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Citation: American Journal of Physics **69**, 322 (2001); doi: 10.1119/1.1328351
View online: http://dx.doi.org/10.1119/1.1328351
View Table of Contents: http://scitation.aip.org/content/aapt/journal/ajp/69/3?ver=pdfcov
Published by the American Association of Physics Teachers

Self-adjoint extensions of operators and the teaching of quantum mechanics

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(Received 8 December 1999; accepted 12 September 2000)

For the example of the infinite well potential, we point out some paradoxes which are solved by a careful analysis of what is a truly self-adjoint operator. We then describe the self-adjoint extensions and their spectra for the momentum and the Hamiltonian operators in different settings. Additional physical requirements such as parity, time reversal, and positivity are used to restrict the large class of self-adjoint extensions of the Hamiltonian.
[DOI: 10.1119/1.1328351]

I. INTRODUCTION

In most of the French universities, quantum mechanics is usually taught in the third-year courses, separately from its applications to atomic, molecular, and subnuclear physics, which are dealt with during the fourth year. In such ''first contact'' lectures, many mathematical subtleties are necessarily left aside. However, even in the so commonly used examples of infinitely deep potential wells, overlooking the mathematical problems leads to contradictions which may be detected by a careful student and which have to do with a precise definition of the ''observables,'' i.e., the self-adjoint operators.

Of course, experts in the mathematical theory of unbounded operators in Hilbert spaces know the correct answer to these questions, but we think it could be useful to popularize these concepts among the teaching community and the more mature students of fourth-year courses. In particular, the role of the boundary conditions that lead to self-adjoint operators is missed in most of the available textbooks, the one by Ballentine (Ref. 1, p. 11) being a notable exception as it includes a discussion of the momentum operator. In this very review we could find only two references relevant to the subject. The first one (Ref. 2) considers a particular self-adjoint extension of the momentum and of the Hamiltonian for a particle in a box, which is interpreted as describing a situation with spontaneous symmetry breaking. The second one (Ref. 3) mentions the self-adjoint extensions of the Hamiltonian for a particle in a half-axis and its relevance, first pointed out by Jackiw,[4] to the renormalization of the two-dimensional delta potential.

The aim of this paper is to emphasize the importance of the boundary conditions in the proper definition of an operator and to make available to an audience of physicists basic results which are not so easily extracted from the large amount of mathematical literature on the subject.

The paper is organized as follows: In Sec. II we discuss some paradoxes met in the study of the infinite potential well. Then, in Sec. III, we present a first analysis of the boundary conditions for the self-adjoint extensions of the momentum operator.

In Sec. IV we introduce the concept of deficiency indices and state von Neumann's theorem. In Sec. V we apply it to the self-adjoint extensions of the momentum operator for which the spectra, the eigenfunctions, and some physical consequences of these are given. We hope that, despite some technicalities needed for precision (which can be omitted in a first reading), the results are easily accessible. The reader interested in these technical aspects may consult Refs. 5 and 6.

Then, in Sec. VI, we describe the self-adjoint extensions of the Hamiltonian operator in various settings (on the real axis, on the positive semiaxis, and in a box) and in Sec. VII we use several constraints from physics to reduce the set of all its possible self-adjoint extensions. In the Appendix we have gathered some technical details on the extensions of the momentum operator.

II. THE INFINITE POTENTIAL WELL: PARADOXES

Let us consider the standard problem (see, for example, Ref. 7, p. 299 or Ref. 8, p. 109) of a particle of mass m in a one-dimensional, infinitely deep, potential well of width L:

$$V(x)=0,\ \ x\in\left]-\frac{L}{2},+\frac{L}{2}\right[;\quad V(x)=\infty,\ \ |x|\geqslant\frac{L}{2}. \qquad (1)$$

Stationary states are obtained through the Schrödinger (eigenvalue) equation

$$H\phi(x)=E\phi(x)$$

and the vanishing of their wave functions at both ends. This means that the action of the Hamiltonian operator for a free particle, unbounded on the closed interval $[-L/2,+L/2]$, is defined by

$$H \equiv -\frac{\hbar^2}{2m} D^2,$$

$$\mathcal{D}(H) = \left\{ \phi, H\phi \in \mathcal{L}^2\left(-\frac{L}{2}, +\frac{L}{2}\right), \quad \phi\left(\pm\frac{L}{2}\right) = 0 \right\}, \tag{2}$$

where D is the differential operator d/dx and $\mathcal{D}(H)$ is the definition domain of the operator H.

Two series of normalized eigenfunctions of opposite parity are obtained. They vanish outside the well and for $x \in [-L/2, +L/2]$ can be written as follows:

$$\begin{aligned} &\textit{odd ones}: \quad \Phi_n(x) = \sqrt{\frac{2}{L}} \sin\left[\frac{2n\pi x}{L}\right], \\ &\qquad E_n = \frac{\hbar^2}{2m}\left(\frac{2n\pi}{L}\right)^2, \\ &\textit{even ones}: \quad \Psi_n(x) = \sqrt{\frac{2}{L}} \cos\left[\frac{(2n-1)\pi x}{L}\right], \\ &\qquad E'_n = \frac{\hbar^2}{2m}\left(\frac{(2n-1)\pi}{L}\right)^2, \end{aligned} \tag{3}$$

where n is a strictly positive integer. The functions $\Phi_n(x)$ and $\Psi_n(x)$ are continuous at $x = \pm L/2$ where they vanish.

