Revista Brasileira de Ensino de Física, vol. 46, e20230316 (2024)
www.scielo.br/rbef
DOI: https://doi.org/10.1590/1806-9126-RBEF-2023-0316

Did you really miss a Delta function here?

Você esqueceu mesmo uma função Delta?

M. Amaku[1,2], F.A.B. Coutinho[*1,3], P.C.C. dos Santos[1], E. Massad[1,3]

[1]Universidade de São Paulo, Faculdade de Medicina, São Paulo, SP, Brasil.
[2]Universidade de São Paulo, Faculdade de Medicina Veterinária e Zootecnia, São Paulo, SP, Brasil.
[3]Fundação Getúlio Vargas, Escola de Matemática Aplicada, Rio de Janeiro, RJ, Brasil.

Received on October 23, 2023. Revised on December 20, 2023. Accepted on December 22, 2023.

This is the third article in a series dedicated to examining the use of the delta function in the physics literature. Here we discuss the appearance of a delta function in the second derivative of the wave function if its derivative is discontinuous. When this happens it is often claimed in the literature that the proposed wave function must be eigenfunction of an operator that contains a delta function and, in some cases, it is rejected. We study in this paper what we believe are alternatives ways to deal with this situation.
Keywords: Dirac delta function, time independent Schrodinger equation.

Este é o terceiro artigo de uma série dedicada a examinar o uso da função delta na literatura física. Aqui discutimos o aparecimento de uma função delta na segunda derivada da função de onda se a sua derivada for descontínua. Quando isto acontece, é frequentemente afirmado na literatura que a função de onda proposta deve ser uma função própria de um operador que contém uma função delta e, em alguns casos, é rejeitada. Neste artigo estudamos o que consideramos serem formas alternativas de lidar com esta situação.
Palavras-chave: Função delta de Dirac, equação de Schrodinger independente do tempo.

1. Introduction

The use of the Dirac delta function in an intuitive way is found very often in the literature, more often in the literature dedicated to the teaching of Physics. But the intuitive use of the Dirac delta function may lead to some wrong statements as we have been discussing in this series of papers [1, 2]. In this paper we present yet another interesting problem that can lead to errors.

There are two ways to view the time independent Schrodinger (TISE). Take for example the TISE for a particle moving on the line under the influence of some potential $V(x)$

$$H\psi = E\psi \tag{1}$$

or more explicitly

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\psi(x) = E\psi(x). \tag{2}$$

The most common point of view found in the literature is to consider that the TISE is a differential equation that must be solved satisfying some mysterious boundary conditions and finding out the values of E for which the solution satisfy these boundary conditions.

Another one is to consider the $\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]$ as an operator acting on functions that belong to some class of functions that is the domain of the operator. From this point of view the boundary conditions are included automatically in the definition of the operator domain and so the boundary conditions are not arbitrary. As we shall see the domain of the operator must be such that makes it self- adjoint. We shall expand on this on section 4 of this paper.

Suppose someone, following the first point of view, solves the time independent Schrodinger (TISE) equation and finds a solution that has, for example, the first derivative discontinuous. Then one can hear (awfully frequently) that since "as is well known the second derivative will have a delta function at the point of discontinuity and so the TISE equation is not satisfied".

There is an immediate problem with this statement. As we will see, if the potential in the TISE has an infinite discontinuity, then the derivative of the solution of the TISE equation may have a discontinuity. But potentials with discontinuities are very common in the examples presented to students. We shall see some examples in this paper but to warm, from the top of our heads, up we can say that the infinite square well potential is an example (see below). In section 2 we present an overview of the papers dealing with discontinuities in the potential and its effect on the wave function. Then in section 3 we present some examples where the discontinuity of the first derivative is not obvious. In section 4 we briefly review operator theory needed to understand the arguments presented in section 5.

*Correspondence email address: coutinho@dim.fm.usp.br

We show that the sentence in the title of this paper should be answered "Really, you got to be kidding. Not so fast because maybe you are the one that is wrong."

In fact, from the second point of view, as we shall see in detail, the domain of the operator may include functions or derivatives of functions with the discontinuity and there is no need to talk about delta function.

The reader can easily work out the case of the infinite square well potential defined

$$V(x) = \begin{cases} \infty & \text{for } -\infty < x < -L \\ 0 & \text{for } -L \leq x \leq L \\ \infty & \text{for } L < x < \infty \end{cases}. \tag{3}$$

This **potential** has discontinuities at $x = -L$ and $x = L$ and the **first** derivative of the wave function has discontinuities at those points. So naïve use of the Dirac function concludes that the usual solution, found in almost every book on quantum mechanics, is not a solution of the TISE because the second derivative of the wave functions has delta functions at $-L$ and L. (If the reader is intrigued by this he/she can see a solution, different from the considerations carried out in this paper, in [2]).

Other more complicated case will be discussed later, but first let's discuss some other results found in the literature about the wave function at discontinuities of the potential.

2. Some Results Found in the Literature About the Behavior of the Wave Function and its Derivative at Singular Points

The first result we want to discuss is given in a beautiful paper by David Branson [3]. He discusses the continuity of the wave function and of its derivative at points where the potential is discontinuous and concludes the **wave functions** must be continuous. His complete result is the justification of the two results found in the literature:

a) If the discontinuity is finite then both the wave function and its derivative are continuous
b) If the discontinuity is infinite the wave function must vanish at this point

These results are discussed by M. Andrews [4] from a more physical point view, but we consider Branson's paper [3] more general.

The second result is by D. Home and S. Sengupta [5]. They examine the discontinuity of the first derivative of the wave function in a few cases by imposing that the **momentum operator** must be self-adjoint. He examines the cases of the infinite square well potential, the Dirac Delta function potential and the one-dimensional Coulomb Potential.

These results however are not general enough and not totally correct. The principles of quantum mechanics require **only** that the operator H in its domain to be self-adjoint.

The paper by T. Cheon and T. Shigehara [6] discuss in simple language how to produce wave functions that are discontinuous without violating self-adjointness.

3. Examples of Questionable Statements

3.1. The infinite spherical square well [7]

The radial part of the TISE for the infinite square well, of radius a, in polar coordinates is

$$\frac{d^2R_\ell(r)}{d^2r} + \frac{2}{r}\frac{dR_\ell(r)}{dr} + \left(k^2 - \frac{\ell(\ell+1)}{r^2}\right)R_\ell(r) = 0, \tag{4}$$

where $k = \sqrt{2m\frac{E}{h}}$, $0 < r < a$, and its general solution is [7]

$$R_\ell(r) = Aj_\ell(kr) + Bn_\ell(kr), \tag{5}$$

where $j_\ell(kr)$ and $n_\ell(kr)$ are the spherical Bessel and spherical Neumann functions of order ℓ. For $\ell \neq 0$ the Neumann solution is unacceptable because it is not square integrable, but for $\ell = 0$ the Neumann solution is integrable.

In the literature there are innumerous arguments for abandoning the $\ell = 0$ Neumann solution. Most of these arguments rest upon the claim that the $\ell = 0$ Neumann wave function produces a delta function in the origin. We shall examine other arguments at the end of this section.

The arguments involving the delta function were put forward by Mohammad Khorrami [8], Antonio Prados and Calos A. Plata [9] and by Jorge Munzenmayer and Derek Frydel [10]. The argument is that when we calculate the Laplacian of the Neumann function

$$\begin{aligned} -\nabla^2((n_0(kr)) &= -\nabla^2\left(\frac{\cos(kr)}{kr}\right) \\ &= \frac{-\nabla^2(\cos(kr))}{kr} - 2(\nabla\cos(kr)) \\ &\quad \cdot\left[\nabla\left(\frac{1}{kr}\right) - \cos(kr)\nabla^2\left(\frac{1}{kr}\right)\right] \\ &= \frac{k\cos(kr)}{r} + \frac{4\pi}{k}\delta(\mathbf{r}) = k^2\,n_0(kr) + \frac{4\pi}{k}\delta(\mathbf{r}) \end{aligned} \tag{6}$$

and hence the appearance of the $\frac{4\pi}{k}\delta(\mathbf{r})$ shows that $n_0(kr)$ is not a solution of the Schrodinger equation.

