Operator domains and self-adjoint operators

Vanilse S. Araujo
Instituto de Fisica da Universidade de Sao Paulo, CP 20516, Sao Paulo, Brazil

F. A. B. Coutinho[a)]
Faculdade de Medicina da Universidade de Sao Paulo, 01246-903, Sao Paulo, Brazil

J. Fernando Perez
Instituto de Fisica da Universidade de Sao Paulo, CP 20516, Sao Paulo, Brazil

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To construct a self-adjoint operator the domain of the operator has to be specified by imposing an appropriate boundary condition or conditions on the wave functions on which the operator acts. We illustrate situations for which different boundary conditions lead to different operators and hence to different physics.
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I. INTRODUCTION

Operators are essential to quantum mechanics. Observables are represented by linear, self-adjoint operators in the Hilbert space of the states of the system under consideration. For mathematicians an operator acting in a Hilbert space consists of its action and its domain. The action refers to what the operator does to the functions on which it acts. The domain is the specified set of functions on which the operator acts. However, most textbooks on quantum mechanics do not mention the domain of the operators. (An exception is the book by Ballentine.[1]) Textbooks usually state that an observable should correspond to a Hermitian operator. The distinction between a self-adjoint operator and a Hermitian operator is not mentioned. The distinction is rather subtle, and we shall see that it has to do with the domain of the operator. We note that a Hermitian operator also is called a symmetric operator in the mathematical literature.

The situation in the physics literature was no better until the recent excellent article by Bonneau, Faraut, and Valent[2] on self-adjoint extensions. We are aware of only two other related articles. One is by Jordan,[3] who pointed out the importance of specifying operator domains and the relationship of the domain with the boundary conditions on the wave functions. The other article is by Capri[4] on self-adjointness and broken symmetry. The concept of self-adjoint operators is essential in quantum mechanics, and we believe that physics students should be aware of it. The construction of self-adjoint operators produces some new and interesting problems. There are also some problems in physics, for instance, the problem of helicity conservation in the Aharonov–Bohm scattering of a Dirac particle, that can be solved only if we consider such technicalities.[5]

The purpose of this paper is to supplement and expand the presentation given in Ref. 2. We examine six examples of the following general procedure. We start with a Hermitian operator, and determine if it can be used to construct a self-adjoint operator by modifying its domain. If the answer is positive, we say that the operator can be extended, and we construct self-adjoint operators by imposing suitable boundary conditions on the wave functions. Usually the result is a family of operators that depend on one or more parameters. Different values of the parameters result in different domains, differing in the boundary conditions satisfied by the wave functions, and hence in different operators. These operators represent new and interesting physics.

In Sec. II we explain what a self-adjoint operator is by comparing it with an operator that is merely Hermitian. In the rest of the paper we show by example how to construct self-adjoint operators. In Sec. III we explain how to determine whether a certain Hermitian operator may be extended, that is, if it is possible to obtain a family of self-adjoint operators that depends on one or more parameters. In Sec. IV we discuss, again by example, how to obtain the family of boundary conditions that characterize the family of self-adjoint operators. Finally in Sec. V we consider the relevance of these operators to physics. The solution of each example is done in parts and is divided over Secs. III–V. In Appendix A we give additional discussion that shows why the prescriptions given in the main body of the paper work, and in Appendix B we give the solution of an exercise.

II. WHAT IS A SELF-ADJOINT OPERATOR?

Most students think that the domain of an operator is automatically specified. They think that, if $\hat{A}$ is an operator and if $\hat{A}\varphi$ belongs to the Hilbert space, then φ belongs to the domain of $\hat{A}$, which, as we shall see, is rarely so. In general, the set of functions to which $\hat{A}\varphi$ belongs to the Hilbert space is too large. The reason for specifying the domain is that we want the operator to be self-adjoint. Furthermore, it is possible for operators with the same action to be different self-adjoint operators if they have different domains.

Let us explain the above considerations with an example. Consider a free particle moving on the one-dimensional half line. The kinetic energy operator of the particle is $H_0 = -(h^2/2m)\, d^2/dx^2$. Consider the set of functions, $\varphi(x)$, defined for $0 \leqslant x < \infty$ such that $\int_0^\infty |\varphi(x)|^2 dx$ is finite, that is, they are square integrable. This set of functions forms a Hilbert space denoted by mathematicians by $L_2[0,\infty]$. There are functions in this space for which

$$\int_0^\infty \left| -\frac{h^2}{2m}\frac{d^2\varphi(x)}{dx^2}\right|^2 dx = \infty,$$

and hence the operator H_0 omits some functions $\varphi(x)$ from the Hilbert space.

However, the condition that $\hat{A}\varphi$ belongs to the Hilbert space is not sufficient even for physicists. It is quite reasonable to argue that for the particle to be confined to the half line, $0 \leqslant x < \infty$, there must be an infinite barrier at $x=0$. This barrier forces us to impose the condition $\varphi(0)=0$. Mathematically, however, this condition makes H_0 self-adjoint as we shall see.

Because we are going to integrate by parts, we must remove various sets of functions from $L_2[0,\infty]$. First we remove all the functions that although square integrable, do not go to zero as $x \to \infty$. An example of such a function can be found in Ref. 6. Second we remove all functions that are not absolutely continuous. A function is absolutely continuous if it is the integral of its derivative, that is, $f(x)$ is absolutely continuous if $f(x)=\int_0^x [df(t)/dt]\, dt + f(0)$. An example of a function that is continuous, but does not have a derivative, is given in Refs. 7 and 8. We call Ω the subset of $L_2[0,\infty]$ that is so formed.

Consider two functions $\varphi_1(x)$ and $\varphi_2(x)$ such that $\varphi_1(0)=0$, but $\varphi_2(0)\neq 0$, both belonging to Ω. Consider the matrix element

$$(\varphi_2, H_0\varphi_1) = \int_0^\infty \varphi_2^*(x)\left[-\frac{h^2}{2m}\frac{d^2\varphi_1(x)}{dx^2}\right]dx. \tag{1}$$

The adjoint of the operator H_0 can be obtained by doing an integration by parts and having it act on $\varphi_2^*(x)$ (from now on we use units such that $h^2/2m=1$). We have

$$\frac{d}{dx}\left[\varphi_2^*(x)\left(\frac{d}{dx}\varphi_1(x)\right)\right] = \frac{d\varphi_2^*(x)}{dx}\frac{d\varphi_1(x)}{dx} + \varphi_2^*(x)\frac{d^2\varphi_1(x)}{dx^2}, \tag{2}$$

$$\frac{d}{dx}\left[\left(\frac{d\varphi_2^*(x)}{dx}\right)(\varphi_1(x))\right] = \frac{d\varphi_2^*(x)}{dx}\frac{d\varphi_1(x)}{dx} + \frac{d^2\varphi_2^*(x)}{dx^2}\varphi_1(x). \tag{3}$$

If we subtract Eq. (3) from Eq. (2), we obtain

$$-\frac{d^2\varphi_2^*(x)}{dx^2}\varphi_1(x) = \varphi_2^*(x)\left[-\frac{d^2\varphi_1(x)}{dx^2}\right] + \frac{d}{dx}\left(\varphi_2^*(x)\frac{d\varphi_1(x)}{dx}\right) - \frac{d}{dx}\left(\frac{d\varphi_2^*(x)}{dx}\varphi_1(x)\right). \tag{4}$$

We then integrate both sides and obtain

$$\int_0^\infty -\frac{d^2\varphi_2^*(x)}{dx^2}\varphi_1(x)dx - \int_0^\infty \varphi_2^*(x)\left[-\frac{d^2\varphi_1(x)}{dx^2}\right]dx = \varphi_2^*(0)\frac{d\varphi_1(0)}{dx} - \frac{d\varphi_2^*(0)}{dx}\varphi_1(0). \tag{5}$$

The reader can easily verify that if $\varphi_2^*(0)$ and $\varphi_1(0)$ are both zero, we have

$$\int_0^\infty \left[-\frac{d^2\varphi_2(x)}{dx^2}\right]^*\varphi_1(x)dx = \int_0^\infty \varphi_2^*(x)\left[-\frac{d^2\varphi_1(x)}{dx^2}\right]dx, \tag{6}$$

or

$$(H_0\varphi_2, \varphi_1) = (\varphi_2, H_0\varphi_1). \tag{7}$$

The important point here is that the boundary condition for the function on the right, $\varphi_1(x)$, is exactly the same as the boundary condition for the function to the left, $\varphi_2(x)$. In other words, when the action and the domain of the operator that acts on the right is equal to the action and the domain of its adjoint, that is, the operator that acts on the left, the operator is said to be self-adjoint. So the operator $-d^2/dx^2$ defined in the domain Ω' of functions of Ω that vanish at the origin is self-adjoint.