A question of fundamental importance arises: Is the Hamiltonian operator H a truly self-adjoint operator? To discuss this question more thoroughly let us consider a particle in the state defined by the even, normalized wave function:

$$\begin{aligned} &\Psi(x) = -\sqrt{\frac{30}{L^5}}\left(x^2 - \frac{L^2}{4}\right), \quad |x| \leqslant \frac{L}{2}; \\ &\Psi(x) = 0, \quad |x| \geqslant \frac{L}{2}. \end{aligned} \tag{4}$$

It may be expanded[9] on the complete basis of eigenfunctions of H given in (3):

$$\Psi(x) = \sum_{n=1}^{\infty} b_n \Psi_n(x),$$

$$b_n = (\Psi_n, \Psi) = \frac{(-1)^{n-1}}{(2n-1)^3} \frac{8\sqrt{15}}{\pi^3}. \tag{5}$$

Let us define also, for further use,

$$\tilde{\Psi}(x) = -\frac{\hbar^2}{2m} D^2 \Psi(x) = \frac{\hbar^2}{m}\sqrt{\frac{30}{L^5}}, \quad -L/2 < x < +L/2, \tag{6}$$

and let us begin with some elementary computations: the mean value of the energy and its mean-square deviation in state (4). On the one hand we have

$$\langle E \rangle = \sum_{n=1}^{\infty} |b_n|^2 E'_n = \frac{480\hbar^2}{m\pi^4 L^2} \sum_{n=1}^{\infty} \frac{1}{(2n-1)^4} = \frac{5\hbar^2}{mL^2}, \tag{7}$$

but on the other hand

$$\begin{aligned} \langle E \rangle &= (\Psi, H\Psi) \\ &= (\Psi, \tilde{\Psi}) \\ &= -\frac{30\hbar^2}{mL^5} \int_{-L/2}^{+L/2} \left[x^2 - \frac{L^2}{4}\right] dx = \frac{5\hbar^2}{mL^2} = \frac{10}{\pi^2} E'_1. \end{aligned}$$

These results are coherent. Things are different for the energy mean-square fluctuation. On the one hand

$$\begin{aligned} \langle E^2 \rangle &= \sum_{n=1}^{\infty} |b_n|^2 (E'_n)^2 \\ &= \frac{240\hbar^4}{m^2\pi^2 L^4} \sum_{n=1}^{\infty} \frac{1}{(2n-1)^2} = \frac{30\hbar^4}{m^2 L^4}, \end{aligned} \tag{8}$$

leads to

$$\Delta E \equiv \sqrt{\langle E^2 \rangle - \langle E \rangle^2} = \sqrt{5}\frac{\hbar^2}{mL^2}, \tag{9}$$

and on the other hand

$$\langle E^2 \rangle = (\Psi, H^2 \Psi) = (\Psi, H\tilde{\Psi}) = 0!!$$

In order to understand the origin of the paradox, let us come back to the definitions. The probability of being in the eigenstate ϕ_n of energy ϵ_n being given by $|(\phi_n, \Psi)|^2$, one obtains

$$\begin{aligned} \langle E^2 \rangle &= \sum_{n=1}^{\infty} \epsilon_n^2 |(\phi_n, \Psi)|^2 = \sum_{n=1}^{\infty} \epsilon_n^2 (\phi_n, \Psi)(\Psi, \phi_n) \\ &= \sum_{n=1}^{\infty} (H\phi_n, \Psi)(\Psi, H\phi_n), \end{aligned}$$

where the reality of the eigenvalues of the Hamiltonian has been used. If H were self-adjoint, one would obtain with the help of the closedness relation

$$\begin{aligned} \langle E^2 \rangle &= \sum_{n=1}^{\infty} (\phi_n, H\Psi)(H\Psi, \phi_n) \\ &= (H\Psi, H\Psi) = (\tilde{\Psi}, \tilde{\Psi}) = \frac{30\hbar^4}{m^2 L^4}, \end{aligned} \tag{10}$$

in agreement with the direct calculation (9). But, if the self-adjointness of H were used once more, one would get

$$\langle E^2 \rangle = (H\Psi, H\Psi) = (\Psi, H^2\Psi) = 0, \tag{11}$$

which is necessarily wrong. In fact, in (10), we used (correctly, as shown by the standard proof using an integration by parts) the self-adjointness of H when it acts in the set of functions that vanish at both end points of the well,

$$(H\phi_n, \Psi) = (\phi_n, H\Psi), \quad (\Psi, H\phi_n) = (H\Psi, \phi_n).$$

In contrast, in (11) the function $\tilde{\Psi}$ does not belong to that set and, consequently, in the integration by parts, the integrated term remains and

$$(H\Psi, \tilde{\Psi}) \neq (\Psi, H\tilde{\Psi}).$$

These simple calculations show that the problem lies in the definition of the action of the operator H on a function $\tilde{\Psi}$ that does not vanish at the end points.

To summarize, we came up against the difficulty of the definition of a self-adjoint operator in a closed interval $[-L/2, +L/2]$ as an extension of a differential operator $-(\hbar^2/2m)D^2$, a question already solved by mathematicians in the thirties. Before explaining this theory in a simple manner, in Sec. III we analyze the momentum operator $-i\hbar D$.

III. SELF-ADJOINT EXTENSIONS OF THE MOMENTUM OPERATOR: A FIRST APPROACH

Let us consider the one-dimensional momentum operator $P=-i\hbar D$ in a closed x interval. Let us take for domain $\mathcal{D}$ the following space:

$$\mathcal{D}(P)=\{\phi,\phi'\in\mathcal{L}^2([0,L]);\phi(0)=\phi(L)=0\}.$$

The vanishing of

$$\begin{aligned}(\psi,-i\hbar D\phi)-(-i\hbar D\psi,\phi)\\ &=\int_0^L dx\left[\overline{\psi}(x)\left(-i\hbar\frac{d\phi(x)}{dx}\right)-\left(i\hbar\frac{d\overline{\psi}(x)}{dx}\right)\phi(x)\right]\\ &=-i\hbar\int_0^L dx\frac{d}{dx}[\overline{\psi}(x)\phi(x)]\\ &=-i\hbar[\overline{\psi}(L)\phi(L)-\overline{\psi}(0)\phi(0)]\end{aligned}\tag{12}$$

implies that P is a symmetric operator in $\mathcal{D}$. But P is not a self-adjoint operator even if its adjoint $P^\dagger=-i\hbar D$ has the same formal expression *but it acts on a different space of functions*. Indeed,

$$\mathcal{D}(P^\dagger)=\{\psi,\psi'\in\mathcal{L}^2([0,L]);\ \text{no other restriction on } \psi(x)\}.$$

With (12), one easily sees that the adjoint of the operator $P_\lambda=-i\hbar D$ acting on the subspace of $\mathcal{L}^2([0,L])$ such as

$$\phi(L)=\lambda\phi(0),\quad \text{where } \lambda\in\mathbb{C},$$

is the operator $P_{\lambda'}$ where $\lambda'=1/\overline{\lambda}$. As a consequence, a candidate family of self-adjoint extensions of the operator $-i\hbar D$, depending on a complex parameter $\lambda\equiv1/\overline{\lambda}$, i.e., a phase $\lambda=e^{i\theta}$, $\theta\in[0,2\pi]$ is:

$$\begin{aligned}&P_\theta\phi(x)=-i\hbar D\phi(x),\\ &\mathcal{D}(P_\theta)=\{\phi,\phi'\in\mathcal{L}^2([0,L]),\quad \phi(L)=e^{i\theta}\phi(0)\}.\end{aligned}\tag{13}$$

Notice that for $\theta=0$, one recovers the usual periodic boundary conditions.