In fact, equation (4) is the result of transforming to spherical polar coordinates. Since this transformation is singular at the origin, we can define the domain of the operator to be functions on the **open interval** $(0, \infty)$ that are square integrable in this interval. Note that to include zero do not alter the value of the integral that proves that this solution is square integrable, technically $L^2(0, \infty) = L^2[0, \infty)$. Taking the open interval eliminates the delta function. If, however we include the zero for the functions that are the domain of the operator then self-adjointness demands $R(r = 0) = 0$, but if we exclude the origin other self-adjoint extensions are possible. This is a rather technical and **mysterious** point that will be discussed in the section 5 of this paper.

3.2. Singular behavior of the Laplace operator in Polar spherical coordinates

In a series of papers [11–13], the authors claim that not only the solutions of the TISE equation may have unnoticed delta functions, but the differential expressions of the equation may have "unnoticed" delta functions.

They consider the transformation of the Laplacian in cartesian coordinates to polar spherical coordinates and conclude that unless you impose an extra-condition to the radial part of the wave function you get a non-solution. They notice that the solution to the TISE in polar coordinates can be written in two forms, viz.

$$\Psi(r) = R_\ell(r)\Upsilon_\ell^m(\theta,\varphi) \tag{7}$$

or we can write

$$\Psi(r) = \frac{u_\ell(r)}{r}\Upsilon_\ell^m(\theta,\varphi). \tag{8}$$

In the above expressions $\Upsilon_\ell^m(\theta,\varphi)$ are spherical harmonics. The problem, according to the authors appears when you try to write an equation for $u_\ell(r)$. The equation for $R_{\ell=0}(r) = R(r)$ is

$$\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr} + \frac{2m}{\hbar^2}(E - V(r))R = 0. \tag{9}$$

Making the substitution $R(r) = \frac{u_{\ell=0}(r)}{r} = \frac{u(r)}{r}$, we get

$$\begin{aligned}\frac{1}{r}\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)u(r) + u(r)\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\frac{1}{r}\\ + 2\frac{du}{dr}\frac{1}{r} + \frac{2m}{\hbar^2}\left(E - V(r)\right)\frac{u}{r} = 0.\end{aligned} \tag{10}$$

The first derivatives disappear, and we are left with

$$\begin{aligned}\frac{1}{r}\left(\frac{d^2}{dr^2}\right)u(r) + u(r)\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\frac{1}{r}\\ + \frac{2m}{\hbar^2}\left(E - V(r)\right)\frac{u}{r} = 0.\end{aligned} \tag{11}$$

The term

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\frac{1}{r} = \frac{1}{r}\frac{d^2}{dr^2}\left(r\frac{1}{r}\right) = 0. \tag{12}$$

So that we get

$$\frac{d^2u(r)}{dr^2} + \frac{2m}{\hbar^2}(E - V(r))u(r) = 0. \tag{13}$$

But the relation (12) is only valid for $r \neq 0$. If we include the point $r = 0$, that the authors claim to be essential based on the fact that the equation in rectangular coordinates do include this point, equation (12) becomes

$$\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)\frac{1}{r} = -4\pi\delta^3(\mathbf{r}), \tag{14}$$

because the operator $\left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr}\right)$ is the radial part of the Laplacian and as is well known $\nabla^2\left(\frac{1}{r}\right) = -4\pi\delta^3(\mathbf{r})$.

Then equation (11) becomes

$$\frac{1}{r}\left(\frac{d^2}{dr^2}\right)u(r) - u(r)4\pi\delta^3(\mathbf{r}) + \frac{2m}{\hbar^2}(E - V(r))\frac{u}{r} = 0. \tag{15}$$

Note that at this point we cannot multiply equation (15) by r to take advantage of the fact that $r\delta^3(\mathbf{r}) = 0$ cannot be used because we would get $0 = 0$. One is then forced, according to the authors, to conclude that $u(r = 0) = 0$ to eliminate the spurious delta.

Again, the problem here is that the transformation to polar coordinates is singular. As show in the section 4 of this paper, the use of polar coordinates **essentially** excludes the origin and then we can or cannot put the delta function and if we decide to put it, we eliminate it by requiring the wave function vanishes at the origin. In fact, we must require that $\lim_{r\to 0} u(r) = 0$.

3.3. The infinite spherical square well again

A paper by Jorge Munzenmayer and Derek Frydel [10] also consider the Neumann solution of the TISE and find equation (6) and conclude that the Neumann solution is not a solution of the TISE. But then they ask themselves what is the equation that has the Neumann function as solution. To answer this, they manipulate equation (6) as follows

$$\left[-\nabla^2 - \frac{4\pi}{k}\frac{\delta(\mathbf{r})}{n_0(kr = 0)}\right]n_0(kr) = k^2 n_0(kr). \tag{16}$$

Since as r approaches $r = 0$ the Neumann function $n_0(kr)$ behaves as $\frac{1}{kr}$ they write equation (16) as

$$\left[-\nabla^2 - 4\pi r\delta(\mathbf{r})\right]n_0(kr) = k^2 n_0(kr). \tag{17}$$

To conclude that the origin of the divergence in $n_0(kr)$ as r approaches zero is that there is a hidden potential for $r = 0$, which is

$$V(r) = -4\pi r\delta(\mathbf{r}). \tag{18}$$

They argue that since $r\delta(\mathbf{r}) = 0$ this potential should be considered invisible. But, since the matrix element of this $V(r)$ is infinite, viz.

$$\langle|V|\rangle = \int_0^\infty \left(-4\pi r\delta(\mathbf{r})\right)\left(n_0(kr)\right)^2 r^2 dr = -2\pi C\lim_{r\to 0}\frac{1}{r}, \tag{19}$$

where C is a normalization constant, we can argue that this matrix element diverges, and that this divergence exactly cancel the divergence of the kinetic energy, which they consider a sign that the potential (18) should be taken seriously. Nevertheless, they consider the (18) potential as unphysical and therefore the Neumann solution should be rejected because, according to them, it is this unphysical potential that produces its divergence.

As can be seen the argument in paper [10] is a hybrid of the two arguments discussed above. It rejects the Neumann solution because it diverges at the origin and because it is produced by a potential that they discuss and conclude is not physical.

A more sophisticated argument to eliminate the singular solution is to say as noted by [10] that the expectation value of the kinetic energy with such a function ($n_0(kr)$) is infinite. This is a very serious argument and can be found early in the classical book by S. Flugge [14]. However, we can circumvent this argument by using other self-adjoint extensions that are different from zero at the origin. The physical significance of these self-adjoint extensions is that we renormalize the kinetic energy by adding a point interaction (also known as zero range interaction, but not a delta function) to the Hamiltonian [15]. But as show in the section 4 of this paper this is equivalent to finding self-adjoint extensions of the Laplacian when we exclude the origin, so that the two solutions are acceptable.

The example of the biharmonic oscillator is laborious and so it is presented later in the paper as a final example. It is better to read this final example after reading the two sections that follow.

4. Finding the Domain of the Operators Associated with a Differential Expression

In this section we quickly recapitulate some operator theory that we need to explain in more detail the second point of view regarding the time independent Schrodinger equation presented in the introduction.

According to this point of view the TISE is just a search for the eigenvalues and eigenfunctions of an operator which is something that acts on function and produces another function, as explained below.