Another operator can be obtained by imposing on the functions Ω the conditions $\varphi_1(0)=0$ and $d\varphi_1(0)/dx=0$. This operator is called Hermitian. However, it is not self-adjoint, because $\varphi_2^*(0)$ and $d\varphi_2^*(0)/dx$ can take any finite value and Eq. (6) is nevertheless satisfied, that is, the domain of the adjoint is larger than the domain of the operator. In fact, the domain of the adjoint is all functions of Ω that remain in Ω after acted on by $-d^2/dx^2$.

Note that we have defined Ω' by removing sets of functions from $L_2[0,\infty]$ and requiring that the functions vanish at the origin. However, we must be sure that the resulting set is dense in $L_2[0,\infty]$, which means that given an arbitrary function $f(x)\in L_2[0,\infty]$ and an arbitrary positive number $\delta>0$, there is always a function $\varphi(x)$ belonging to Ω' such that $\int_0^\infty |f(x)-\varphi(x)|^2 dx < \delta$. The domain of an operator has to be dense in order that the adjoint exists (see Ref. 9 for a proof). The reader should not worry about this point. Mathematicians have proved that all sets used in this work[10] are dense in the relevant Hilbert space. In many cases given a function of the Hilbert space, a plot of it together with a plot of a convenient function of Ω' will convince the reader.

We now rewrite Eq. (5) as

$$\int_0^\infty -\frac{d^2\varphi_2^*(x)}{dx^2}\varphi_1(x)dx = \int_0^\infty \varphi_2^*(x)\left[-\frac{d^2\varphi_1(x)}{dx^2}\right]dx + \varphi_2^*(0)\varphi_1(0) \times \left[\frac{1}{\varphi_1(0)}\frac{d\varphi_1(0)}{dx} - \frac{1}{\varphi_2^*(0)}\frac{d\varphi_2^*(0)}{dx}\right]. \tag{8}$$

We see that if we let

$$\frac{1}{\varphi(0)}\frac{d\varphi(0)}{dx} = \kappa, \tag{9}$$

where κ can be any real number, we obtain another operator. In fact, we obtain a family of operators that depend on κ. They all have the same action $-d^2/dx^2$, but they act on different domains characterized by κ. As we have said, the case $\kappa=\infty$ ($\varphi(0)=0$) is usually identified with an infinite wall at $x=0$.

We can now define what is a Hermitian operator and what is a self-adjoint operator. Consider an operator $\hat{A}$ defined in a dense domain $D(\hat{A})$ of a Hilbert space. Its adjoint $\hat{A}^+$, whose domain is $D(\hat{A}^+)$, is such that for all ϕ and $\varphi \in D(\hat{A})$,

$$(\hat{A}^+\phi,\varphi)=(\phi,\hat{A}\varphi). \tag{10}$$

The operator $\hat{A}$ is Hermitian if its action is the same as the action of $\hat{A}^+$ and if the domain of its adjoint $\hat{A}^+$, $D(\hat{A}^+)$, is such that $D(\hat{A})\subset D(\hat{A}^+)$, that is, the domain of the operator is contained in the domain of the adjoint. If the action of $\hat{A}$ is the same as the action of $\hat{A}^+$ and $D(\hat{A})=D(\hat{A}^+)$, the operator is self-adjoint. The domain of the adjoint is deduced from Eq. (10) as we shall see in the examples.

III. HOW DO WE KNOW IF AN OPERATOR IS SELF-ADJOINT?

We now show by examples how we can determine if an operator has a family of self-adjoint extensions and the number of parameters on which this family depends. As a bonus we learn how to tell if an operator is self-adjoint.

A. Example 1, part 1: A free particle in the right half of the real line

Consider the operator $-d^2/dx^2$ defined in the domain of functions $\varphi(x)$, $0\leqslant x<\infty$, such that φ vanishes near the origin.[11] The functions $\varphi(x)$ are continuous and infinitely differentiable. All the functions in the domain vanish in a small, but finite interval $[0,a]$ where $a>0$ is an arbitrary real number, and also for $x>b>a$, another arbitrary real number. The condition $\int_0^\infty|\varphi(x)|^2dx<\infty$ is automatically satisfied. An example of such a function is $u_{ab}(x)=0$ for $0\leqslant x\leqslant a$ and $x\geqslant b$ and $u_{ab}(x)=\exp[1/((x-a)(x-b))]$ for $a<x<b$.

This operator is Hermitian as we have seen in Sec. II. Let $\varphi_1(x)$ be a function in the domain defined above. Then $\varphi_1(x)$ vanishes in the neighborhood of $x=0$ and so does $d\varphi_1(x)/dx$. Therefore the right-hand side of Eq. (5) is zero even if $\varphi_2(x)\neq 0$, and hence, the domain of the adjoint is a subset of absolutely continuous functions that vanish as $x\to\infty$ of $L_2[0,\infty]$ and that remain in the domain when acted on by the operator.

To see if this operator can be extended to a family of self-adjoint operators, that is, if we can construct self-adjoint operators from it, we consider

$$-\frac{d^2\Psi_+(x)}{dx^2}=i\eta\Psi_+(x), \tag{11}$$

$$-\frac{d^2\Psi_-(x)}{dx^2}=-i\eta\Psi_-(x), \tag{12}$$

where η is a real number introduced for dimensional reasons only.

Let n_+ and n_- be the numbers of linearly independent solutions of Eqs. (11) and (12), respectively, that are in the domain of the adjoint. The numbers n_+ and n_- are called deficiency indexes. If $n_+=n_-=n$, the operator can be extended, and n^2 is equal to the number of the parameters of the resulting family of self-adjoint operators. As we shall see, the parameters appear in the boundary conditions imposed on the functions at $x=0$. If $n_+=n_-=0$, the operator is self-adjoint.

It is easy to see that Eqs. (11) and (12) have solutions in the domain of the adjoint:

$$\Psi_+(x)=e^{-e^{-(\pi/4)i}\eta^{(1/2)}x}, \tag{13}$$

$$\Psi_-(x)=e^{-e^{(\pi/4)i}\eta^{(1/2)}x}. \tag{14}$$

So $n_+=n_-=1$, and we conclude that the operator can be extended, that is, there is a one parameter family of self-adjoint operators. The operators depend on the boundary condition at $x=0$, which contains one parameter. As we know the boundary condition is

$$\frac{d\varphi(0)}{dx}=\kappa\varphi(0), \tag{15}$$

where κ can be any real number.

B. Example 2, part 1: The delta function potential as a self-adjoint extension

We will now show an example of an Hermitian operator that when extended, will correspond to a free particle except for a delta function at the origin. Consider the operator $-d^2/dx^2$ defined in the following domain. Let $f(x)$ be a function of the domain. Then $f(x)$ and $df(x)/dx$ are absolutely continuous, $d^2f(x)/dx^2\in L_2[0,\infty]$, and $f(0)=0$. This operator is Hermitian and the domain of the adjoint can be calculated as follows. We use Eq. (4) and integrate from $-\infty\to 0^-$ and from $0^+\to\infty$ to obtain

$$\begin{aligned}\int_{-\infty}^{+\infty}-\frac{d^2\varphi_2^*(x)}{dx^2}\varphi_1(x)dx-\int_{-\infty}^{+\infty}\varphi_2^*(x)\left[-\frac{d^2\varphi_1(x)}{dx^2}\right]dx\\ =\varphi_2^*(0^-)\frac{d\varphi_1(0^-)}{dx}-\varphi_2^*(0^+)\frac{d\varphi_1(0^+)}{dx}\\ -\frac{d\varphi_2^*(0^-)}{dx}\varphi_1(0^-)+\frac{d\varphi_2^*(0^+)}{dx}\varphi_1(0^+).\end{aligned} \tag{16}$$

We set the right hand side of Eq. (16) to zero. Because $\varphi_1(0^-)=\varphi_1(0^+)=0$, we have that $d\varphi_2^*(0^+)/dx-d\varphi_2^*(0^-)/dx=\delta$ (where δ is any number); because $d\varphi_1(0^-)/dx=d\varphi_1(0^+)/dx$, we have $\varphi_2^*(0^-)=\varphi_2^*(0^+)$. Therefore, the domain of the adjoint consists of functions that are absolutely continuous with first derivatives absolutely continuous except at the origin where they have an arbitrary discontinuity. Therefore the operator is Hermitian.