Conclusion: Given a symmetric differential operator acting on a given functional space, it is not automatically a self-adjoint operator and may have many self-adjoint extensions.

IV. DEFICIENCY INDICES AND VON NEUMANN'S THEOREM

Since what follows is more abstract and makes use of (maximally reduced) mathematical terminology, we would like to motivate the reader to such an effort. This section is devoted to the concept of ''deficiency indices'' for an operator P. The concept itself is very simple: it is an ordered pair of positive integers (n_+,n_-). Its knowledge, upon use of an important theorem due to von Neumann, immediately gives the answer to the difficult question: How many self-adjoint extensions does the operator P admit?

Let us begin with some necessary definitions.

Let us consider a Hilbert space $\mathcal{H}$. An operator $(A,\mathcal{D}(A))$ defined on $\mathcal{H}$ is said to be densely defined if the subset $\mathcal{D}(A)$ is dense in $\mathcal{H}$, i.e., that for any $\psi\in\mathcal{H}$ one can find in $\mathcal{D}(A)$ a sequence ϕ_n which converges in norm to ψ.

An operator $(A,\mathcal{D}(A))$ is said to be *closed* if ϕ_n is a sequence in $\mathcal{D}(A)$ such that

$$\lim_{n\to\infty}\phi_n=\phi,\qquad \lim_{n\to\infty}A\phi_n=\psi,$$

then $\phi\in\mathcal{D}(A)$ and $A\phi=\psi$.

Let us recall the definition of the adjoint operator of an (in general not bounded) operator H with dense domain $\mathcal{D}(H)$. The domain $\mathcal{D}(H^\dagger)$ is the space of functions ψ such that the linear form

$$\phi\to(\psi,H\phi)$$

is continuous for the norm of $\mathcal{H}$. Hence there exists a $\psi^\dagger\in\mathcal{H}$ such that

$$(\psi,H\phi)=(\psi^\dagger,\phi).$$

One defines $H^\dagger\psi=\psi^\dagger$. A useful result is that the adjoint of any densely defined operator is closed, see Ref. 5, p. 80, Vol. 1.

An operator $(H,\mathcal{D}(H))$ is said to be *symmetric* if for all ϕ, $\psi\in\mathcal{D}(H)$ we have

$$(H\phi,\psi)=(\phi,H\psi).$$

If $\mathcal{D}(H)$ is dense, it amounts to saying that $(H^\dagger,\mathcal{D}(H))$ is an extension of $(H,\mathcal{D}(H))$.

The operator H with dense domain $\mathcal{D}(H)$ is said to be self-adjoint if $\mathcal{D}(H^\dagger)=\mathcal{D}(H)$ and $H^\dagger=H$.

In this section we will assume that $(A,\mathcal{D}(A))$ is densely defined, symmetric, and closed and let $(A^\dagger,\mathcal{D}(A^\dagger))$ be its adjoint.

One defines the deficiency subspaces $\mathcal{N}_\pm$ by

$$\mathcal{N}_+=\{\psi\in\mathcal{D}(A^\dagger),\quad A^\dagger\psi=z_+\psi,\quad \operatorname{Im}z_+>0\},$$

$$\mathcal{N}_-=\{\psi\in\mathcal{D}(A^\dagger),\quad A^\dagger\psi=z_-\psi,\quad \operatorname{Im}z_-<0\},$$

with respective dimensions n_+,n_-. These are called the deficiency indices of the operator A and will be denoted by the ordered pair (n_+,n_-).

The crucial point is that n_+ (n_-) is completely independent of the choice of z_+ (z_-) as far as it lies in the upper (lower) half complex plane. In practice one takes $z_+=i\lambda$ and $z_-=-i\lambda$ with an arbitrary strictly positive constant λ needed for dimensional reasons, and the determination of the deficiency indices of the operator A just boils down to the counting of how many solutions of the equation $A^\dagger\psi=z\psi$ have finite norm!

The following theorem, first discovered by Weyl[10] in 1910 for second-order differential operators and generalized by von Neumann[11] in 1929, is of paramount importance.

Theorem 1: For an operator A with deficiency indices (n_+,n_-) there are three possibilities:

(1) If $n_+=n_-=0$, then A is self-adjoint (in fact this is a necessary and sufficient condition).
(2) If $n_+=n_-=n\geqslant1$, then A has infinitely many self-adjoint extensions, parametrized by a unitary $n\times n$ matrix (i.e., n^2 real parameters).
(3) If $n_+\neq n_-$, then A has no self-adjoint extension.

The concrete application of this theorem to differential operators still requires some work because one has to solve three problems:

(1) Find a domain $\mathcal{D}(P)$ for which the formally self-adjoint operator P is symmetric and closed.
(2) Compute its adjoint $(P^\dagger,\mathcal{D}(P^\dagger))$ and determine the deficiency indices of P.
(3) When they do exist, describe the domains of all the self-adjoint extensions.

A whole body of theory has been built up to solve these problems for differential operators and is given in many textbooks (for instance Refs. 5 and 6).

In Sec. V we describe the results for the simplest case of the momentum operator $P=-i\hbar D$, referring for the proofs to Ref. 5, Vol. 1, pp. 106–111. The reader should be comforted by the simplicity of the determination of the deficiency indices.

