of which cannot be zero due to the Wronskian relation, so the only solution is the trivial one; for the region in question, of course. On the other hand, the solution to Eq. (17) in the region $x \leq 0$ vanishes at $x = 0$ but its derivative does not, *i.e.*, $u'(0-) \neq 0$; for this reason, we have a non trivial solution on the negative real semi-axis.

In conclusion, the solutions to the Schrödinger equation (17) (on the whole real axis), with the "boundary potential" term given by Eq. (16) (and a regular well potential at $x \leq 0$) and satisfying only the Dirichlet boundary condition at $x = 0$, *i.e.*, $u(0) = 0$ (this boundary condition is considered a critical part of the domain of $\hat{H}_\delta$) must be written as $u(x) = F(x)\,\Theta(-x)$, where $F(x)$ satisfies the Schrödinger equation (13) on the half line $x \leq 0$. We identified this function in that region as $F(x) \equiv f(x)$ with potential $v(x)$ and satisfies $F(0) = 0$. In this manner, the delta term or point interaction in Eq. (16), with $u(0) = 0$ situates the extensive infinite wall on the right-hand side of the real axis. If we change the term: $-u'(0-)\,\delta(x) \to +u'(0+)\,\delta(x)$ (see Eq. (18) and subsequent comments), the impenetrable barrier could be placed on the left-hand side of the real axis; this simple result will be useful in constructing an infinite square-well potential in Sec. 5 of this paper.

Finally, it is worth while (and important) to insist that we obtain the same solution (12) from the Schrödinger eigenvalue equation (11) (with operator $\hat{H}$) as well as from Eq. (17) (with operator $\hat{H}_\delta$). These two different Hamiltonian operators (with their corresponding singular potentials) are essentially equivalent because, in this situation, they lead to equal results. On the other hand, the formal operator $\hat{H}_\delta$ with its heuristic perturbation at the origin is certainly not a proper operator in $L^2(\Re)$, that is, $\left\|\hat{H}_\delta u\right\| = \infty$. In fact, with $v(x) = 0$,

$$\left\|\hat{V}u\right\|^2 = \|\, Vu \,\|^2 = \lim_{g\to\infty} g\,(\hbar^2/2m)^2 |\, u'(0-)\,|^2 = \infty;$$

thus, it is not strictly correct to write $\hat{H}_\delta$ with the distributional potential given by Eq. (16). Nevertheless, our $\hat{H}_\delta$ yields a solution [Eq. (12)] that makes sense quantum mechanically. The operator $\hat{H}_\delta$ (with the boundary potential term $V(x)\,u(x) \propto u'(0-)\,\delta(x)$) acting on (suitable) functions $u(x)$ satisfying $u(x = 0) = 0$, is not self-adjoint. We provide some mathematical details in Appendix B.

The operator $\hat{h}$ (defined to act on an appropriate set of functions belonging to $L^2(\Omega)$) does not have this kind of problem. Notably, however, when we use $\hat{h}$, there is not a consistent canonical quantization procedure (that can be carried out in the interval Ω, see Ref. 4). Indeed, for a particle on a half-line, there is no (self-adjoint) momentum operator of the form $\hat{p} \equiv -i\hbar(d/dx)$ (see, for example, Refs. 4 and 5); nevertheless, the operator $\hat{h} \neq (\hat{p})^2/2m$ (with the domain given by $D(\hat{h})$) is self-adjoint (see, for example, Refs. 5, 6 and 7). This last requirement appears to be the most important reason for using the operator $\hat{h}$, since the particle can only be in the region $x \leq 0$ in the end.

5. Construction of an infinite square-well potential

In this same framework, what can we say about the infinite square-well potential, *i.e.* two infinite walls which are separated by a distance L? By supposing that the walls are placed at $x = 0$ and $x = L$, which implies

$$V(x) = \lim_{V_0\to\infty} V_0\,(\Theta(-x) + \Theta(x - L)),$$

we can throw away the Schrödinger equation on the whole real axis with this infinite square-well potential. That is, we can discard a non-self-adjoint Hamiltonian operator $\hat{H}$ (see Ref. 8) with the "strong" boundary condition $u(x \leq 0) = u(x \geq L) = 0$ inside its domain $D(\hat{H})$ and replace it with the following:

$$(\hat{H}_\delta\, u)(x) \equiv -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) + V(x)\,u(x) = E\,u(x) \tag{22}$$

(also on the real line), where the boundary potential term is given by

$$V(x)\,u(x) = \frac{\hbar^2}{2m}(u'(0+)\,\delta(x) - u'(L-)\,\delta(x - L)) \tag{23}$$

(we took the potential zero inside the interval $(0, L)$, *i.e.*, $v(x) = 0$) and the solution $u(x)$ satisfies the Dirichlet boundary condition $u(0) = u(L) = 0$. Consequently, this solution has the form $u(x) = F(x)\,(\Theta(x) - \Theta(x - L))$, where $F(x) \equiv f(x)$ specifically satisfies the free Schrödinger equation on the one-dimensional box ($0 \leq x \leq L$)

$$(\hat{h}\, f)(x) \equiv -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} f(x) = E\, f(x), \qquad (24)$$

and also satisfies the Dirichlet boundary condition $f(0) = f(L) = 0$. We know without a doubt which the eigenfunctions of the Hamiltonian $\hat{h}$ are in this traditional case.