An operator consists of an action (what it does to function where it acts) and a domain that is the specification of a set of function where it acts.

A differential expression of order two in one dimension acting on a function $\phi(x)$ produces another function $\psi(x)$. It is an object like

$$O\{\phi(x)\} = \left[a_2(x)\frac{d^2}{dx^2} + a_1(x)\frac{d}{dx} + a_0(x)\right]\phi(x) = \psi(x). \tag{20}$$

It is clearly linear, because $O\{a\,\phi_1(x) + b\,\phi_2(x)\} = a\,O\{\phi_1(x)\} + b\,O\{\phi_2(x)\}$ where a and b are numbers.

A **differential expression** is the **action** of a differential operator, that is, what it does when acting on function. But to be an operator we **must** specify the domain, that is the set of function where it is allowed to act. In quantum mechanics the space of functions of a system is a Hilbert space.

Consider a set of complex valued functions $\psi(x)$ defined in an interval $[a, b]$. Later we are going to consider cases where a or b can be ∞ or both $a = -\infty$ and $b = +\infty$. The "scalar product" of two such a function in this set, $\varphi(x)$ and $\psi(x)$, is defined as

$$(\varphi, \psi) = \int_a^b \varphi^*(x)\psi(x)dx. \tag{21}$$

The set of function for which (21) is finite (with some others technical conditions not important for us now) is called square integrable and is denoted $L^2(a, b)$.

Consider now the *linear*, second order, "differential expression", already mentioned in (20) and repeated here.

$$a_2(x)\frac{d^2}{dx^2} + a_1(x)\frac{d}{dx} + a_0(x). \tag{22}$$

This "differential expression" when acting on a function, say $f(x)$ produces another function, say $g(x)$, that is

$$L(f(x)) = a_2(x)\frac{d^2f(x)}{dx^2} + a_1(x)\frac{df(x)}{dx} + a_0(x)f(x) = g(x). \tag{23}$$

The "differential expression" (23) is the **action** of an operator which is defined by this action and by a set of functions, the domain of the operator so that if $f(x)$ belongs to the **domain** the set of functions g(x) constitute the **range** of the operator. The domain is usually given by **boundary conditions** that the functions and its first derivatives satisfy at the end points, $x = a$, and $x = b$, plus some continuity conditions on $f(x)$ and $\frac{df(x)}{dx}$.

The adjunct of this operator, annotated as $L^+(f_1(x))$, is given by another "differential expression" that acts on a function $f_1(x)$ as follows

$$\begin{aligned} L^+(f_1(x)) = {} & \frac{d^2}{dx^2}\left(a_2(x)f_1(x)\right) \\ & + \frac{d}{dx}\left(a_1(x)f_1(x)\right) + a_0(x)f_1(x) = g_1(x) \end{aligned} \tag{24}$$

and the set of functions $f_1(x)$ that constitute its domain. This set of function is not arbitrary, as we show below. In fact, we have that, given the scalar products

$$(L^+u, v) = \left(L^+u(x), v(x)\right) = \int_a^b \left(L^+u(x)\right)^* v(x)dx \tag{25}$$

and

$$(u, Lv) = (u(x), L(v(x))) = \int_a^b u^*(x)L(v(x))dx. \tag{26}$$

 DOI: https://doi.org/10.1590/1806-9126-RBEF-2023-0316

We have that Lagrange formula

$$(L^{+}u, v) - (u, Lv) = J(u, v) \tag{27}$$

where

$$J(u, v) = a_2(x)\frac{du(x)}{dx} - u(x)\frac{d(a_2(x))}{dx} + a_1(x)u(x)v(x) \tag{28}$$

is obeyed. This follows from integration by parts, so we must **restrict** ourselves to functions u(x) so that integration by parts can be carried out.

Now we insist that the domain of L^{+} are all the functions $u(x)$ that make

$$J(u(b), v(b)) - J(u(a), v(a)) = 0 \tag{29}$$

for all the function $v(x)$ of the domain of L. This is the **definition** of the domain of L^{+}. Note that the action and the domain of L^{+} are usually different from the action and the domain of L.

But the action of L^{+} and L can be the same. For example, if we take $a_2(x) = -\frac{\hbar^2}{2m}$ and $a_1(x) = a_0(x) = 0$ we have that both L^{+} and L have the **same action**, namely $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$. But we must examine the domains. If the domain of L^{+} is not the same domain of L (but by definition obeys (29)) then the operator is called Hermitian by Physicists (symmetric by mathematicians). If the domains are the **same** the operators are called self-adjoint. By the **same** domain we mean that if we change the functions of the domain of the operator, we must make a **different** change on the functions in the domain of the adjunct. Then the domains of L and L^{+} become different because the change is not the same. See the examples below.

4.1. Examples

Consider two operators with the same action is $-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$ and whose domain are specified in the examples. We call O_1 and O_2 the first and second operators respectively.

Example (1) The first operator O_1 has as domain functions $\phi_1(x)$ that vanish together with its derivative at $x = a$ and $x = b$. This operator is symmetric but not self-adjoint. In fact, let $\phi_2(x)$ be the functions in the domain of the adjunct. Then integration by parts (Lagrange formula, see above) show that

$$\begin{aligned}
&(O_1^{+}\phi_2, \phi_1) - (\phi_2, O_1\phi_1)\\
&\quad= \int_a^b \left(-\frac{\hbar^2}{2m}\frac{d^2\phi_2(x)}{dx^2}\right)^{*}\phi_1(x)dx\\
&\qquad- \int_a^b (\phi_2(x))^{*}\left(-\frac{\hbar^2}{2m}\frac{d^2\phi_1(x)}{dx^2}\right)dx\\
&\quad= \left[(\phi_2(a))^{*}\frac{d\phi_1(a)}{dx} - \left(\frac{d\phi_2(a)}{dx}\right)^{*}\phi_1(a)\right]\\
&\qquad- \left[(\phi_2(b))^{*}\frac{d\phi_1(b)}{dx} - \left(\frac{d\phi_2(b)}{dx}\right)^{*}\phi_1(b)\right] = 0
\end{aligned} \tag{30}$$

regardless of the values of $\phi_2(x)$ at $x = a$ and $x = b$. So, the domain of the adjunct is larger than the domain of the operator and hence O_1 is not self-adjoint, that is $O_1 \neq O_1^{+}$ and the operator is just symmetric. Of course, since we used integration by parts, we must impose some conditions on both functions.

Example (2) The second operator has as domain functions $\phi_1(x)$ that vanish at a and b. This operator is self-adjoint. In fact, let $\phi_2(x)$ be the functions in the domain of the adjunct. Then integration by parts (Lagrange formula) show that

$$\begin{aligned}
&(O_2^{+}\phi_2, \phi_1) - (\phi_2, O_2\phi_1)\\
&\quad= \int_a^b \left(-\frac{\hbar^2}{2m}\frac{d^2\phi_2(x)}{dx^2}\right)^{*}\phi_1(x)dx\\
&\qquad- \int_a^b (\phi_2(x))^{*}\left(-\frac{\hbar^2}{2m}\frac{d^2\phi_1(x)}{dx^2}\right)dx\\
&\quad= \left[(\phi_2(a))^{*}\frac{d\phi_1(a)}{dx} - \left(\frac{d\phi_2(a)}{dx}\right)^{*}\phi_1(a)\right]\\
&\qquad- \left[(\phi_2(b))^{*}\frac{d\phi_1(b)}{dx} - \left(\frac{d\phi_2(b)}{dx}\right)^{*}\phi_1(b)\right] = 0,
\end{aligned} \tag{31}$$

when $\phi_2(x)$ vanishes at $x = a$ and $x = b$ regardless of its derivative. So, both O_2^{+} and O_2 has the same **action** and the same **domain**, and hence $O_2 = O_2^{+}$ and the operator is self-adjoint. To carry the integration by parts and some other technicalities we must also demand that the functions and the first derivatives are absolutely continuous (see below) so that the second derivative belong to $L^2(a, b)$.