V. SELF-ADJOINT EXTENSIONS OF THE MOMENTUM OPERATOR

Let us apply the previous analysis to the momentum operator $P=-i\hbar D$, in three different ''physical'' situations: first on the whole real axis and in this case we conclude to a unique self-adjoint extension, second on the positive semi-axis and in this case there is no self-adjoint extension, and third in a finite interval $[0, L]$ in which case there are infinitely many self-adjoint extensions, parametrized by $U(1)$, i.e., a phase. The momentum operator is certainly the simplest differential operator to begin with and it already exhibits all the possibilities described in von Neumann's theorem. For each physical situation corresponding to position space being some interval $[a, b]$, finite or not, the maximal domain on which the operator $P=-i\hbar D$ has a well-defined action will be called $\mathcal{D}_{\max}(a,b)$, and is given in the Appendix. In this section, we merely apply the previous theorem, postponing some mathematical details to the Appendix.

Let us consider the Hilbert space $\mathcal{H}=L^2(a,b)$. To use von Neumann's theorem we have to determine the functions $\psi_\pm(x)$ given by

$$P^\dagger\psi_\pm(x)=-i\hbar D\psi_\pm(x)=\pm i\frac{\hbar}{d}\psi_\pm(x).$$

For dimensional reasons we have introduced the constant $d>0$, homogeneous to some length.

An easy integration gives $\psi_\pm(x)=C_\pm e^{\mp x/d}$. Then we have to discuss the different intervals $[a, b]$.

A. The operator *P* on the whole real axis

None of the functions $\psi_\pm(x)$ belongs to the Hilbert space $L^2(\mathbb{R})$ and therefore the deficiency indices are (0, 0). Hence we conclude that the operator $(P,\mathcal{D}_{\max}(\mathbb{R}))$ is indeed self-adjoint, in agreement with the heuristic considerations given in the standard textbooks on quantum mechanics. Moreover, the spectrum of P on the real axis is continuous, with no eigenvalues.

B. The operator *P* on the positive semi-axis

Among the functions $\psi_\pm(x)$, only ψ_+ belongs to $L^2(0,+\infty)$. We conclude that the deficiency indices are (1, 0) and therefore, by the von Neumann theorem, that P has no self-adjoint extension. This is a fairly surprising conclusion, since it implies that the momentum is not a measurable quantity in that situation!

C. The operator *P* on a finite interval

Since we are working on a finite interval, both $\psi_\pm(x)=C_\pm e^{\mp x/d}$ belong to $L^2(0,L)$ and the deficiency indices are (1, 1).

From von Neumann's theorem, we know that the self-adjoint extensions are parametrized by $U(1)$, i.e., a phase $e^{i\theta}$, in agreement with the result of Sec. III. Denoting these extensions by $P_\theta=(P,\mathcal{D}_\theta)$, they are given by

$$\mathcal{D}_\theta=\{\psi\in\mathcal{D}_{\max}(0,L),\quad \psi(L)=e^{i\theta}\psi(0)\},\quad \theta\in[0,2\pi]. \tag{14}$$

Moreover, the spectra are purely discrete. Using the boundary condition (14), the eigenvalues and eigenfunctions are easily shown to be

$$\begin{gathered} P_\theta\phi_n(x,\theta)=\frac{2\pi\hbar}{L}\nu\phi_n(x,\theta),\\ \nu=n+\frac{\theta}{2\pi},\quad n=0,\pm1,\pm2,...,\\ \phi_n(x,\theta)=\frac{1}{\sqrt{L}}\exp\left[2i\pi\nu\frac{x}{L}\right],\quad (\phi_m,\phi_n)=\delta_{mn}. \end{gathered} \tag{15}$$

As the phase θ appears in the eigenfunctions any measurement of the momentum of a given system should, in general, depend on it. To display this, let us go back to the state (4). After a translation, we are left with the wave function

$$\Psi(x)=\sqrt{\frac{30}{L^5}}x(L-x).$$

Its eigenfunction expansion is

$$\Psi(x)=\sum_{n=-\infty}^{n=+\infty}c_n(\theta)\phi_n(x,\theta),$$

with coefficients

$$c_n(\theta)=-\frac{\sqrt{30}}{2\pi^2\nu^2}\left[\cos(\theta/2)-\frac{\sin(\theta/2)}{\pi\nu}\right]e^{-i\theta/2}\quad \text{for}\quad \theta\neq0, \tag{16}$$

and

$$c_0=\frac{\sqrt{30}}{6},\quad c_n=-\frac{\sqrt{30}}{2\pi^2n^2},\quad n=1,2,...\quad \text{for}\quad \theta=0. \tag{17}$$

So the probability of finding the particle with a momentum $2\pi\nu\hbar/L$, being equal to $|c_n(\theta)|^2$, is really θ dependent. Of course one would like to have a physical argument which gives some preferred value of θ.

Let us conclude with the following remarks.

(1) The textbooks which do study the momentum operator in a box (Ref. 1 and Ref. 12, Vol. 2, p. 1202) usually consider (using physical arguments) only the self-adjoint extension corresponding to the periodic boundary condition (i.e., $\theta=0$) which is certainly the simplest (but still arbitrary) choice. The antiperiodic boundary condition (i.e., $\theta=\pi$) has been considered by Capri in Ref. 2.

(2) For a particle in a box, it is often argued that the ''physical'' wave function should vanish on the walls $x=0$

and $x=L$, ensuring that the position probability vanishes continuously for $x\leqslant 0$ and for $x\geqslant L$. One should realize that the continuity of the measurable quantity

$$\Pr(0\leqslant x\leqslant u)=\int_0^u|\phi(x)|^2dx,\quad u\in[0,L]$$

is ensured as soon as the integral $\int_0^L|\phi(x)|^2\,dx$ converges and does not require any continuity property of $\phi(x)$. Specializing this remark to the eigenfunctions of P_θ, we observe that $|\phi_n(x,\theta)|^2$ does not vanish continuously at $x=0$ but nevertheless the physical quantity

$$\Pr(0\leqslant x\leqslant u)=\frac{u}{L}$$

vanishes continuously, as it should, for $u\to 0$.