6. Discussion and summary

We have seen that an impenetrable barrier is a singular potential, *i.e.*, infinite, on some extremely large region contained in $\Re$. Mathematically, we can characterize this large, solid, impenetrable barrier by the wave function vanishing in that extremely large region. Since the particle is actually confined to the rest of the whole real line, one can study the problem only in that region (the allowed region) and the wave function is zero only on the solid wall. Certainly, this is a usual and natural procedure and we do not need a singular potential in this case. Besides, the representative Hamiltonian operator for the confined particle in this region is self-adjoint with the Dirichlet boundary condition and also with other several types of boundary conditions (see, for example, Ref. 6). As we have demonstrated, an impenetrable barrier is also a distributional (singular potential) at the wall with a very precise strength (see Eq. (16)). With the wave function vanishing there, the corresponding Hamiltonian operator is not self-adjoint (it is not also a proper operator, as was explained early). Thus, we have identified three Hamiltonian operators which describe an impenetrable barrier at a point in $\Re$ ($\hat{h}$), or in a big region contained in $\Re$ ($\hat{H}$ and $\hat{H}_\delta$). As we have seen, these ideas also work when we have several impenetrable barriers on the real line, specifically, when we have two impenetrable barriers for building an infinite square well (a box). We believe that the subject may be of interest to teachers and students of quantum mechanics; to our knowledge, it has not been sufficiently discussed in quantum mechanics textbooks.

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Appendix A

The (Hamiltonian) operator $\hat{H}$ has a natural domain (for simplicity's sake, we shall consider only the "free" Hamiltonian, *i.e.*, $v(x) = 0$, and naturally we take the impenetrable barrier as a boundary condition in the region $x \geq 0$):

$$D(\hat{H}) = \{u | u \in L^2(\Re),\ u \in AC^2(\Re),$$
$$(\hat{H}u) \in L^2(\Re),\ u(x \geq 0) = 0\},$$

however, this operator is not self-adjoint; to check this, we use some results obtained in Ref. 9. In fact, we can write any $u \in L^2(\Re)$ (and $u \in AC^2(\Re)$) as:

$$u(x) = u_1(x)\,\Theta(-x) + u_2(x)\,\Theta(x),$$

where $u_1(x)$ and $u_2(x)$ belong to $L^2(\Re)$ and $AC^2(\Re)$. Hence, a boundary condition like $u(x \geq 0) = 0$ can be obtained from $u_1(x = 0) = 0$ and $u_2(x{=}0){=}u_2'(x{=}0){=}0$. It could be useful to read the discussion that follows Eq. (21). However, this boundary condition is not included in any of the boundary conditions that are self-adjoint to the globally defined Hamiltonian. All these (confining and transversal) boundary conditions can be written as the following (see Eq. (80) in Ref. 9):

$$\begin{pmatrix} u_1'(0) - \frac{\sqrt{2}}{2}(1 - i)\, u_1(0) \\ u_2'(0) + \frac{\sqrt{2}}{2}(1 - i)\, u_2(0) \end{pmatrix} = U \begin{pmatrix} u_1'(0) - \frac{\sqrt{2}}{2}(1 + i)\, u_1(0) \\ u_2'(0) + \frac{\sqrt{2}}{2}(1 + i)\, u_2(0) \end{pmatrix},$$

where U is a 2×2 unitary matrix and as a result, there is a four parameter family of boundary conditions.

Appendix B

The operator $\hat{H}_\delta$ with the boundary potential term $V(x)\,u(x) \propto u'(0-)\,\delta(x)$ acting on (suitable) functions $u(x)$ satisfying $u(x = 0) = 0$, is not self-adjoint. Essentially, this is because the boundary conditions (19) and (21), supplemented with $u(0) = 0$ ($\Rightarrow u(x \geq 0) = 0$), do not coincide with any included in the families of (confining) suitable boundary conditions at the origin and belonging to the domain of the (globally) extended self-adjoint operator $\hat{H}$ in $L^2(\Re)$. See these specific extensions in Eq. (93) of Ref. 9. Certainly, these confining extensions (without the condition $u(x \geq 0) = 0$) could be written in terms of boundary potentials; nevertheless, neither of these should lead to the boundary condition $u(x \geq 0) = 0$ if the two formulations are equivalent.

The problem of infinite walls and confined systems in the context of deformation quantization, as well as in standard quantum mechanics, was initially studied in Ref. 10. The results given by Eq. (16) with $v(x) = 0$ (and also Seki's results) bear a certain resemblance to Dias and Prata's, although ours were obtained in a much simpler manner. They prefer to write the product $V(x)\,u(x)$ in terms of the derivative of a particular Dirac delta function. For instance, Dias and Prata's expression can be obtained from our Eq. (16) if one introduces, as they did in Ref. 11, a new distribution $u'(0-)\,\delta(x) \equiv u'(x-)\,\tilde{\delta}(x)$ which also obeys the Dirac delta property $u'(x-)\,\tilde{\delta}(x) = -u(x-)\,\tilde{\delta}'(x)$; in fact,

$$V(x)\,u(x) = -\frac{\hbar^2}{2m}u'(0-)\,\delta(x)$$
$$= -\frac{\hbar^2}{2m}u'(x-)\,\tilde{\delta}(x) = +\frac{\hbar^2}{2m}u(x-)\,\tilde{\delta}'(x).$$

Note that the presence of this kind of distribution is required because we do not define, in general, the product of the usual Dirac delta $\delta(x)$ with a function which is discontinuous, as is the function $u'(x)$ at $x = 0$ (See Ref. 12). In any case, the product $V(x)\,u(x)$ in our approach, as well as in Dias and Prata's initial formulation, leads to the boundary condition $u(x \geq 0) = 0$ (in the problem of a particle on the whole real line but permanently living on the half-line $x \leq 0$) [10], and (the two formulations) could be considered to be equivalent for this reason alone.

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