Remark 1 *Crudely, a function is absolutely continuous in an interval (a, b) if we can write it as*

$$f(x) = f(a) + \int_a^x \frac{df(x)}{dx}dx. \tag{32}$$

Technically $\frac{df(x)}{dx}$ may exist only almost everywhere, meaning that it may not exist in some points.

Example (3) Consider the operator whose action is $-i\hbar\frac{d}{dx}$. Impose that the domain are differentiable functions $\psi(x)$ defined in an interval $[a, b]$ such that $\int_a^b |\psi(x)|^2 dx$ is finite, that is, the functions $\psi(x)$ belongs to $L^2(|a, b|)$. Now assume that in addition the domain are functions with $\psi(a) = \psi(b) = 0$. In this domain the operator is symmetric but not self-adjoint. To see this calculate

$$\begin{aligned}
&\int_a^b \psi_2^{*}(x)\left(-i\hbar\frac{d}{dx}\psi_1(x)\right)dx\\
&\quad= \psi_2^{*}(b)\psi_1(b) - \psi_2^{*}(a)\psi_1(a)\\
&\qquad+ \int_a^b \left(-i\hbar\frac{d}{dx}\psi_2^{*}(x)\right)\psi_1(x)dx.
\end{aligned} \tag{33}$$

Now if $\psi_1(x)$ is in the imposed domain we have

$$\int_a^b \psi_2^*(x)\left(-i\hbar\frac{d}{dx}\psi_1(x)\right)dx$$
$$= \int_a^b \left(-i\hbar\frac{d}{dx}\psi_2^*(x)\right)\psi_1(x)dx, \qquad (34)$$

regardless of the values of $\psi_2(x)$ at the points $x = a$ and $x = b$. Therefore, the operator is symmetric but not self-adjoint. But, if we take the domain of the operator to be functions such that $\psi(a) = e^{i\theta}\psi(b)$ for arbitrary real θ, $0 < \theta < 2\pi$, then it is easy to see that within this domain, the operator whose action is $-i\hbar\frac{d}{dx}$ is self-adjoint.

The examples show that we need some criteria to find if an operator which is symmetric, is in fact self- adjoint or, more importantly, if it can be modified so it becomes self-adjoint. This is given by the following theorem due to von Neumann.

Let H be a symmetric differential operator such that its domain, $D(H)$, are functions $\phi(x)$ and $\frac{d\phi(x)}{dx}$ are such the $\frac{d^2\phi(x)}{dx^2}$ exists, that is $\phi(x)$ and $\frac{d\phi(x)}{dx}$ are absolutely continuous.

To see if H is self-adjoint in this domain we search for the independent square integrable solutions of the differential equation

$$H^+\phi_+(x) = i\kappa\phi_+(x) \qquad (35)$$

and

$$H^+\phi_-(x) = -i\kappa\phi_-(x), \qquad (36)$$

where H^+ is the action of the adjoint of H, which for simplicity we are assuming here are the have the same action as H. The operator H is assumed to be symmetric because the adjunct may have different domains. The constant κ was introduced to maintain the dimension of the equation.

Now let n_+ and n_- (called deficiency indexes) be the number of linearly independent solutions of (35) and (36), respectively. Then

1) If $n_+ = 0$ and $n_- = 0$ then the operator H in its original domain is essentially self-adjoint. No boundary conditions are needed.

   Example: Take the operator $-i\hbar\frac{d}{dx}$ acting on functions $\phi(x)$ defined in the interval $[-\infty, +\infty]$ and such that $\phi(-\infty) = \phi(+\infty) = 0$ and $\phi(x)$ is square integrable. The equations $-i\hbar\frac{d}{dx}\chi(x) = +i\kappa\chi(x)$ and $-i\hbar\frac{d}{dx}\chi(x) = -i\kappa\chi(x)$ have no solution in $L^2(-\infty, +\infty)$ and so the operator is essentially self-adjoint and no extra conditions are needed.
2) If $n_+ = n_- \neq 0$ the operator is not self-adjoint but we can construct self-adjoint operators with it, usually by specifying the boundary conditions. The resulting operator is called a **self-adjunct extension** of the original symmetric operator.

   Example: The operator with the same action, $-i\hbar\frac{d}{dx}$, operating on functions defined on the interval $[a, b]$ such that $\phi(a) = \phi(b) = 0$ have deficiency indices $(1, 1)$ and modification of original boundary conditions, $\phi(a) = \phi(b) = 0$, are needed. New boundary conditions, which we will see latter how to obtain, are $\phi(a) = e^{i\theta}\phi(b)$, they produce an infinite number of operators one for each different values of θ. They are all different from the original which had the domain fixed by boundary conditions $\phi(a) = \phi(b) = 0$.
3) If $n_+ \neq n_-$ the operator cannot be made self-adjoint.
4) Finally to get the boundary conditions we must find a unitary transformation connecting the solutions of equations (35) and (36). This procedure is illustrated in the examples that follow.

This first example illustrate how we can use the formalism of self-adjoint extension to interpret the quantum mechanics of a particle moving in the real axis form which the zero was singled out or removed. A few more complicated examples can be found in [16].

Example (4) The delta function potential as a self-adjoint extension.

Consider the operator $-\frac{d^2}{dx^2}$ in the following domain: $f(x)$ and $\frac{df(x)}{dx}$ are continuous and $\frac{d^2f(x)}{dx^2}$ belongs to $L^2(-\infty, +\infty)$ and $f(0) = 0$. This last condition is essential to this example because the point $x = 0$ was **singled out**. (In the next example we consider the case where we create a hole in the line by saying that at $x = 0$ the value of the wave function is not specified, that is we remove the point $x = 0$ from the real line.)

This above operator is symmetric. To calculate the domain of its adjoint we integrate its action between a function $\varphi_2^*(x)$ of is adjoint and a function $\varphi_1(x)$ of its domain. We have, integrating by parts

$$\int_{-\infty}^{\infty}\left[-\frac{d^2\varphi_2^*(x)}{dx^2}\right]\varphi_1(x)dx - \int_{-\infty}^{\infty}\varphi_2^*(x)\left[-\frac{d^2\varphi_1(x)}{dx^2}\right]dx$$
$$= \varphi_2^*(0^-)\frac{d\varphi_1(0^-)}{dx} - \varphi_2^*(0^+)\frac{d\varphi_1(0^+)}{dx}$$
$$- \frac{d\varphi_2^*(0^-)}{dx}\varphi_1(0^-) + \frac{d\varphi_2^*(0^+)}{dx}\varphi_1(0^+). \qquad (37)$$

Setting the second member equal to zero and remembering that $\varphi_1(0^-) = \varphi_1(0^+) = \varphi_1(0) = 0$ and that $\frac{d\varphi_1(0^-)}{dx} = \frac{d\varphi_1(0^+)}{dx}$ we have that the domain of the adjoint is given by functions $\varphi_2(x)$ whose derivatives satisfies

$$\frac{d\varphi_2^*(0^+)}{dx} - \frac{d\varphi_2^*(0^-)}{dx} = \delta, \qquad (38)$$

where δ is a real number and the functions themselves satisfy

$$\varphi_2^*(0^-) = \varphi_2^*(0^+) = \varphi_2^*(0). \qquad (39)$$

 DOI: https://doi.org/10.1590/1806-9126-RBEF-2023-0316

In words, the domain of the adjoint are functions that are continuous at $x = 0$ but with derivatives discontinuous at $x = 0$. The domain of the adjunct is different from the domain of the original operator. Therefore, the original operator is not self-adjoint. So let us use von Neumann theory and see if it has extensions that are self-adjoint.