To see if this operator can be extended to a family of self-adjoint operators, that is, if we can construct self-adjoint operators from it, we consider

$$-\frac{d^2\Psi_\pm}{dx^2}=\pm i\eta\Psi_\pm, \tag{17}$$

where the constant η is included for dimensional reasons only. Equation (17) has solutions

$$\Psi_+(x)=\begin{cases} e^{(e^{-i(\pi/4)})\eta^{(1/2)}x} & \text{for } -\infty<x<0\\ e^{-(e^{-i(\pi/4)})\eta^{(1/2)}x} & \text{for } 0<x<\infty,\end{cases} \tag{18}$$

$$\Psi_-(x)=\begin{cases} e^{(e^{i(\pi/4)})\eta^{(1/2)}x} & \text{for } \infty<x<0\\ e^{-(e^{i(\pi/4)})\eta^{(1/2)}x} & \text{for } 0<x<\infty.\end{cases} \tag{19}$$

Thus, $n_+=n_-=1$, and we conclude that the operator can be extended, that is, there is a one parameter family of self-adjoint operators. The operators depend on the boundary condition at $x=0$, which contains one parameter. As we shall see in Sec. IV, the boundary condition corresponds to a delta function at the origin.

In the next example we consider an operator with the same action but with a different domain. We shall see that the deficiency indices are different and in Sec. IV we shall see that the family of self-adjoint extensions is different. In fact, they will contain the present case as a special case. This example and the next illustrate the importance of the domain of the Hermitian operator from which one starts to construct the family of self-adjoint operators.

C. Example 3, part 1: A free particle in the real line from which the origin has been removed

In this example we consider a Hermitian operator that can be extended to a family of four parameter self-adjoint operators. Those operators represent the most general point interaction at the origin. The delta function considered in the previous example is a particular example of a point interaction.

Consider the operator $-d^2/dx^2$ defined in the whole real line with the origin removed.[12] So the functions in this domain are not defined for $x=0$; the functions $u_{abcd}(x)$ belonging to this domain vanish around $x=0$, that is for $-a<x<b$ and also for $x<-c$ and for $x>d$, where a, b, c, and d are arbitrary positive numbers. Therefore the domain of this operator consists of functions that vanish before the point $x=0$ from the negative and positive sides and for large distances in both positive and negative directions.

This operator is clearly Hermitian. Consider $\varphi_1(x)$ belonging to the domain of the operator (as defined above) and an arbitrary absolutely continuous $\varphi_2(x)$. Then using Eq. (4) and integrating from $-\infty$ to 0^- and from 0^+ to ∞, we obtain

$$\int_{-\infty}^{+\infty} - \frac{d^2\varphi_2^*(x)}{dx^2}\varphi_1(x)dx - \int_{-\infty}^{+\infty}\varphi_2^*(x)\left[-\frac{d^2\varphi_1(x)}{dx^2}\right]dx$$
$$=\varphi_2^*(0^-)\frac{d\varphi_1(0^-)}{dx}-\varphi_2^*(0^+)\frac{d\varphi_1(0^+)}{dx}$$
$$-\frac{d\varphi_2^*(0^-)}{dx}\varphi_1(0^-)+\frac{d\varphi_2^*(0^+)}{dx}\varphi_1(0^+). \tag{20}$$

The second line vanishes because $\varphi_1(0^-)=\varphi_1(0^+)=0$; also $d\varphi_1(0^-)/dx=d\varphi_1(0^+)/dx=0$ independent of the corresponding values of $\varphi_2^*(0^\pm)$. Thus we obtain

$$\int_{-\infty}^{+\infty} - \frac{d^2\varphi_2^*(x)}{dx^2}\varphi_1(x)dx - \int_{-\infty}^{+\infty}\varphi_2^*(x)\left[-\frac{d^2\varphi_1(x)}{dx^2}\right]dx$$
$$=0. \tag{21}$$

The domain of the adjoint is the set of all square integrable functions from $-\infty$ to ∞ that vanishes when $x\to\pm\infty$, but are not defined at $x=0$. The functions also are absolutely continuous from $-\infty\to 0^-$ and from $0^+\to\infty$, and remain in the set when acted on by the operator. To see if this operator can be extended to a self-adjoint operator, consider

$$-\frac{d^2\Psi_\pm(x)}{dx^2}=\pm i\eta\Psi_\pm(x). \tag{22}$$

It is easy to see that there are two solutions for the positive sign and two for the negative sign, so that $n_+=n_-=2$. The solutions are

$$\Psi_+^1=\begin{cases}0, & -\infty<x<0\\ e^{-e^{-(\pi/4)i}\eta^{(1/2)}x}, & 0<x<\infty,\end{cases} \tag{23}$$

$$\Psi_+^2=\begin{cases}e^{e^{-(\pi/4)i}\eta^{(1/2)}x}, & -\infty<x<0\\ 0, & 0<x<\infty,\end{cases} \tag{24}$$

$$\Psi_-^1=\begin{cases}0, & -\infty<x<0\\ e^{-e^{+(\pi/4)i}\eta^{(1/2)}x}, & 0<x<\infty,\end{cases} \tag{25}$$

$$\Psi_-^2=\begin{cases}e^{e^{+(\pi/4)i}\eta^{(1/2)}x}, & -\infty<x<0\\ 0, & 0<x<\infty.\end{cases} \tag{26}$$

Therefore, as we shall see, we can create self-adjoint operators by imposing suitable boundary conditions on the wave functions at the origin. The boundary conditions will depend on four parameters.

D. Example 4, part 1: A free particle in the plane from which the origin has been removed

In this example we consider an example of a Hermitian operator that can be extended to one parameter family of self-adjoint extensions which represent a renormalized two-dimensional delta function.

Consider the operator $-\nabla^2$ in two dimensions. In polar coordinates the radial part of the action of this operator (for angular momentum zero) is given by

$$H=-\frac{1}{r}\frac{d}{dr}\left(r\frac{d}{dr}\right). \tag{27}$$

To complete the definition we specify the domain which we take to be $C_0^\infty\{R^2\backslash\{0\}\}$, that is, functions that are continuous, infinitely differentiable, and vanish before the point $r=0$ and for $r>b$, where b is an arbitrary positive number that varies from function to function. In Example 2, we removed the origin from the real line. In the present case we remove the point $r=0$ from the plane.

It is easy to check that this operator is Hermitian. Take $\varphi_1(r)$ belonging to the domain of the operator (as we defined) and an arbitrary $\varphi_2(r)$. If we use integration by parts, we obtain

$$(H\varphi_2(r),\varphi_1(r))-(\varphi_2(r),H\varphi_1(r))$$
$$=-\int_0^\infty dr\, r\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}\right)\varphi_2^*(r)\varphi_1(r)$$
$$+\int_0^\infty dr\, r\varphi_2^*(r)\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}\right)\varphi_1(r)$$
$$=\lim_{r\to 0} r\left[\frac{d\varphi_2^*(r)}{dr}\varphi_1(r)-\varphi_2^*(r)\frac{d\varphi_1(r)}{dr}\right]. \tag{28}$$

The second line vanishes for all values of $\varphi_2^*(0)$ and $d\varphi_2^*(0)/dr$ because $\varphi_1(0)=0$ and $d\varphi_1(0)/dr=0$. Thus we obtain

$$(H\varphi_2(r),\varphi_1(r))-(\varphi_2(r),H\varphi_1(r))=0. \tag{29}$$

The domain of the adjoint is all absolutely continuous functions of $L_2([0,\infty);r\,dr)$, that is, functions $\varphi(r)$ that vanish when $r \to \infty$ such that $\int_0^\infty |\varphi(r)|^2 r\, dr < \infty$. To see if this operator can be extended, we have to examine the solutions of

$$-\frac{1}{r}\frac{d}{dr}\left(r\frac{d}{dr}\right)\Psi_{\pm}(r) = \pm i\eta\Psi_{\pm}(r), \tag{30}$$

or

$$-\frac{d^2}{dr^2}\Psi_{\pm}(r) - \frac{1}{r}\frac{d}{dr}\Psi_{\pm}(r) - (\pm i)\eta\Psi_{\pm}(r) = 0. \tag{31}$$

Equation (31) has two normalizable solutions, namely,

$$\Psi_{\pm}(r) = K_0(e^{\mp i(\pi/4)}\eta^{1/2} r). \tag{32}$$

Therefore, $n_+ = n_- = 1$, and the operator given by Eq. (27) has a one-parameter family of self-adjoint extensions.