(3) The existence of normalizable eigenfunctions of the momentum operator has an important consequence: The Heisenberg inequality $\Delta X\Delta P\geqslant\hbar/2$ no longer holds. Indeed, for the state $\phi_n(x,\theta)$ given in relation (15), one has $\Delta P=0$ and $\Delta X=L/2$. On the contrary, on the whole real axis the spectrum is fully continuous (no normalizable eigenfunctions), and the momentum probabilities are related to the Fourier transformed wave function. As the widths in x space and in p space are inversely proportional, the Heisenberg inequality follows.

(4) If one identifies the variable x with the angular variable $\varphi\in[0,2\pi]$ of polar coordinates, then the angular momentum is $L_z=-i\hbar(d/d\varphi)$. The previous remark shows that the inequality $\Delta\varphi\Delta L_z\geqslant\hbar/2$ can be violated, even by wave functions periodic in the angle φ.

VI. SELF-ADJOINT EXTENSIONS OF THE HAMILTONIAN

In the same setting as in Sec. V, we consider now the Hamiltonian operator $H=-D^2$. We work in the Hilbert space $L^2(a,b)$. The maximal domain in which the operator D^2 is defined will again be called $\mathcal{D}_{\max}(a,b)$. To compute the deficiency indices we solve

$$-D^2\phi(x)=\pm ik_0^2\phi(x),\quad k_0>0, \tag{18}$$

and get

$$\phi_\pm=a_\pm e^{k_\pm x}+b_\pm e^{-k_\pm x},\quad k_\pm=\frac{(1\mp i)}{\sqrt{2}}k_0. \tag{19}$$

A. The Hamiltonian on the whole real axis

Let us consider a free particle moving in a one-dimensional space. The Hilbert space is $\mathcal{H}=L^2(\mathbb{R})$, which implies $\phi_\pm\notin\mathcal{H}$ and the deficiency indices (0,0). It follows that on the real axis there is a *unique* self-adjoint extension of the Hamiltonian, with a fully continuous spectrum, in full agreement with the physicist's understanding of this case.

B. The Hamiltonian on the positive semi-axis

Let us now consider a free particle in front of an infinitely high wall for $x<0$. In the Hilbert space $\mathcal{H}=L^2(0,+\infty)$, the solutions to Eq. (18) are given by

$$\phi_\pm=b_\pm e^{-k_0x/\sqrt{2}}e^{\pm ik_0x/\sqrt{2}},$$

leading to the deficiency indices (1,1), and therefore to infinitely many self-adjoint extensions parametrized by $U(1)$.

The corresponding boundary conditions are

$$(\phi'(0)-i\phi(0))=e^{i\alpha}(\phi'(0)+i\phi(0)),\quad \alpha\in[0,2\pi],$$

which are equivalent to

$$\phi(0)=\lambda\phi'(0),\quad \lambda=-\tan(\alpha/2),\quad \lambda\in\mathbb{R}\cup\{\infty\}, \tag{20}$$

see Ref. 5, Vol. 2, pp. 187, 204. The boundary condition $\phi'(0)=0$ corresponds to $\lambda=\infty$. Physicists use the particular extension with $\lambda=0$; see, for instance, Ref. 7, p. 328 and Ref. 13, p. 33.

Let us now discuss the energy spectra of a particle confined in the region $x\geqslant 0$. When the particle energy E is positive, we can compute the reflection coefficient for this infinitely high barrier in order to compare the predictions given by the different extensions. The wave function is

$$\phi(x)=Ae^{-ikx}+Be^{ikx},\quad E=\frac{\hbar^2k^2}{2m},\quad k>0. \tag{21}$$

Let us define the reflection amplitude and reflection probability by

$$r(k)=\frac{A}{B},\quad R(k)=|r(k)|^2.$$

Imposing the boundary condition (20) we get

$$r(k)=-\frac{1+i\lambda k}{1-i\lambda k}\Rightarrow R=1. \tag{22}$$

Remarkably enough the physical content (i.e., $R=1!$) of all the extensions is the same: The wall acts as a perfect reflector.

This is not quite true for the bound states

$$E=-\frac{\hbar^2\rho^2}{2m},\quad \rho>0,\quad \phi(x)=Ae^{-\rho x},$$

for which (20) implies $(1+\lambda\rho)A=0$. There will be a bound state with $\rho=-1/\lambda$ only for $\lambda<0$ and different from ∞. Its energy and normalized wave function are

$$E=-\frac{\hbar^2}{2m\lambda^2},\quad \lambda<0,\quad \phi(x)=\sqrt{\frac{2}{|\lambda|}}e^{-x/|\lambda|}. \tag{23}$$

As far as an infinitely high wall is feasible experimentally, the existence (or nonexistence) of this negative energy will act as a selector of some self-adjoint extensions.

If experiment could rule out the negative energy state, or if one is reluctant to accept negative energies for the Hamiltonian, there are still many possible extensions, with $\lambda\geqslant 0$ or $\lambda=\infty$.

C. The Hamiltonian on a finite interval

This last case corresponds to a particle in a box: $x\in[0,L]$. From a mathematical standpoint the situation is quite similar to the one already experienced with the momentum operator in Sec. V C, but to our knowledge, it did not appear before in the literature. So we give some details in the main text.

One starts from the operator $(H,\mathcal{D}_0(H))$ such that

$$\mathcal{D}_0(H)=\{\phi\in\mathcal{D}_{\max}(0,L) \quad \text{and} \quad \phi(0)=\phi(L)=\phi'(0)=\phi'(L)=0\}.$$

It is densely defined and closed, with adjoint

$$H^\dagger=H, \quad \mathcal{D}(H^\dagger)=\mathcal{D}_{\max}(0,L).$$

Since all the solutions of Eq. (18) belong to $L^2(0,L)$, the deficiency indices are now (2,2) and the self-adjoint extensions are parametrized by a $U(2)$ matrix.