According to the above recipe we must ask if the equations

$$-\frac{d^2\Psi_\pm(x)}{dx^2} = \pm i\chi\Psi_\pm(x) \tag{40}$$

has solution belonging to $L^2(-\infty, \infty)$, that is square integrable.

Each equation has a solution each, viz

$$\Psi_+(x) = \begin{cases} e^{\left(e^{-i\frac{\pi}{4}}\chi^{\frac{1}{2}}x\right)} & \text{for } -\infty < x < 0 \\ e^{-\left(e^{-i\frac{\pi}{4}}\chi^{\frac{1}{2}}x\right)} & \text{for } 0 < x < +\infty \end{cases} \tag{41}$$

and

$$\Psi_-(x) = \begin{cases} e^{\left(e^{i\frac{\pi}{4}}\chi^{\frac{1}{2}}x\right)} & \text{for } -\infty < x < 0 \\ e^{-\left(e^{i\frac{\pi}{4}}\chi^{\frac{1}{2}}x\right)} & \text{for } 0 < x < +\infty \end{cases} \tag{42}$$

Since each equation has one solution, we have that the deficiency indices are $(1, 1)$. So, the original operator has a one parameter, let's call it α, family of self-adjoint operators that are extension of it. To find this family we use the following prescription: We begin by finding a unitary transformation that connect the solutions with $i\chi$ with the solutions with $-i\chi$. Since we have just one solution for each of the equations (4.13) the unitary transformation connecting then is just a phase $e^{i\alpha}$.

Let $\varphi(x)$ be a function on the domain we are seeking. We impose

$$\int_{-\infty}^{+\infty}\left[-\frac{d^2(\Psi_+(x) + e^{i\alpha}\Psi_-(x))^*}{dx^2}\right]\varphi(x)dx = \int_{-\infty}^{+\infty}(\Psi_+(x) + e^{i\alpha}\Psi_-(x))^*\left[-\frac{d^2\varphi(x)}{dx^2}\right]dx \tag{43}$$

and using equation (37) with $\varphi_2^*(x)$ replaced with $\left(\Psi_+(x) + e^{i\alpha}\Psi_-(x)\right)^*$ and $\varphi_1(x)$ by $\varphi(x)$ we have (see [16, p. 208])

$$\varphi(0^-) = \varphi(0^+) = \varphi(0) \tag{44}$$

and

$$\frac{d\varphi(0^+)}{dx} - \frac{d\varphi(0^-)}{dx} = -\frac{2\alpha^{\frac{1}{2}}\cos\left(\frac{\pi}{4} + \frac{\alpha}{2}\right)}{\cos\left(\frac{\alpha}{2}\right)}\varphi(0) = g\varphi(0), \tag{45}$$

where g is a real arbitrary number.

The boundary conditions (44) and (45) can be obtained by adding to the operator a delta function, namely $-\frac{d^2}{dx^2} + g\delta(x)$, and by doing standard manipulations.

This is our main result: The problem can be solved by saying that we have an operator with an action and a domain, or you can say, no, you have an action plus a delta function. This second interpretation requires that you promote the wave functions and everything else to generalized functions if you want to be mathematically rigorous (see [2]). Furthermore, in some cases it takes a lot of work to identify the delta function interactions that reproduces the boundary conditions, as we shall see in the next example, and in more complicate case the interaction to be added to the action is not a delta function as we shall see further in this paper.

Example (5) A free particle in the real line with the point $x = 0$ removed.

In this example we examine the operator whose action is again $-\frac{d^2}{dx^2}$ whose domain are function $u_{abcd}(x)$ which vanishes from $-\infty$ to $x = a < 0$, are continuously and infinitely differentiable between $x = a$ and $x = b$ with $u_{abcd}(a) = u_{abcd}(b) = 0$, vanish between $x = b < 0$ and $x = c > 0$ (containing the origin) and is continuously differentiable from $x = c$ to $x = d$ with $u_{abcd}(c) = u_{abcd}(d) = 0$ and finally vanished for $x = d$ to $x = \infty$. This domain in called by mathematicians $C_0^\infty(R/0)$. The points $x = b$ and $x = c$ can be arbitrarily close to zero so that these functions are zero in an arbitrarily small interval $[b, c]$. The point $x = 0$ was thus removed from the domain of the operator.

The operator is clearly symmetric because if $\varphi_1(x)$ is in its domain then

$$\int_{-\infty}^{\infty}\left[-\frac{d^2\varphi_2^*(x)}{dx^2}\right]\varphi_1(x)dx - \int_{-\infty}^{\infty}\varphi_2^*(x)\left[-\frac{d^2\varphi_1(x)}{dx^2}\right]dx = \varphi_2^*(0^-)\frac{d\varphi_1(0^-)}{dx} - \varphi_2^*(0^+)\frac{d\varphi_1(0^+)}{dx} - \frac{d\varphi_2^*(0^-)}{dx}\varphi_1(0^-) + \frac{d\varphi_2^*(0^+)}{dx}\varphi_1(0^+) \tag{46}$$

$$\varphi_1(0^-) = \varphi_1(0^+) = 0 \tag{47}$$

and

$$\frac{d\varphi_1(0^-)}{dx} = \frac{d\varphi_1(0^+)}{dx} = 0 \tag{48}$$

because $\varphi_1(x)$ is continuous and infinitely differentiable.

Therefore, the right-hand side of the above equation vanishes independently of $\varphi_2(x)$ and so, the domain of the adjunct is larger than the domain of the operator. In fact, the domain of the adjunct are functions $\varphi_2(x)$ that vanishes when $x \to \pm\infty$, are not defined at $x = 0$, are square integrable from $-\infty$ to $+\infty$ and have square integrable second derivatives.

According to the von Neumann theory to see if this operator has self-adjoint extensions we investigate the number of solutions of the equations

$$-\frac{d^2\Psi_\pm(x)}{dx^2} = \pm i\chi\Psi_\pm. \tag{49}$$

But now, because we excluded the point $x = 0$, there are four solutions.

$$\Psi_+^1(x) = \begin{cases} 0 & \text{for } -\infty < x < 0 \\ e^{-\left(e^{-i\frac{\pi}{4}}\chi^{\frac{1}{2}}x\right)} & \text{for } 0 < x < +\infty \end{cases} \tag{50}$$

$$\Psi_+^2(x) = \begin{cases} e^{-\left(e^{-i\frac{\pi}{4}}\chi^{\frac{1}{2}}x\right)} & \text{for } -\infty < x < 0 \\ 0 & \text{for } 0 < x < +\infty \end{cases} \tag{51}$$

$$\Psi_-^1(x) = \begin{cases} 0 & \text{for } -\infty < x < 0 \\ e^{-\left(e^{+i\frac{\pi}{4}}\chi^{\frac{1}{2}}x\right)} & \text{for } 0 < x < +\infty \end{cases} \tag{52}$$

$$\Psi_-^2(x) = \begin{cases} e^{-\left(e^{+i\frac{\pi}{4}}\chi^{\frac{1}{2}}x\right)} & \text{for } -\infty < x < 0 \\ 0 & \text{for } 0 < x < +\infty \end{cases} \tag{53}$$

Therefore, the deficiency indices are $(2, 2)$ and so there is a four parameter self-adjoint extensions of the original operator.