Exercise 1: Consider the operator given by Eq. (27). Use the unitary transformation,

$$U: L_2([0,\infty); r\, dr) \to L_2([0,\infty); dr) \quad (Uf)(r) = r^{-1/2} f(r), \tag{33}$$

to show that the action of the operator becomes

$$-\frac{d^2}{dr^2} - \frac{1}{4r^2}. \tag{34}$$

Define its domain as $C_0^\infty((0,\infty)/\{0\})$ and show that the deficiency indices are $n_+ = n_- = 1$.

E. Example 5, part 1: A free Dirac particle in the real line from which the origin has been removed

The kinetic energy operator is given by

$$H_D = -i\alpha\frac{d}{dx} + \beta m, \tag{35}$$

where

$$\alpha = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \tag{36}$$

$$\beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \tag{37}$$

We take the domain to be $(C_0^\infty(R\backslash\{0\}))^2$, which means that the two components are both continuous, infinitely differentiable, and vanish for $r < a < b$ and for $r > b$ and also for $r > -a' > -b$ and $r > -b'$, where a, b, a', and b' are arbitrary positive numbers that depend on the function. Note that the constants for the upper components need not be equal to the constants for the lower component. In this domain the operator of Eq. (35) is Hermitian. Consider $\varphi_1(x)$ belonging to the domain of the operator (as we defined) and an arbitrary $\varphi_2(x)$. Then if we use integration by parts, we obtain

$$[H_D\varphi_2(x), \varphi_1(x)) - (\varphi_2(x), H_D\varphi_1(x)] = \varphi_2^*(0^+)\alpha\varphi_1(0^+) - \varphi_2^*(0^-)\alpha\varphi_1(0^-). \tag{38}$$

The expression in Eq. (38) vanishes because $\varphi_1(0^-) = \varphi_1(0^+) = 0$, independent of the values of $\varphi_2^*(0^\pm)$.

To see if we can extend the operator H_D, we look at a square-integrable, two-component function that satisfies

$$H_D\Psi_+(r) = +i\eta\Psi_+(r), \tag{39}$$

$$H_D\Psi_-(r) = -i\eta\Psi_-(r). \tag{40}$$

It is not very difficult to see that $n_+ = n_- = 2$. So again we have a four parameter family of self-adjoint extensions. We define the function (note that the zero has been removed)

$$\xi(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{if } x < 0. \end{cases} \tag{41}$$

The solutions are

$$\Psi_+^1 = \begin{pmatrix} e^{-(\eta^2+m^2)^{(1/2)}x}\xi(x) \\ -\left[\dfrac{m-i\eta}{m+i\eta}\right]^{1/2} e^{-(\eta^2+m^2)^{(1/2)}x}\xi(x) \end{pmatrix}, \tag{42}$$

$$\Psi_+^2 = \begin{pmatrix} e^{(\eta^2+m^2)^{1/2}x}\xi(-x) \\ +\left[\dfrac{m-i\eta}{m+i\eta}\right]^{1/2} e^{-(\eta^2+m^2)^{(1/2)}x}\xi(-x) \end{pmatrix}, \tag{43}$$

$$\Psi_-^1 = \begin{pmatrix} e^{-(\eta^2+m^2)^{(1/2)}x}\xi(x) \\ -\left[\dfrac{m-i\eta}{m+i\eta}\right]^{1/2} e^{-(\eta^2+m^2)^{1/2}x}\xi(x) \end{pmatrix}, \tag{44}$$

$$\Psi_-^2 = \begin{pmatrix} e^{(\eta^2+m^2)^{(1/2)}x}\xi(-x) \\ +\left[\dfrac{m-i\eta}{m+i\eta}\right]^{1/2} e^{(\eta^2+m^2)^{(1/2)}x}\xi(-x) \end{pmatrix}. \tag{45}$$

F. Example 6, part 1: A free Dirac particle in a plane from which the origin has been removed

In polar coordinates the radial part of the action of the kinetic energy operator for the zero angular momentum part is

$$H_{2D} = \begin{pmatrix} m & -\left(\dfrac{d}{dr} + \dfrac{1}{r}\right) \\ \dfrac{d}{dr} & -m \end{pmatrix}. \tag{46}$$

It is easy to see that

$$H_{2D}\Psi_{\pm} = \pm im\Psi_{\pm}, \tag{47}$$

(where m has been introduced for dimensional reasons) has solutions

$$\Psi_{\pm} = \begin{pmatrix} K_0(\sqrt{2}mr) \\ -e^{\mp i(\pi/4)}K_1(\sqrt{2}mr) \end{pmatrix}, \tag{48}$$

but these solutions are not normalizable. So the operator is self-adjoint. As we shall see, the above result means that, for instance, we cannot put a δ function at the origin.[13]

IV. BOUNDARY CONDITIONS

We now show how the boundary conditions can be determined. As we have seen in Sec. III, a Hermitian operator can be extended to a self-adjoint operator if the number of square-integrable solutions of $\hat{A}\Psi_{\pm} = \pm i\eta\Psi_{\pm}$, which we called n_+ and n_-, are equal. The first step in determining the boundary conditions is to construct a unitary operator U that relates functions Ψ_+ and Ψ_-.

A. Example 1, part 2: A free particle in the right half of the real line

As we have seen, the solutions of Eqs. (11) and (12) for this case are

$$\Psi_+(x)=e^{-e^{-(\pi/4)i}\eta^{(1/2)}x}, \quad \Psi_-(x)=e^{-e^{(\pi/4)i}\eta^{(1/2)}x}. \tag{49}$$

The unitary matrix relating the subspace generated by $\Psi_+(x)$ to the subspace generated by $\Psi_-(x)$ is therefore one-dimensional, that is, just a complex number of modulus one. Hence, the self-adjoint extensions depend on one parameter only. We set $U=\alpha$ with $|\alpha|=1$.

The prescription for obtaining the boundary conditions is simply to require that

$$\int_0^\infty -\frac{d^2(\Psi_+(x)+\alpha\Psi_-(x))^*}{dx^2}\varphi(x)dx = \int_0^\infty (\Psi_+(x)+\alpha\Psi_-(x))^*\left[-\frac{d^2\varphi(x)}{dx^2}\right]dx. \tag{50}$$

Equation (50) is equivalent to Eq. (6) with φ_2's replaced by $\Psi_+(x)+\alpha\Psi_-(x)$. We use Eq. (5) to obtain

$$(\Psi_+(0)+\alpha\Psi_-(0))^*\frac{d\varphi(0)}{dx} - \frac{d(\Psi_+(0)+\alpha.\Psi_-(0))^*}{dx}\varphi(0)=0. \tag{51}$$

If we replace the values of $\Psi_+(0)$, $\Psi_-(0)$, $d\Psi_+(0)/dx$, and $d\Psi-(0)/dx$ by using Eq. (49), we obtain

$$(1+\alpha^*)\frac{d\varphi(0)}{dx}+(e^{(\pi/4)i}\eta^{1/2}+\alpha^* e^{-(\pi/4)i}\eta^{1/2})\varphi(0)=0, \tag{52}$$

or if we let $\alpha=e^{i\vartheta}$,

$$\frac{1}{\varphi(0)}\frac{d\varphi(0)}{dx}=\eta^{1/2}\cos\left(\frac{\vartheta}{2}+\frac{\pi}{4}\right)\Big/\cos\frac{\vartheta}{2}=\kappa, \tag{53}$$

in agreement with the result obtained in Eq. (9). Note that the constant η was absorbed in the constant κ. The fact that the constant η can be absorbed is general and is the reason why mathematicians set $\eta=1$ from the very beginning.