To describe these self-adjoint extensions, it is natural to introduce the sesquilinear form, for ϕ and ψ in $\mathcal{D}_{\max}(0,L)$,

$$B(\phi,\psi)=\frac{1}{2i}((H^\dagger\phi,\psi)-(\phi,H^\dagger\psi)), \tag{24}$$

which depends only on the boundary values of ϕ and ψ. Specializing to $\psi=\phi$ we have

$$B(\phi,\phi)=\frac{1}{2i}(\phi'(L)\overline{\phi(L)}-\phi(L)\overline{\phi'(L)} - \phi'(0)\overline{\phi(0)}+\phi(0)\overline{\phi'(0)}). \tag{25}$$

The identity

$$\frac{1}{2i}(x\bar{y}-\bar{x}y)=\frac{1}{4}(|x+iy|^2-|x-iy|^2), \tag{26}$$

applied to $x=L\phi'(L)$, $y=\phi(L)$, and $x=L\phi'(0)$, $y=\phi(0)$ brings relation (25) to

$$4LB(\phi,\phi)=|L\phi'(0)-i\phi(0)|^2+|L\phi'(L)+i\phi(L)|^2 -|L\phi'(0)+i\phi(0)|^2 -|L\phi'(L)-i\phi(L)|^2. \tag{27}$$

The domain of a self-adjoint extension is a maximal subspace of $\mathcal{D}_{\max}(0,L)$ on which the form $B(\phi,\phi)$ vanishes identically. These self-adjoint extensions are parametrized by a unitary matrix U, and will be denoted $H_U=(H,\mathcal{D}(U))$, in which $\mathcal{D}(U)$ is the space of functions ϕ in $\mathcal{D}_{\max}(0,L)$ satisfying the following boundary conditions:

$$\begin{pmatrix} L\phi'(0)-i\phi(0) \\ L\phi'(L)+i\phi(L)\end{pmatrix}=U\begin{pmatrix} L\phi'(0)+i\phi(0) \\ L\phi'(L)-i\phi(L)\end{pmatrix}. \tag{28}$$

Notice the arbitrariness in the choice of the ordering of the coordinates $L\phi'(0)\pm i\phi(0)$ and $L\phi'(L)\mp i\phi(L)$. The crucial observation is that whatever the choice of coordinates is, the arbitrariness of the self-adjoint extensions remains described by a $U(2)$ matrix.

These boundary conditions describe all the self-adjoint extensions $H_U=(H,\mathcal{D}(U))$ of a particle in a box. Moreover, thanks to the useful theorem, proved in Ref. 6, Vol. 2, p. 90, stating that for a differential operator of order n with deficiency indices (n,n), all of its self-adjoint extensions have a discrete spectrum, we know that all the spectra of the H_U are fully discrete. Leaving the details to the reader, we only give the results.

Let us parametrize the unitary matrix U as:

$$U=e^{i\psi}M, \quad \det M=1, \quad \Rightarrow \det U=e^{2i\psi}, \quad \psi\in[0,\pi], \tag{29}$$

where M is an element of $SU(2)$, i.e., a unitary matrix of determinant 1. The range of ψ is restricted to π instead of 2π because the couples (ψ,M) and $(\psi+\pi,-M)$ give rise to the same unitary matrix U. Notice also that it follows that the points $\psi=0$ and $\psi=\pi$ are to be identified.

In what follows we will use the Pauli matrices

$$\tau_1=\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad \tau_2=\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad \tau_3=\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix},$$

and the notation

$$\mathbf{n}\cdot\boldsymbol{\tau}=n_1\tau_1+n_2\tau_2+n_3\tau_3.$$

We found it convenient to use the coordinates $m=(m_0,\mathbf{m})$ such that

$$M=\begin{pmatrix} m_0-im_3 & -m_2-im_1\\ m_2-im_1 & m_0+im_3\end{pmatrix}=m_0I-i\mathbf{m}\cdot\boldsymbol{\tau}, \tag{30}$$

constrained by

$$m_0^2+\mathbf{m}\cdot\mathbf{m}=1\Leftrightarrow m\in\mathbb{S}^3. \tag{31}$$

Then, starting from the boundary conditions (28), we obtain the spectra for the Hamiltonian in a box.

(a) $E=s^2/L^2>0$:

$$2s[\sin\psi\cos s-m_1]=\sin s[\cos\psi(s^2+1)-m_0(s^2-1)].$$

(b) $E=0$: $s\to 0 \Leftrightarrow$

$$2\sin\psi-\cos\psi=2m_1+m_0. \tag{32}$$

(c) $E=-r^2/L^2<0$: $s=ir \Leftrightarrow$

$$2r[\sin\psi\cosh r-m_1]=\sinh r[-\cos\psi(r^2-1) +m_0(r^2+1)].$$

Remarks:

(1) The eigenvalue equations are independent of the parameters (m_2,m_3). As shown in Ref. 14, this follows from their invariance under the transformation

$$M\to M'=e^{-\theta\tau_1/2i}Me^{+\theta\tau_1/2i}.$$

Let us point out that this invariance is specific of the spectra, not of the eigenfunctions.

(2) The existence of negative energies seems rather surprising since $P^2=-D^2$ is a formally positive operator. That this is not generally true can be seen by computing

$$(\phi,H\phi)-(P\phi,P\phi)=\bar{\phi}(0)\phi'(0)-\bar{\phi}(L)\phi'(L), \quad \phi\in D_U.$$

If the right-hand side of this relation is positive, the spectrum will be positive, an issue which depends on the extension H_U considered (see Sec. VII C).

(3) The discrete spectra s_n can be classified as ''simple'' when their analytic form can be given, or ''generic'' when this is not the case. The detailed analysis of the spectra may be found in Ref. 14.

VII. RESTRICTIONS FROM PHYSICS ON THE SELF-ADJOINT EXTENSIONS

In Sec. VI we have described all the possible self-adjoint extensions of the operator H_U as they follow from operator theory. Now we examine which extensions are likely to play an interesting role according to arguments from physics.

A. Extensions preserving time reversal

Let $\Psi(x,t)$ be a solution of the Schrödinger equation

$$i\hbar \frac{\partial \Psi}{\partial t}(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2}(x,t) \tag{33}$$

inside the box. The time reversal invariance of this equation means that if $\Psi(x,t)$ is a solution of (33), then $\overline{\Psi}(x,t)$ is also a solution. If we consider a stationary state of definite energy E with the wave function

$$\Psi(x,t) = \phi_E(x)\exp\left(-i\frac{Et}{\hbar}\right),$$

the previous statement implies that $\phi_E(x)$ and $\overline{\phi_E}(x)$ are two eigenfunctions of the Hamiltonian H with the same eigenvalue E. One can therefore choose *real* eigenfunctions by taking the linear combination $\phi_E(x) + \overline{\phi_E}(x)$.