The unitary operator connecting the two solutions is now a 4×4 unitary matrix Depending on four parameters viz.

$$U = \begin{Bmatrix} u_{11} & u_{12} \\ u_{21} & u_{22} \end{Bmatrix} = \begin{bmatrix} \cos b e^{i(a+b)} & i \sin b e^{i(d-a)} \\ i \sin b e^{i(d+a)} & \cos b e^{i(c-a)} \end{bmatrix}. \tag{54}$$

The boundary conditions are obtained by enforcing that if $\varphi(x)$ is a function in the domain of the operator we seek then

$$\int_{-\infty}^{\infty} \left[-\frac{d^2 \left(\Psi_+^1(x) + u_{11}\Psi_-^1(x) + u_{12}\Psi_-^2(x)\right)^*}{dx^2} \right] \varphi(x) dx = \int_{-\infty}^{\infty} \left(\Psi_+^1(x) + u_{11}\Psi_-^1(x) + u_{12}\Psi_-^2(x)\right)^* \left[-\frac{d^2\varphi(x)}{dx^2} \right] dx \tag{55}$$

and

$$\int_{-\infty}^{\infty} \left[-\frac{d^2 \left(\Psi_+^1(x) + u_{21}\Psi_-^1(x) + u_{22}\Psi_-^2(x)\right)^*}{dx^2} \right] \varphi(x) dx = \int_{-\infty}^{\infty} \left(\Psi_+^1(x) + u_{21}\Psi_-^1(x) + u_{22}\Psi_-^2(x)\right)^* \left[-\frac{d^2\varphi(x)}{dx^2} \right] dx \tag{56}$$

After some algebra (see [16]) we find finally that

$$\begin{bmatrix} \frac{d\varphi(0^+)}{dx} \\ \varphi(0^+) \end{bmatrix} = e^{i\theta} \begin{vmatrix} \alpha & \beta \\ \gamma & \delta \end{vmatrix} \begin{bmatrix} \frac{d\varphi(0^-)}{dx} \\ \varphi(0^-) \end{bmatrix}, \tag{57}$$

where $\alpha\gamma - \beta\delta = 1$, and where the parameters in Greek letters α, β, δ, γ and θ are related to the parameters in Roman letters a, b, c, d and to the constant χ by

$$\beta = \sqrt{2}\chi^{1/2} \left[\frac{\cos\left(a + \frac{\pi}{4}\right) - \cos b \sin\left(c - \frac{\pi}{4}\right)}{\sin b} \right]$$

$$\alpha = \sqrt{2}\chi^{1/2} \left(\frac{\sin a - \cos b \cos c}{\sin b} \right)$$

$$\delta = \sqrt{2}\frac{1}{\chi^{1/2}} \left(\frac{\cos a + \cos b \cos c}{\sin b} \right)$$

$$\gamma = \sqrt{2}\frac{1}{\chi^{1/2}} \left[\frac{\cos\left(a + \frac{\pi}{4}\right) + \cos b \sin\left(c + \frac{\pi}{4}\right)}{\sin b} \right]$$

$$\theta = d.$$

The physics of the Hamiltonian defined by the action $-\frac{d^2}{dx^2}$ whose domain are functions in the holed real line with boundary conditions given by (57) was given in [17, 18]. Note that until this point, we didn't speak of zero range interactions or more specifically, in this case, of delta functions. But if the reader wishes he/she can see interpret the above result as a Hamiltonian with the action $-\frac{d^2}{dx^2}$ plus a contact interaction (or zero range interactions) that includes not only the delta function but also derivatives of the delta function. The complete result can be found in a beautiful paper by S. De Vincenzo and C. Sánchez [19] and will be reproduced latter in this paper.

The above procedures are only prescriptions, that are described in more detail in [16]. The reader can find detailed treatments in the following reference in ascending order of mathematical complexity: [20], [21] and [22].

Now we can proceed and examine the problems raised in the literature and described above in section 3 and in section 6.

5. Alternative Solutions to the Questionable Statements Presented Before in Section 3

Now we are ready to decipher as promised the mystery of how transforming the Laplacian operator, $-\nabla^2$, from cartesian coordinates to polar coordinates allow us to modify the problem tremendously.

In cartesian coordinates the action of operator is

$$-\nabla^2 = -\left\{ \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right\}. \tag{58}$$

Now, when we transform to spherical polar coordinates (or to cylindrical polar coordinates) the point $(x = 0, y = 0, z = 0)$ becomes singular because the Jacobian of the transformation tends to zero as we approach the origin. Therefore, we must remove the point $(x = 0, y = 0, z = 0)$ and the plane becomes a holed plane which is different from our original space. In fact, **translation invariance is lost**.

Therefore, we **must** first study the self-adjointness of the operator (58) in the space of function $\psi(\mathbf{r}) = \psi(x, y, z)$ defined by

$$\int \psi^*(\mathbf{r})\psi(\mathbf{r})d^3\mathbf{r} = \text{finite}, \tag{59}$$

that is the space $L^2(R^3)$, that has no holes in it.

We shall examine the operator in the space with a hole in the point $\mathbf{r} = \mathbf{0}$ after examining the action of the Laplacian in polar coordinates. In spherical polar coordinates we have

$$-\nabla^2 = -\left(\frac{d^2}{dr^2} + 2r\frac{d}{dr} + \frac{1}{r^2 \sin^2\varphi}\frac{d^2}{d\theta^2} + \frac{1}{r^2 \sin\varphi}\frac{d}{d\varphi}\left(\sin\varphi\frac{d}{d\varphi}\right)\right). \tag{60}$$

After separation of variables, we recovered the operator given by equation (4) which is the radial part of the action of the differential expression given by (60), viz.

$$\frac{d^2R_\ell(r)}{d^2r} + \frac{2}{r}\frac{dR_\ell(r)}{dr} + \left(k^2 - \frac{\ell(\ell+1)}{r^2}\right)R_\ell(r)(r). \tag{61}$$

Then we **must** work with functions defined in the space $L^2(R^3\backslash(0,0,0))$ which means that the origin $(0,0,0)$ was removed.

We shall now show that the operator given by the action (58) and domain (59) is essentially self-adjoint whereas the operator given by the action (61) (for $\ell = 0$) in the domain $L^2(r^2dr\backslash 0))$ that is functions of r such that

$$\int_0^\infty R_0^2(r)r^2dr = \text{finite} \tag{62}$$

is not. For $\ell \neq 0$ the operator is essentially self-adjoint because one of the equations of the most general solution is not square integrable.

Consider the following equations

$$-\frac{\hbar^2}{2m}\left\{\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right\}\psi(x, y, z) = \mp iE\psi(x, y, z). \tag{63}$$

This equation separates if we write $\psi(x, y.z)$ as $\psi(x, y.z) = X(x)Y(y)Z(z)$ and gives

$$\frac{d^2X(x)}{dx^2} = \pm il^2X(x)$$
$$\frac{d^2Y(y)}{dy^2} = \pm im^2Y(y)$$
$$\frac{d^2Z(z)}{dz^2} = \pm i(k^2 - l^2 - m^2)Z(z)$$

where $k^2 = \frac{2mE}{\hbar^2}$.

The equations have no square integrable solution, so the deficiency indices are $(0,0)$ the operator given whose action is given by (58) and the domain are function that square integrable, that is $L^2(R^3)$, is essentially self-adjoint.

Now, when we remove the origin by going to spherical coordinates, we must consider the equations

$$\frac{d^2R_0(r)}{d^2r} + \frac{2}{r}\frac{dR_0(r)}{dr} \mp ik^2R_0(r) = 0. \tag{64}$$

Each of the two above equations admits one linearly independent solution and so, we have that the deficiency indices are $(1,1)$, and hence the operator admits a one parameter family of self-adjoint extensions, whose wave functions are given by

$$R_{\ell=0}(r) = j_0(kr) + \alpha n_0(kr), \quad r > 0, \tag{65}$$

each member of the family being characterized by a value of the parameter α.