B. Example 2, part 2: The delta function potential as a self-adjoint extension

We now explain how to obtain the boundary conditions. As we shall see, the boundary conditions will be the ones obtained heuristically by considering a delta function at the origin.

We found in Sec. III that Eq. (17) has one solution each in the domain of the adjoint. The unitary matrix relating the subspace generated by $\Psi_+(x)$ to the subspace generated by $\Psi_-(x)$ is therefore one-dimensional, that is, just a complex number of modulus one, $e^{i\alpha}$. The prescription to obtain the boundary conditions is simply to require that

$$\int_{-\infty}^\infty -\frac{d^2(\Psi_+(x)+e^{i\alpha}\Psi_-(x))^*}{dx^2}\varphi(x)dx = \int_{-\infty}^\infty (\Psi_+(x)+e^{i\alpha}\Psi_-(x))^*\left[-\frac{d^2\varphi(x)}{dx^2}\right]dx. \tag{54}$$

If we use Eq. (16), we find

$$\begin{aligned}(\Psi_+(0^-)+e^{i\alpha}\Psi_-(0^-))^*\frac{d(\varphi(0^-)}{dx}-(\Psi_+(0^+)\\ +e^{i\alpha}\Psi_-(0^+))^*\frac{d(\varphi(0^+)}{dx}\\ -\frac{d(\Psi_+(0^-)+e^{i\alpha}\Psi_-(0^-))^*}{dx}\varphi(0)\\ +\frac{d(\Psi_+(0^+)+e^{i\alpha}\Psi_-(0^+))^*}{dx}\varphi(0)=0.\end{aligned} \tag{55}$$

We replace the values of $\Psi_+(0^+)$, $\Psi_-(0^+)$, $d\Psi_+(0^+)/dx$, etc., and obtain

$$\frac{d\varphi(0^+)}{dx}-\frac{d\varphi(0^-)}{dx}=-\frac{2\eta^{1/2}\cos\left(\frac{\pi}{4}+\frac{\alpha}{2}\right)}{\cos\left(\frac{\alpha}{2}\right)}\varphi(0) = g\varphi(0), \tag{56}$$

where g is an arbitrary real number. Equation (56) is the boundary condition when we treat the Schrödinger equation formally, by considering heuristically a delta function at the origin. However, as will be explained in Sec. V, the heuristic procedure for obtaining the boundary conditions is not strictly correct.

C. Example 3, part 2: A free particle in the real line from which the origin has been removed

We found in Sec. III that Eq. (22) of Example 2 has two linearly independent solutions for each sign. Therefore the subspace generated by $\Psi_+^1(x)$ and $\Psi_+^2(x)$ is two-dimensional, and so is the subspace generated by $\Psi_-^1(x)$ and $\Psi_-^2(x)$. The mapping between the two subspaces is given by a 2×2 unitary matrix U given by

$$U=\begin{pmatrix} u_{11} & u_{12}\\ u_{21} & u_{22}\end{pmatrix}=\begin{pmatrix} \cos b e^{i(c+a)} & i\sin b e^{-i(d-a)}\\ i\sin b e^{i(d+a)} & \cos b e^{-i(c-a)}\end{pmatrix}. \tag{57}$$

Then the boundary conditions can be obtained by enforcing

$$\int_{-\infty}^{+\infty}\left[\frac{d^2}{dx^2}(\Psi_+^1(x)+u_{11}\Psi_-^1(x)+u_{12}\Psi_-^2(x))\right]^*\varphi(x)dx = \int_{-\infty}^{+\infty}[\Psi_+^1(x)+u_{11}\Psi_-^1(x)+u_{12}\Psi_-^2(x)]^*\frac{d^2\varphi}{dx^2}dx, \tag{58}$$

$$\int_{-\infty}^{+\infty}\left[\frac{d^2}{dx^2}(\Psi_+^2(x)+u_{21}\Psi_-^1(x)+u_{22}\Psi_-^2(x))\right]^*\varphi(x)dx$$
$$=\int_{-\infty}^{+\infty}[\Psi_+^2(x)+u_{21}\Psi_-^1(x)+u_{22}\Psi_-^2(x)]^*\frac{d^2\varphi}{dx^2}dx. \tag{59}$$

That is, we enforce Eq. (21) with φ_2 replaced by $\Psi_+^1(x)+u_{11}\Psi_-^1(x)+u_{12}\Psi_-^2(x)$, and $\Psi_+^2(x)+u_{21}\Psi_-^1(x)+u_{22}\Psi_-^2(x)$, respectively, where $\Psi_+^1(x)$, $\Psi_+^2(x)$, $\Psi_-^1(x)$, and $\Psi_-^2(x)$ are given by Eqs. (23)–(26).

If we use Eq. (20) and Eqs. (23)–(26), we find from Eqs. (58) and (59) that

$$(1+u_{11}^*)\varphi'(0^+)+(e^{i(\pi/4)}+e^{-i(\pi/4)}\eta^{1/2}u_{11}^*)\varphi(0^+)$$
$$-u_{12}^*\varphi'(0^-)+e^{-i(\pi/4)}\eta^{1/2}u_{12}^*\varphi(0^-)=0, \tag{60}$$

$$u_{21}^*\varphi'(0^+)+e^{-i(\pi/4)}\eta^{1/2}u_{21}^*\varphi(0^+)-(1+u_{22}^*)\varphi'(0^-)$$
$$+(e^{i(\pi/4)}+e^{-i(\pi/4)}u_{22}^*\eta^{1/2})\varphi(0^-)=0, \tag{61}$$

where $\varphi'(0^\pm)=d\varphi(0^\pm)/dx$.

To bring Eqs. (60) and (61) to a more familiar form, we multiply Eq. (60) by $e^{-i(\pi/4)}u_{21}^*$ and Eq. (61) by $e^{i(\pi/4)}(1-iu_{11}^*)$. Then we subtract the two resultant equations and replace u_{11}^* by its value given by Eq. (57), assuming that $\sin b\neq 0$:

$$\varphi'(0^+)=e^{id}\left[\sqrt{2}\left(\frac{\cos\left(a+\frac{\pi}{4}\right)-\cos b\,\sin\left(c-\frac{\pi}{4}\right)}{\sin b}\right)\right]$$
$$\times\varphi'(0^-)$$
$$+e^{id}\left[\sqrt{2}\left(\frac{\sin a-\cos b\,\cos c}{\sin b}\right)\right]\varphi(0^-)\,\eta^{1/2}. \tag{62}$$

We let

$$\alpha'=\sqrt{2}\left(\frac{\cos\left(a+\frac{\pi}{4}\right)-\cos b\,\sin\left(c-\frac{\pi}{4}\right)}{\sin b}\right), \tag{63}$$

$$\beta'=\sqrt{2}\left(\frac{\sin a-\cos b\,\cos c}{\sin b}\right), \tag{64}$$

$$\vartheta'=d. \tag{65}$$

Then Eq. (62) can be written as

$$\varphi'(0^+)=e^{i\vartheta'}[\alpha'\varphi'(0^-)+\beta'\eta^{1/2}\varphi(0^-)]. \tag{66}$$

Similarly, if we multiply Eq. (60) by u_{21}^* and Eq. (61) by $(1-u_{11}^*)$ and subtract the resulting equations, we obtain

$$\eta^{1/2}\varphi(0^+)=-e^{id}\left[\sqrt{2}\left(\frac{\cos a+\cos b\,\cos c}{\sin b}\right)\right]\varphi'(0^-)$$
$$+e^{id}\left[\sqrt{2}\left(\frac{\cos\left(a+\frac{\pi}{4}\right)+\cos b\,\sin\left(c+\frac{\pi}{4}\right)}{\sin b}\right)\right]$$
$$\times\varphi(0^-)\,\eta^{1/2}. \tag{67}$$

We let

$$\delta'=-\sqrt{2}\left(\frac{\cos a+\cos b\,\cos c}{\sin b}\right), \tag{68}$$

$$\gamma'=\sqrt{2}\left(\frac{\cos\left(a+\frac{\pi}{4}\right)+\cos b\,\sin\left(c+\frac{\pi}{4}\right)}{\sin b}\right), \tag{69}$$

and write Eq. (67) as

$$\eta^{1/2}\varphi(0^+)=e^{i\vartheta'}\big(\delta'\varphi'(0^-)+\gamma'\eta^{1/2}\varphi(0^-)\big). \tag{70}$$

Thus we can express the results of Eqs. (66) and (70) as follows:

$$\begin{pmatrix}\varphi'(0^+)\\ \eta^{1/2}\varphi(0^+)\end{pmatrix}=e^{i\vartheta'}\begin{pmatrix}\alpha' & \beta'\\ \delta' & \gamma'\end{pmatrix}\begin{pmatrix}\varphi'(0^-)\\ \eta^{1/2}\varphi(0^-)\end{pmatrix}, \tag{71}$$

and it is easy to verify that the real parameters α', β', γ', and δ' satisfy $\alpha'\gamma'-\beta'\delta'=1$.