The shortcoming in this argument is that the boundary conditions (28) do not lead *necessarily* to real eigenfunctions $\phi_E(x)$. Among all of the self-adjoint extensions of the Hamiltonian only some subclass will have real eigenfunctions. These extensions will be said to be time reversal invariant.

To determine all of these extensions, we merely observe that, using the notations

$$\psi_\pm(x) = L\phi'(x) \pm i\phi(x),$$

the reality of $\phi(x)$ implies $\overline{\psi_\pm}(x) = \psi_\mp(x)$. Taking the complex conjugate of relation (28) gives

$$\begin{pmatrix}\psi_+(0)\\ \psi_-(L)\end{pmatrix} = \overline{U}\begin{pmatrix}\psi_-(0)\\ \psi_+(L)\end{pmatrix} = \overline{U}U\begin{pmatrix}\psi_+(0)\\ \psi_-(L)\end{pmatrix}. \tag{34}$$

Since $\psi_+(0)$ and $\psi_-(L)$ cannot vanish simultaneously, we conclude to

$$\det(\mathbb{I} - \overline{U}U) = 0. \tag{35}$$

Using for U the coordinates given by (30), easy computations give $m_2 = 0$ and, correspondingly, the matrix

$$U = e^{i\psi}\begin{pmatrix} m_0 - im_3 & -im_1 \\ -im_1 & m_0 + im_3\end{pmatrix}$$
$$\text{with} \quad \psi \in [0,\pi] \quad \text{and} \quad m_0^2 + m_1^2 + m_3^2 = 1. \tag{36}$$

B. Extensions preserving parity

The potential $V(x)$, vanishing inside the box, is symmetric with respect to the point $x = L/2$. To make this symmetry explicit we shift the coordinate x to

$$u = \frac{x}{L} - \frac{1}{2}, \quad u \in \left[-\frac{1}{2}, +\frac{1}{2}\right],$$

and define

$$\tilde{V}(u) = V(x), \quad \tilde{\phi}_E(u) = \phi_E(x).$$

In the new variable u, the potential is even: $\tilde{V}(-u) = \tilde{V}(u)$. It follows that, for a given energy, the eigenfunctions $\tilde{\phi}_E(u)$ and $\tilde{\phi}_E(-u)$ are solutions of the same differential equation and we can choose linear combinations of definite parity $\tilde{\phi}_E(u) \pm \tilde{\phi}_E(-u)$.

As was already the case in the discussion of time reversal invariance, this argument is wrong since it overlooks the possibility for the boundary conditions (28) to break parity. Note that this point is often forgotten in quantum mechanics textbooks: There, one generally finds that, as soon as the potential is symmetric, the solution of the Schrödinger equation is of definite parity. It should be clear that the boundary conditions are essential. A good example to think about is the finite square well. The wave functions of its bound states are subject to the boundary conditions $\int|\phi(x)|^2 dx < \infty$. As this condition is symmetric, the wave functions do have a definite parity. This is not the case for the diffusion eigenfunctions, for which one has an incoming and reflected wave for $x \to -\infty$, while for $x \to +\infty$ one has only a transmitted wave. In this second case the symmetry between x and $-x$ is broken by the very conditions which characterize a diffusion experiment.

We will therefore define parity preserving extensions of the Hamiltonian H_U as the ones for which the eigenfunctions $\tilde{\phi}_E(u)$ verify

$$|\tilde{\phi}_E(-u)|^2 = |\tilde{\phi}_E(u)|^2. \tag{37}$$

Here one can show[14] that all parity preserving extensions are given by $m_3 = 0$ and so correspond to the matrix

$$U = e^{i\psi}\begin{pmatrix} m_0 & -m_2 - im_1 \\ m_2 - im_1 & m_0\end{pmatrix}, \quad \psi \in [0,\pi],$$
$$m_0^2 + m_1^2 + m_2^2 = 1. \tag{38}$$

C. Extensions preserving positivity

One of the most surprising facts for a physicist is the appearance of extensions with negative energies (see Secs. VI B and VI C).

From a theorem proved in Ref. 6 (theorem 16, Vol. 2, p. 44) one knows that only a finite number of negative energies can appear and that the sum of their multiplicities is at most 2. However, the determination of the U matrices with no negative eigenvalues involves lengthy graphical discussions of Eq. (32), which are fairly tedious.

A partial answer to this problem is offered by an interesting theorem due to von Neumann (see Ref. 5, p. 97). It states that if A is densely defined and closed, then $A^\dagger A$ is self-adjoint (and obviously positive).

Let us apply this result to the operator $(P = -iD, \mathcal{D}_0(P))$ defined in Sec. V C, whose adjoint was $(P, \mathcal{D}_{\max}(0,L))$. It follows that the operator

$$(P^2, \mathcal{D}_1(P^2)),$$
$$\mathcal{D}_1(P^2) = \{\phi \in \mathcal{D}_{\max}(0,L) \quad \text{with} \quad \phi(0) = \phi(L) = 0\},$$

will be self-adjoint. It corresponds to the extension with $U = \mathbb{I}$.

If we take for the operator $(P, \mathcal{D}_{\max}(0,L))$, with adjoint $(P, \mathcal{D}_0(P))$, we are led to

$$(P^2, \mathcal{D}_2(P^2)),$$
$$\mathcal{D}_2(P^2) = \{\phi \in \mathcal{D}_{\max}(0,L) \quad \text{with} \quad \phi'(0) = \phi'(L) = 0\},$$

a self-adjoint extension corresponding to $U = -\mathbb{I}$.

As a last example, we may start from $(P, \mathcal{D}_\theta)$, in which case von Neumann's theorem gives the self-adjoint extension

$$(P^2,\mathcal{D}_3(P^2)),$$

$$\mathcal{D}_3(P^2)=\{\phi\in\mathcal{D}_{\max}(0,L) \quad \text{with} \quad \phi(L)=e^{i\theta}\phi(0),$$
$$\phi'(L)=e^{i\theta}\phi'(0)\},$$

corresponding to the matrix

$$U=\begin{pmatrix} 0 & e^{-i\theta} \\ e^{i\theta} & 0 \end{pmatrix}, \quad \theta\in[0,2\pi].$$

It can be shown[14] that for this choice of the matrix U, the operators $(P^2,\mathcal{D}_U)$ and $(P,\mathcal{D}_\theta)$ have the same eigenfunctions. These extensions, $(P^2,\mathcal{D}_U)$, are really the squares of the ones of the momentum operator $(P,\mathcal{D}_\theta)$.