Now we see that the Neumann function appears naturally. It is part of the eigenfunction of an extension of the Laplacian characterized by the parameter α.

If we take $\alpha = 0$ we have the eigenfunctions of the usual operator Hamiltonian, used in the literature.

To find the eigenvalues and eigenfunction of the extended operator it is easier to calculate the extension of the operator obtained by making the transformation

$$R(r) = \frac{u(r)}{r}, \text{valid for } r > 0 \tag{66}$$

in equation (45), for $\ell = 0$.

The resulting operator is

$$\frac{d^2u(r)}{dr^2} \mp ik^2u(r) = 0, \tag{67}$$

which again show us that the operator $-\frac{d^2}{dr^2}$ in the space of function $L^2(0,\infty)$, note that the origin was removed, have deficiency indexes $(1,1)$ and so has a one parameter family of self-adjoint extensions.

We have now three options

1. Seek for a contact interaction (with zero range) that cancels the infinity of the kinetic energy that appears if we calculate the expectation value of $\frac{\hbar^2}{2m}\frac{d^2}{dr^2}$ with functions of the form $\frac{u(r)}{r}$.
   This contact interaction is constructed for example by adding to the kinetic energy a square well potential with length ϵ and whose depth is fine tuned.

   This contact interaction will depend on a parameter that we denote by α and the new Hamiltonian is

   $$H(\alpha) = -\lim_{\epsilon\to 0}\frac{\hbar^2}{2m}\left[\frac{d^2}{dr^2} - \frac{\pi^2}{4\epsilon^2} + \frac{2\alpha}{\epsilon} + \frac{4\alpha^2}{\pi^2} + \alpha^2\right] \quad \text{for } r < \epsilon$$

   and

   $$H(\alpha) = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} \text{ for } r > \epsilon.$$

For more details, see references [15] for three dimensions, and [23] and [24] for two dimensions.

2. To extend the operator domain by imposing that $\frac{\frac{du(0)}{dr}}{u(0)} = \alpha$. This is a general result. When we restrict the range of the functions where the action of your operator acts you must put boundary conditions. These boundary conditions are easily deduced if you can solve the equations that give the deficiency indexes. In this case they can be derived by integration by parts. Assume that $\phi_1(r)$ and $\phi_2(r)$ are in the domain we search. Then we have

$$\int_0^\infty \left(-\frac{d^2\phi_2^*(x)}{dx^2}\right)\phi_1(x)dx - \int_0^\infty \phi_2^*(x)\left(-\frac{d^2\phi_1^*(x)}{dx^2}\right)dx = \phi_2^*(0)\phi_1(0)\left[\frac{\frac{d\phi_1(0)}{dx}}{\phi_1(0)} - \frac{\frac{d\phi_2(0)}{dx}}{\phi_2(0)}\right]$$

and so $\frac{\frac{d\phi_1(0)}{dx}}{\phi_1(0)} = \alpha$ real (see [16] for details).

3. By giving up arguing and to declare that there is a delta function in the Hamiltonian that forces us to take $u(0) = 0$. This last option is not entirely correct because as is well know the delta function is too strong in three dimensions and it is more restrictive than the one described above.

Remark 2 *The same problem as the one discussed above occurs in two dimensions and the alternative solutions to problems that occur is the same as the ones given above. Consider the Laplacian in two dimensions. When we transform to polar coordinates, translation invariance is lost, because the point ($x = 0$ and $y = 0$) becomes singular. Therefore, the Kinetic energy operator must be studied carefully. The solutions obtained to the problem described above are the same as the ones described above for three dimensions, namely*

1) *Seek for a contact interaction that cancels the infinity of the kinetic energy if we want to use the singular solution. This was done in [23].*
2) *Look for self-adjoint extensions of the operator extensions This was done in [16, 24].*
3) *To give up arguing. But in this case, we cannot say that there is a delta function at the origin, because as explained in [23] the delta function is too strong in two dimensions.*

6. A Final Example

In this final example we discuss a more complicated case using the machinery developed before.

The problem is the asymmetric, or biharmonic, harmonic oscillator in one dimension and was presented in the article by W. Edward Gettys and H.H. Graben [25]. The Hamiltonian of this problem is

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}mx^2\left(\omega_1^2\theta(x) + \omega_2^2\theta(-x)\right). \quad (68)$$

As explained already the above should be interpreted as a differential expression of an operator. To be an operator we must specify its domain. For the above differential expression when $\omega_1 = \omega_2$ we don't need to add any boundary condition, the domain are functions that are square integrable on the line. To require that the eigenfunctions can be normalized is sufficient to guarantee the self-adjointness of the operator. See V.S. Araujo et al. [26]. In fact, the operator whose action is (68) in the domain $L^2(-\infty, +\infty)$ is essentially self-adjoint.

To find the eigenvalues and eigenfunctions of the above operator before specifying its domain we solve the two differential equations

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + \frac{1}{2}m\omega_1^2x^2\Psi(x) = E\Psi(x), \quad \text{for } -\infty < x < 0 \quad (69a)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + \frac{1}{2}m\omega_2^2x^2\Psi(x) = E\Psi(x), \quad \text{for } 0 < x < \infty. \quad (69b)$$

However, let's first consider the usual solution of the simple harmonic oscillator. This is relevant for the problem, because to solve the problem described above one must solve the Schrödinger equation for the harmonic oscillator in some range. Let's therefore briefly recall the solution of the harmonic oscillator.

6.1. The standard harmonic oscillator

The equation to be solved in standard notation is:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\Psi(x) + \frac{1}{2}m\omega^2x^2\Psi(x) = E\Psi(x), \quad \text{for } -\infty < x < \infty. \quad (70)$$

The point $x = 0$ is an ordinary point of the equation (70) and so have two linear independent solutions that can be obtained as a series expansion [27].

By making different, but related, transformations we get the usual versions of the harmonic oscillator equation. We are going to need all of them for clarity, because they are all used in different textbooks and because as have seen these transformations may change the domain of the operators.

1. The Weber equation

Change to $\xi = \left(\frac{2m\omega}{\hbar}\right)^{\frac{1}{2}} x$ and $\varepsilon = \frac{E}{\hbar\omega}$ to get the Weber equation

$$\frac{d^2\psi}{d\xi^2} + \left(\varepsilon - \frac{\xi^2}{4}\right)\psi = 0. \quad (71)$$

This form is used in [28].

2. The Hermite equation

Change to $\xi = \left(\frac{m\omega}{\hbar}\right)^{\frac{1}{2}} x$ and $\psi(x) = e^{-\frac{\xi^2}{2}} f(\xi)$ to get

$$\frac{d^2 f}{d\xi^2} - 2\xi \frac{df}{d\xi} + \left(\frac{2E}{\hbar\omega} - 1\right) f = 0. \tag{72}$$

The point $x = 0$ is an ordinary point of the equation 1 [27] and so have two linear independent solutions that can be obtained as a series expansion. This equation was used in the book by Eugen Merzbacher [29] to solve the so-called double oscillator.

3. The confluent hypergeometric equation

Change in the Hermite equation $z = \xi^2$ and $u(z) = f(\xi)$ to get

$$z\frac{d^2 u}{dz^2} + \left(\frac{1}{2} - z\right)\frac{du}{dz} + \frac{\nu}{2}u = 0, \tag{73}$$

where $E = \left(\nu + \frac{1}{2}\right)\hbar\omega$, which is the confluent hypergeometric equation [30, chapter VI].

Each of these forms are equations that have been studied very thoroughly in the 19$^{\text{th}}$ century, and each of these forms have been used to solve similar problems to the bi-harmonic oscillator. For example, as mentioned before, the Hermite equation was used by Eugen Merzbacher [29] to solve the so-called double oscillator.