On the other hand, if $u_{12}=u_{21}=0$, that is, if $\sin b=0$, Eqs. (60) and (61) become

$$\varphi'(0^\pm)=\varkappa^\pm\varphi(0^\pm), \tag{72}$$

where $\varkappa^\pm$ is any real number. The meaning of Eq. (72) is that the two sides of the real line became decoupled.

The constant η in Eq. (71) can be easily absorbed in the constants β' and δ' by dividing the second equation by $\eta^{1/2}$. As mentioned, the fact that the constant can be absorbed is general and the constant η could have been set equal to unity from the beginning. From Eq. (71) we have

$$\begin{pmatrix}\varphi'(0^+)\\ \varphi(0^+)\end{pmatrix}=e^{i\vartheta}\begin{pmatrix}\alpha & \beta\\ \delta & \gamma\end{pmatrix}\begin{pmatrix}\varphi'(0^-)\\ \varphi(0^-)\end{pmatrix}, \tag{73}$$

where $\alpha'=\alpha$, $\beta=\beta'\eta^{1/2}$, $\delta=\delta/\eta^{1/2}$, $\gamma=\gamma'$, and $\vartheta=\vartheta'$.

The physics of the boundary conditions given by Eq. (73) was studied in Refs. 14 and 15. We shall return to the physics of the above boundary conditions in Sec. V.

D. Example 4, part 2: A free particle in the plane from which the origin has been removed

As we have shown, the solutions of Eq. (31) are

$$\Psi_\pm(r)=K_0(e^{\mp i(\pi/4)}\eta^{1/2}r). \tag{74}$$

The subspace generated by $\Psi_+(r)$ is one-dimensional and so is the space generated by $\Psi_-(r)$. Therefore the unitary matrix mapping the two subspaces is just a complex number of modulus one, $e^{i\theta}$. Thus the self-adjoint extensions depend on one parameter only.

The boundary conditions are obtained by enforcing:

$$-\int_0^\infty drr\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}\right)(\Psi_+(r)+e^{i\theta}\Psi_-(r))^*\varphi(r)$$
$$=-\int_0^\infty drr(\Psi_+(r)+e^{i\theta}\Psi_-(r))^*\left(\frac{d^2}{dr^2}+\frac{1}{r}\frac{d}{dr}\right)\varphi(r), \tag{75}$$

which is the condition of Eq. (29) with $\varphi_2(r)$ replaced by $\Psi_+(r)+e^{i\theta}\Psi_-(r)$. If we use Eq. (28), we obtain

$$\lim_{r\to 0} r\left[\frac{d}{dr}(\Psi_+(r)+e^{i\theta}\Psi_-(r))^*\varphi(r)\right.$$
$$\left. -\left(\left[\Psi_+(r)+e^{i\theta}\Psi_-(r)\right]^*\frac{d}{dr}\varphi(r)\right)\right]=0. \tag{76}$$

We replace $\Psi_\pm(r)$ by using Eq. (32) and take into account the behavior at the origin of the functions[16]

$$K_0(z)\sim -\ln\frac{z}{2}-\gamma, \tag{77}$$

$$K_1(z)\sim\frac{1}{z}, \tag{78}$$

where $\gamma=0.5772$ is the Euler constant. If we also use that[16]

$$\frac{d}{dz}K_0(z)=-K_1(z), \tag{79}$$

we find that Eq. (76) gives

$$\lim_{r\to 0}\left\{\varphi-r\frac{d\varphi}{dr}\{\ln r+\beta\}\right\}=0, \tag{80}$$

where $\beta=-(\pi/4)\,\mathrm{tg}(\theta/2)+\ln(\eta/2)+\gamma$ can be any real number.

The physics of the boundary conditions given by Eq. (80) was studied by a limiting procedure in Refs. 13 and 17.

Exercise 2: Show that the one parameter family of boundary conditions for the operator given by Eq. (34) is

$$\alpha\phi_0+\phi_1=0, \tag{81}$$

where

$$\phi_0=\lim_{r\to 0}(r^{1/2}\ln r)^{-1}\varphi(r),$$
$$\phi_1=\lim_{r\to 0} r^{-1/2}[\varphi(r)-\phi_0 r^{1/2}\ln r]. \tag{82}$$

(See p. 98 of Ref. 18 and Appendix B for the solution.)

E. Example 5, part 2: A free Dirac particle in the real line from which the origin has been removed

As shown in Sec. III, each of Eqs. (39) and (40) has two linearly independent solutions. Thus the subspace generated by $\Psi_+^1(x)$ and $\Psi_+^2(x)$ is two-dimensional, and so is the subspace generated by the solutions $\Psi_-^1(x)$ and $\Psi_-^2(x)$. The mapping between the two subspaces is given by a 2×2 unitary matrix U.

Let us take U to be identical to Eq. (57) of Example 3:

$$U=\begin{pmatrix} u_{11} & u_{12}\\ u_{21} & u_{22}\end{pmatrix}=\begin{pmatrix}\cos b e^{i(c+a)} & i\sin b e^{-i(d-a)}\\ i\sin b e^{i(d+a)} & \cos b e^{-i(c-a)}\end{pmatrix}. \tag{83}$$

Thus the boundary conditions are obtained by enforcing

$$(H_D(\Psi_+^1(x)+u_{11}\Psi_-^1(x)+u_{12}\Psi_-^2(x))^*,\varphi(x))$$
$$=((\Psi_+^1(x)+u_{11}\Psi_-^1(x)+u_{12}\Psi_-^2(x))^*,H_D\varphi(x)), \tag{84}$$

$$[H_D(\Psi_+^2(x)+u_{21}\Psi_-^1(x)+u_{22}\Psi_-^2(x))^*,\varphi(x)]$$
$$=[(\Psi_+^2(x)+u_{21}\Psi_-^1(x)+u_{22}\Psi_-^2(x))^*,H_D\varphi(x)]. \tag{85}$$

That is, we enforce Eq. (38) to vanish with φ_2 replaced by $\Psi_+^1(x)+u_{11}\Psi_-^1(x)+u_{12}\Psi_-^2(x)$ and $\Psi_+^2(x)+u_{21}\Psi_-^1(x)+u_{22}\Psi_-^2(x)$, respectively, where $\Psi_+^1(x),\Psi_-^1(x),\Psi_+^2(x)$, and $\Psi_-^2(x)$ are given by Eqs. (42)–(45).

If we write

$$\varphi(x)=\begin{pmatrix}\varphi_1(x)\\ \varphi_2(x)\end{pmatrix}, \tag{86}$$

and use Eq. (38) and Eqs. (42)–(45), then Eqs. (84) and (85) become

$$(1+u_{11}^*)\varphi_2(0^+)+(e^{i\arctan(\eta/m)}$$
$$+e^{-i\arctan(\eta/m)}u_{11}^*)\varphi_1(0^+)-u_{12}^*\varphi_2(0^-)$$
$$+e^{-i\arctan(\eta/m)}u_{12}^*\varphi_1(0^-)=0, \tag{87}$$

$$u_{21}^*\varphi_2(0^+)+e^{-i\arctan(\eta/m)}u_{21}^*\varphi_1(0^+)-(1+u_{22}^*)\varphi_2(0^-)$$
$$+(e^{i\arctan(\eta/m)}+e^{-i\arctan(\eta/m)}u_{22}^*)\varphi_1(0^-)=0. \tag{88}$$

If we take $\eta=m$, then Eqs. (87) and (88) become similar to Eqs. (60) and (61). To write Eqs. (87) and (88) in the form of Eq. (71), we have

$$\begin{pmatrix}\varphi_1(0^+)\\ \varphi_2(0^+)\end{pmatrix}=U\begin{pmatrix}\varphi_1(0^-)\\ \varphi_2(0^-)\end{pmatrix}, \tag{89}$$

where

$$U=e^{i\vartheta}\begin{pmatrix}\delta & \gamma\\ \alpha & \beta\end{pmatrix}, \tag{90}$$

where α, β, γ, δ, and ϑ are any real numbers satisfying $\beta\delta-\alpha\gamma=1$. On the other hand, if $u_{12}=u_{21}=0$, Eqs. (87) and (88) become

$$\varphi_2(0^\pm)=\varkappa^\pm\varphi_1(0^\pm), \tag{91}$$

where $\varkappa^\pm$ is any real number. The meaning of Eq. (91) is that the two sides of the real line became decoupled. The physics of the boundary conditions given by Eq. (89) was studied in Ref. 19.

F. Example 6, part 2: A free Dirac particle in a plane from which the origin has been removed

In this case the operator given by Eq. (46) was found to be self-adjoint. Some consequences of this fact will be considered in Sec. V.

V. PHYSICAL INTERPRETATION

We now discuss the implication of the different self-adjoint extensions of an operator. In all the examples we have presented the self-adjoint extensions were constructed by modifying the boundary conditions at one point. An interpretation of this modification is that there is an interaction that acts at that point. That is why the theory of self-adjoint extensions is particularly suitable for studying point interactions. For a good but advanced review see Ref. 18. Let us examine how our examples illustrate the concept of point interactions.

A. Example 1, part 3: A free particle in the right half of the real line

As we have seen the particle is confined to the half line $0 \leqslant x < \infty$ and does not cross the origin. This situation can be realized by imposing the boundary condition

$$\frac{1}{\varphi(0)} \frac{d\varphi(0)}{dx} = \kappa. \tag{92}$$

If κ is a finite negative number, the point $x=0$ is impenetrable, but attracts the particle. On the other hand, if κ is a finite positive number, the point $x=0$ is impenetrable but repels the particle. To see this we calculate the phase shift $\delta(k)$. It is easy to see that $k\cot(\delta(k))=\kappa$ and the scattering length is $a=-1/\kappa$. This effective range expansion is exact. If $\kappa<0$, there is a bound state as shown in Ref. 2. The scattering length is positive. If $\kappa>0$, there is no bound state and the effective interaction is repulsive.

B. Example 2, part 3: The delta function potential as a self-adjoint extension

In this example we found a family of self-adjoint extensions whose boundary conditions are the ones described in the literature for a particle moving in the line with a delta function in the origin. The treatment found in the literature is however not strictly correct as we shall now see.

The Schrödinger equation for the $\delta(x)$ interaction is

$$-\frac{d^2\varphi}{dx^2} + g\,\delta(x)\varphi(x) = E\varphi(x). \tag{93}$$

We integrate both sides of Eq. (93) from $-\epsilon$ to ϵ and let $\epsilon \to 0$ to determine the boundary conditions, assuming the continuity of $\varphi(x)$. However $g\,\delta(x)$ is not a proper operator in the Hilbert space, because

$$\int_{-\infty}^{\infty} |g\,\delta(x)\varphi(x)|^2 dx = g^2 \int_{-\infty}^{\infty} |\varphi(0)|^2 dx = \infty, \tag{94}$$

unless $\varphi(0)=0$.

C. Example 3, part 3: A free particle in the real line from which the origin has been removed

We saw in Example 3 that a particle moving on the real line from which the origin has been removed admits a four parameter family of self-adjoint extensions. Let us choose one set: $\alpha=1$, $\beta=g$, $\gamma=1$, $\delta=0$, and $\theta=0$. Then the boundary conditions reduce to

$$\varphi'(0^+) - \varphi'(0^-) = g\varphi(0^+), \tag{95}$$

and $\varphi(0^+)=\varphi(0^-)=\varphi(0)$. These are the boundary conditions obtained by formally manipulating the Schrödinger equation with a Dirac delta function potential of strength g at the origin. However, as already explained, it is not strictly correct to write

$$H = -\frac{d^2}{dx^2} + g\,\delta(x), \tag{96}$$

because the delta function potential is not a proper operator in the Hilbert space.

Other combinations of α, β, γ, δ, and θ can be used. Each combination results in a different point interaction at $x=0$. It is difficult to give an expression for the potentials represented by these boundary conditions. The reason is that the result of a delta function when acting in a discontinuous function is undefined as shown in Ref. 20. In particular, it is difficult to obtain the boundary conditions for the derivative of the delta function,

$$-\frac{d^2}{dx^2} + g'\frac{d\,\delta(x)}{dx}, \tag{97}$$

by formally manipulating the operator as was done for the delta function potential above.[14] However by renormalizing the strength of the delta functions and taking appropriate limits, it is possible to get a feeling for these generalized point interactions.[21]

D. Example 4, part 3: A free particle in the plane from which the origin has been removed

We now discuss the physical interpretation of the one family of self-adjoint extensions of a particle moving in the plane from which the origin has been removed. As mentioned, it is not possible in this case to make sense of the delta function potential at the origin. As shown in Ref. 17, if we assume a square-well potential of depth V_0 and radius ρ at the origin and take the limit $\rho \to 0$ and $V_0 \to -\infty$ such that $V_0\delta^2 \to -g$ so that the potential approaches $-g\,\delta^2(r)$, we find that the energy of the ground state goes to $-\infty$. This result means that the delta function potential in two dimensions is too strong. To remedy this problem we can make V_0 diverge more slowly. This limiting procedure is the meaning of the boundary condition given in Eq. (80) and obtained in Ref. 17, using a different method that we now explain in more detail.

Consider a particle moving in a plane, and assume that there is a point interaction at the origin, $\delta^2(\mathbf{r})$, which is the delta function in two dimensions,

$$-\frac{\hbar^2}{2m}\nabla^2\phi(\mathbf{r}) + g\,\delta^2(\mathbf{r})\phi(\mathbf{r}) = E\phi(\mathbf{r}). \tag{98}$$

We introduce polar coordinates (r,θ) and replace the $\delta^2(x)$ potential by a square well of depth V_0 and radius ρ. Because this potential is attractive in two dimensions, it always has at least one bound state.[22] Let $|E_b|$ be its energy. Because we are going to let $\rho \to 0$, we consider s waves only, because states with $l \neq 0$ will not be affected by the potential. We let

$$k = \left(\frac{2m}{\hbar^2}|E_b|\right)^{1/2}, \tag{99}$$

$$k_0 = \left(\frac{2m}{\hbar^2}(V_0 - |E_b|)\right)^{1/2}. \tag{100}$$

If we match the solutions at $r=\delta$, we have

$$-k_0[J_1(k_0\rho)/J_0(k_0\rho)] = -k[K_1(k\rho)/K_0(k\rho)]. \tag{101}$$

If we now let $\rho \to 0$ such that $|V_0|\rho^2 \to g$, so that the potential would approach $-g\,\delta^2(\mathbf{r})$, we find that the bound state energy diverges. So we have to renormalize the delta function. As explained in Ref. 17, we do this by letting $V_0 \to \infty$ as a function of ρ such that

$$\lim_{\rho\to 0} -k[K_1(k\rho)/K_0(k\rho)] = \lim_{\rho\to 0}\left[\rho\left(\ln\left(\frac{k\rho}{2}+\gamma\right)\right)\right]^{-1}. \tag{102}$$

Thus the limiting procedure (the renormalized delta function in two dimensions) is the physical meaning of the boundary condition given by Eq. (80).

Exercise 3: Compare Eq. (102) with Eq. (80) to obtain a physical interpretation for the arbitrary constant β of Eq. (80).

E. Example 5, part 3: A free Dirac particle in the real line from which the origin has been removed

The four parameter family of self-adjoint extensions of a Dirac particle moving in a line from which the origin has been removed is very similar to the Schrödinger case studied in Example 3. The different self-adjoint extensions are point interactions placed at the origin. Two particular cases were studied in Ref. 18, p. 400. The nonrelativistic limit of these interactions was studied in Ref. 19.