We prefer to use equation (73). It has two independent solutions [30, Chapter 6]. They are ${}_1F_1\left(-\frac{\nu}{2};\frac{1}{2};z\right)$ and $U\left(-\frac{\nu}{2};\frac{1}{2};z\right)$ where ${}_1F_1\left(-\frac{\nu}{2};\frac{1}{2};z\right)$ is the hypergeometric function, and $U\left(-\frac{\nu}{2};\frac{1}{2};z\right)$ is defined by

$$\begin{aligned} U\left(-\frac{\nu}{2};\frac{1}{2};z\right) =& \sqrt{\pi}\left\{\frac{{}_1F_1\left(-\frac{\nu}{2};\frac{1}{2};z\right)}{\Gamma\left(\frac{1}{2}-\frac{\nu}{2}\right)}\right. \\ & \left. -\ z^{\frac{1}{2}}\,\frac{{}_1F_1\left(\frac{1}{2}-\frac{\nu}{2};\frac{3}{2};z\right)}{\Gamma\left(-\frac{\nu}{2}\right)}\right\}, \end{aligned} \tag{74}$$

where Γ stands for the gamma function.

When $z \to \infty$, ${}_1F_1\left(-\frac{\nu}{2};\frac{1}{2};z\right)$ diverges like e^z, while $U\left(-\frac{\nu}{2};\frac{1}{2};z\right) \to 0$; hence, since $\psi(x)$ must be normalized we are left with $U\left(-\frac{\nu}{2};\frac{1}{2};z\right)$. This can be checked in [30, p. 289].

Hence

$$\psi(\xi) = Ce^{\frac{-\xi^2}{2}} U\left(-\frac{\nu}{2};\frac{1}{2};z\right), \tag{75}$$

where C is a constant and so equation (75) is the solution of the problem. (See in this connection [25])

Note that ν, and hence E, are still arbitrary. These are not determined by the normalizability of ψ. We emphasize this because the usual treatment in the literature gives the impression (see for example [31, Chapter 4]) that the convergence of ψ for $x \to \infty$ determines the eigenvalue.

When the potential is continuous the derivative of the wave function should not have a discontinuity, hence we must examine the derivative of $\psi(\xi)$, $\frac{d\psi(\xi)}{d\xi}$, that is

$$\begin{aligned} \frac{d\psi(\xi)}{d\xi} =& -2C\xi e^{-\frac{\xi^2}{2}}\left\{U\left(-\frac{\nu}{2};\frac{1}{2};z\right)\right. \\ & \left. +\ \nu U\left(1-\frac{\nu}{2};\frac{1}{2};z\right)\right\}. \end{aligned} \tag{76}$$

When $z \to 0$, we find

$$\frac{d\psi(\xi)}{d\xi} \sim \frac{\sqrt{\pi}C\nu}{\Gamma\left(\frac{1}{2}-\frac{\nu}{2}\right)\Gamma\left(1-\frac{\nu}{2}\right)}\frac{\xi}{|\xi|}, \tag{77}$$

which is discontinuous at $\xi = 0$!

Then since we are examining equation (77), the demonstration on the paper by D. Branson [3] requires that this discontinuity should be eliminated by requiring that

$$\frac{\nu}{\Gamma\left(\frac{1}{2}-\frac{\nu}{2}\right)\Gamma\left(1-\frac{\nu}{2}\right)} = 0. \tag{78}$$

This will hold when ν is a negative integer and we get the usual harmonic oscillator solution. In more detail, when ν is an integer only the first term of equation (74) remains, and the function U becomes an even function of z. When $-\nu$ is odd only the second term survives, and U becomes an odd function of z. Furthermore when ν is an integer the Fs in equation (74) turns out to be the Hermite polynomials and the equation (75) becomes the usual solution of the harmonic oscillator.

3.1. The bi harmonic oscillator

The reader must by now becoming a bit uncomfortable, because we can write the potential of the bi harmonic oscillator as

$$V(x) = \frac{1}{2}mx^2\left(\omega_1\theta(x) + \omega_2\theta(-x)\right), \tag{79}$$

where $\theta(x)$ is the Heaviside step function whose derivative, at $x = 0$, is discontinuous. In fact, the solution of equation (69a) is given by equation (73) with ω replaced by ω_1 and the solution of equation (69b) is given by the same equation (73) with ω replaced by ω_2 and x replaced by $-x$.

We have now three options:

1) The eigenvalues of the bi harmonic oscillator can be obtained by requiring that the wave functions and their derivatives are continuous at $x = 0$. This is equivalent to retain the point $x = 0$ and therefore the operator whose action is (79) belong to $L^2(-\infty, +\infty)$. This is done in the paper by W. Edward Gettys and H.H. Graben [25].
2) To remove the point $x = 0$. This means that we are in mathematical parlance putting a barrier or frontier at $x = 0$. By doing this we can construct self-adjoint operators by imposing the boundary conditions (57) to the wave functions at the **removed** origin

$$\begin{bmatrix}\frac{d\varphi(0^+)}{dx}\\ \varphi(0^+)\end{bmatrix} = e^{i\theta}\begin{vmatrix}\alpha & \beta\\ \gamma & \delta\end{vmatrix}\begin{bmatrix}\frac{d\varphi(0^-)}{dx}\\ \varphi(0^-)\end{bmatrix}. \tag{80}$$

Let's take the boundary condition given by $\theta = 0$, $\alpha = 1$, and $\gamma = \delta = 0$. Then we have $\varphi(0^+) = \varphi(0^-) = \varphi(0)$ and $\frac{d\varphi(0^+)}{dx} - \frac{d\varphi(0^-)}{dx} = \beta\varphi(0)$, and we have construct a self-adjoint operator, that corresponds to a delta function at the origin. In fact, some people would claim that the solution we got is wrong because we missed a delta function at $x = 0$. To circumvent, or accept this sentence we may declare that the Hamiltonian have a delta function at $x = 0$, with strength α. This option requires that we declare that the wave functions are generalized function (or distribution as they are also called). However, we can ignore this point. See J. Viana-Gomes and N.M.R. Peres [32] or S.H. Patil [33].

We do not want to argue with them but in fact we have construct a five-parameter family of self-adjoint operators that can indeed be interpreted as contact interactions as shown below.

3) These operators can be interpreted as an operator whose action is $-\frac{d^2}{dx^2}$ plus contact interactions (or zero range interactions) that includes not only the delta function but also derivatives of the delta function. These contact interactions given by [19] are

$$\widehat{V}(x) = g_1\delta(x) - (g_2 - ig_3)\delta(x)\frac{d}{dx} + (g_2 + ig_3)\frac{d}{dx}\delta(x) - g_4\frac{d}{dx}\left(\delta(x)\frac{d}{dx}\right) \tag{81}$$

where the four parameters, g_i ($i = 1$ to 4), are related to the parameters given by equation (42), for example, $g_1 = \beta$.

The energy levels of potential (81) are given in reference [18]. The complete analysis is complicated and a recent reference is given by [34].

7. Conclusions

In this paper we examined the claim that some solutions of the TISE are not solutions because they contain a delta function that was forgotten. We showed that these solutions are eigenfunctions of operators that are self-adjoint extensions of an appropriate operator. If you admit that self-adjointness is the only criteria to accept operators and their eigenfunctions in quantum mechanics these solutions are perfectly acceptable.

Another point of view is to accept that these eigenfunctions are eigenfunctions of operators with the same action but with added zero-range or contact iterations. In the case of one-dimensional problems (or problems that can be reduced to one dimensional problems but with barries) it is better to interpret the wave function as generalized functions.

Acknowledgments

The authors acknowledge partial support from CNPq (Conselho Nacional de Desenvolvimento Científico e Tecnológico).

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