Exercise 4: Use the boundary conditions given by Eq. (89) to obtain the bound states and scattering states of a Dirac particle moving in one dimension with a generalized point interaction at the origin.[19]

F. Example 6, part 3: A free Dirac particle in a plane from which the origin has been removed

Finally in Example 6 we saw that it is impossible to extend the Hamiltonian of a Dirac particle in the plane from which the origin has been removed, because the operator so obtained is already self-adjoint. In Ref. 13 this problem was investigated by placing a square well potential at the origin and taking the appropriate limit. By doing this we obtained wave functions that are not normalizable at the origin. Therefore the procedure, unlike in the non-relativistic problem treated in Example 4, fails.

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APPENDIX A: A THEOREM

We show why the prescriptions adopted in Secs. II and III work. We do not give rigorous proofs, but only wish to make the results more natural. Rigorous proofs can be found, for instance, in Ref. 23.

The main result is the following: Let $\hat{O}$ be a Hermitian operator. If the equations,

$$\hat{O}\varphi^{\pm} = \pm i\varphi^{\pm}, \tag{A1}$$

have no square-integrable solutions, then $\hat{O}$ is self-adjoint. We know that if an operator is self-adjoint, then the action and the domain of $\hat{O}$ and $\hat{O}^{+}$ are identical.

Assume that there is a φ that belongs to the domain of $\hat{O}$ such that

$$\hat{O}\varphi = i\varphi. \tag{A2}$$

Then we must have

$$\hat{O}^{+}\varphi = i\varphi, \tag{A3}$$

and

$$-i(\varphi,\varphi) = (i\varphi,\varphi) = (\hat{O}\varphi,\varphi) = (\varphi,\hat{O}^{+}\varphi) = (\varphi,\hat{O}\varphi) = i(\varphi,\varphi), \tag{A4}$$

and hence $\varphi = 0$. So, if $\hat{O}$ is a self-adjoint operator, Eq. (A1) has only trivial solutions, that is, $\varphi^{\pm} = 0$, or has no square-integrable solutions.

Now let $\hat{O}$ be a Hermitian operator such that each of the equations

$$\hat{O}\Psi_{+} = i\Psi_{+}, \tag{A5}$$

$$\hat{O}\Psi_{-} = -i\Psi_{-}, \tag{A6}$$

has (for example) two normalizable linearly independent solutions, in the domain[24] of the $\hat{O}^{+}$ so that the deficiency indexes are $n_{+} = n_{-} = 2$. Let Ψ_{+}^{1} and Ψ_{+}^{2} be the two solutions of Eq. (A5) and Ψ_{-}^{1} and Ψ_{-}^{2} the corresponding solutions of Eq. (A6). We note that $\Psi_{+}^{i}(i=1,2)$ form a vector space of dimension two, and so do $\Psi_{-}^{i}(i=1,2)$. Let $D_{+}(\hat{O})$ be the vector space spanned by $\Psi_{+}^{i}(i=1,2)$ and $D_{-}(\hat{O})$ be the vector space spanned by $\Psi_{-}^{i}(i=1,2)$. Let U be a unitary application of $D_{+}(\hat{O})$ in $D_{-}(\hat{O})$ so that, for instance,

$$U\Psi_{+}^{i} = \sum_{j=1}^{2} u_{ij}\Psi_{-}^{j}. \tag{A7}$$

Define now a new domain for the operator

$$D(\hat{O}) = \{\varphi + \Psi_{+} + U\Psi_{+} \mid \varphi \in D(\hat{O}^{+}), \Psi_{+} \in D_{+}(\hat{O})\}. \tag{A8}$$

Hence the action of $\hat{O}$ in this new domain is

$$\hat{O}(\varphi + \Psi_{+} + U\Psi_{+}) = \hat{O}\varphi + i\Psi_{+} - iU\Psi_{+}. \tag{A9}$$

If we require that $\hat{O}$ be Hermitian in this new domain, then it becomes self-adjoint because in this new domain $\hat{O}\Psi_{\pm} = \pm i\Psi_{\pm}$ has no solution. The boundary conditions stem from the requirement that

$$\left(\hat{O}\left(\Psi_{+}^{i} + \sum_{j=1}^{2} u_{ij}\Psi_{-}^{j}\right),\varphi\right) = \left(\left(\Psi_{+}^{i} + \sum_{j=1}^{2} u_{ij}\Psi_{-}^{j}\right),\hat{O}\varphi\right). \tag{A10}$$

APPENDIX B: SOLUTION OF EXERCISE 2

We show how to go from the boundary condition (80) to the boundary condition (81). Because we are going to work close to the limit, we can write

$$r\frac{d\Psi(r)}{dr} = \Psi(r) - \lim_{r\to 0}\left(\frac{\Psi(r)}{\ln r}\right)\ln r. \tag{B1}$$

We replace Eq. (B1) in Eq. (80) and obtain

$$\lim_{r\to 0}\left(\Psi(r)-\Psi(r)\ln r+\left(\lim_{r\to 0}\frac{\Psi(r)}{\ln r}\right)\ln^2 r+\beta\Psi(r)\right.$$
$$\left.-\beta\left(\lim_{r\to 0}\frac{\Psi(r)}{\ln r}\right)\ln r\right)=0, \tag{B2}$$

which we write as

$$\lim_{r\to 0}\ln r\left[\frac{\Psi(r)}{\ln r}-\Psi(r)+\left(\lim_{r\to 0}\frac{\Psi(r)}{\ln r}\right)\ln r+\beta\frac{\Psi(r)}{\ln r}\right.$$
$$\left.-\beta\left(\lim_{r\to 0}\frac{\Psi(r)}{\ln r}\right)\right]=0. \tag{B3}$$

Because $\lim_{r\to 0}\ln r\to-\infty$, we must have

$$\lim_{r\to 0}\left[\frac{\Psi(r)}{\ln r}-\Psi(r)+\left(\lim_{r\to 0}\frac{\Psi(r)}{\ln r}\right)\ln r+\beta\frac{\Psi(r)}{\ln r}\right]=0, \tag{B4}$$

where we have dropped the last term $-\beta(\lim_{r\to 0}[\Psi(r)/\ln r])$ in comparison with the third term $(\lim_{r\to 0}[\Psi(r)/\ln r])\ln r$. If we replace $\Psi(r)=\phi(r)/r^{1/2}$ in Eq. (B4), we finally obtain

$$\alpha\lim_{r\to 0}\left(\frac{\phi(r)}{r^{1/2}\ln r}\right)-\lim_{r\to 0}\left(\frac{\phi(r)}{r^{1/2}}-\lim_{r\to 0}\left(\frac{\phi(r)}{r^{1/2}\ln r}\right)\ln r\right)=0, \tag{B5}$$

where $\alpha=\beta+1$ is an arbitrary real constant, related to the energy of the unique bound state of this system (see Exercise 3).

[a]Electronic mail: coutinho@dim.fm.usp.br

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[11]We call this domain $C_0^\infty((0,\infty)\backslash\{0\})$. The symbol C means that the functions are continuous. The superscript ∞ means that the functions are infinitely differentiable. The subscript 0, and the removal of the origin, $\backslash\{0\}$, means that all the functions in the domain vanish in a small, but finite interval $[0,a]$ where $a>0$ is an arbitrary real number, and also for $x>b>a$, another arbitrary real number.
[12]We call this domain $C_0^\infty(R\backslash\{0\})$. The meaning of the symbol $R\backslash\{0\}$ is that the point zero has been removed from the real line. So the functions in this domain are not defined for $x=0$. The superscript ∞ and the subscript 0 have the same meanings as before; $\backslash\{0\}$, means that the functions $u_{abcd}(x)$ belonging to $C_0^\infty(R\backslash\{0\})$ vanish around $x=0$, that is for $-a<x<b$ and also for $x<-c$ and for $x>d$, where a, b, c, and d are arbitrary positive numbers. Therefore the domain of this operator consists of functions that vanish before the point $x=0$ from the negative and positive sides and for large distances in both positive and negative directions.
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[24]In the mathematical literature the two equations (A5) and (A6) are written with O replaced by O^+.