D. The infinite well as a limit of the finite one

Let us consider the standard problem of a particle of mass m in a one-dimensional potential well of width L and depth V_0:

$$V(x)=0, \quad x\in]0,L[; \quad V(x)=V_0>0, \quad x\notin]0,L[. \tag{39}$$

A standard computation gives the bound state wave functions

$$x\leqslant 0: \quad \phi_n(x)=d_n e^{\rho x}, \quad \rho^2=\frac{2m(V_0-E)}{\hbar^2},$$
$$x\geqslant L: \quad \phi_n(x)=\pm d_n e^{-\rho(x-L)}, \tag{40}$$
$$0\leqslant x\leqslant L: \quad \phi_n(x)=d_n\left[\cos kx+\frac{\rho}{k}\sin kx\right], \quad k^2=\frac{2mE}{\hbar^2}$$

with

$$d_n=\frac{k}{\rho}\sqrt{\frac{2}{L}}\frac{1}{\sqrt{(1+2/(\rho L))(1+k^2/\rho^2)}}.$$

The positive integer n labels the (finite for a given value of V_0) family of solutions of the transcendental equation:

$$\tan(kL)=\frac{2k\rho}{k^2-\rho^2}$$

and the $\pm$ corresponds to the (opposite) parity of the stationary state n, and to

$$\cos(kL)+\frac{\rho}{k}\sin(kL)=\pm 1.$$

When V_0 is large, one finds for the spectrum

$$\left(\rho\simeq\infty, \ v_0=\sqrt{\frac{2mV_0L^2}{\hbar^2}}\gg 1, \ k \ \text{fixed}\right)$$

$$k_nL\simeq n\pi(1-2/v_0), \quad E_n\simeq E_n^\infty(1-4/v_0), \tag{41}$$

where the E_n^∞'s are the infinite well energy levels (3), and for the stationary states:

$$\phi_n(x\leqslant 0)\sim\sqrt{\frac{2}{L}}\left(\frac{n\pi}{v_0}\right)\exp -v_0|x/L|\sim 0,$$
$$\phi_n(x\geqslant L)\sim\pm\sqrt{\frac{2}{L}}\left(\frac{n\pi}{v_0}\right)\exp -v_0(x/L-1)\sim 0, \tag{42}$$
$$\phi_n(0\leqslant x\leqslant L)\sim\sqrt{2/L}\left[\sin n\pi\frac{x}{L}+\left(\frac{n\pi}{v_0}\right)\right.$$
$$\left.\times\left(\cos n\pi\frac{x}{L}-\frac{1}{n\pi}\sin n\pi\frac{x}{L}\right)\right].$$

In that (fixed energy) infinite limit of the finite well, we see that the standard boundary conditions $\phi(0)=\phi(L)=0$ are recovered. One could have considered a nonsymmetric potential well such that $V(x)=V_0$ for $x<0$ and $V(x)=V_1$ for $x>L$ with $V_0\neq V_1$. Taking the limits $V_0\to\infty$ and $V_1\to\infty$ independently leads to the same conclusions as for the symmetric case $V_0=V_1$ considered here.

This result is hardly a surprise since for fixed V_0 we impose from the beginning the *continuity of the wave function and its first derivative* at $x=0$ and $x=L$. The wave function in the classically forbidden region ($x<0$ and $x>L$) is exponentially decreasing and is damped to zero in the $V_0\to\infty$ limit. Combined with the continuity of $\phi_n(x)$ at the points $x=0$ and $x=L$ this leads to $\phi(0)=\phi(L)=0$. (Notice that in that limit the continuity of the first derivative of the wave function is lost.)

In many textbooks (Ref. 12, Vol. 1, p. 78, Ref. 7, exercise 6.7, p. 396), this limiting process is argued to select the ''right'' boundary conditions for the self-adjoint extension of the Hamiltonian. In the same spirit, it would be tempting to consider the semi-axis case as a limit of a step potential. This selects uniquely the self-adjoint extension of the Hamiltonian such that $\phi(0)=0$ (Sec. VI B). However, for any finite height, the momentum P_x has a unique self-adjoint extension, while for an infinite height, P_x has no self-adjoint extension at all (see Sec. V B)!

This discussion shows that an infinite potential cannot be simply described as the limit of a finite one.

VIII. CONCLUDING REMARKS

The aim of this article was twofold: first to popularize the theory of self-adjoint extensions of operators among people learning and (or) teaching quantum mechanics and second to give concrete examples for some simple potentials encountered in quantum mechanics textbooks.

Further work is obviously needed. For instance the new spectra for a particle in a box could lead to different low temperature behaviors of the specific heat, following the lines of Refs. 15 and 16. Similarly, the boundary effects computed in Ref. 17 should be examined anew.

Certainly the examples considered here are simplified models devised to describe physical phenomena. This process of modeling is at the heart of the physicist's work. Once some simplified model is chosen and becomes part of the teaching activity one should explain the subtleties possibly hidden in it.

Our hope is that our analysis will be extended to the differential operators acting in three-dimensional space which could lead to more realistic physical situations and bring to light new phenomena: These developments could initiate the ''physics of self-adjoint extensions.''

Moreover, as previously seen, an infinite potential cannot be simply described as the limit of a finite one. This enforces interest in the large class of self-adjoint extensions described in this work: They deserve further study since they are all on an equal footing with respect to the principles of quantum mechanics.

Last, but not least, let us mention other difficult problems which are not thoroughly dealt with in the standard teaching of quantum mechanics: the definition of higher powers of operators (to say nothing of their exponential!) and their commutators. This item was encountered in Sec. II, where it was observed that H^2 is not the square of the operator H. By contrast, in Sec. VII C, we have exhibited a specific extension of P^2 which is really the square of the extension P_θ of P.

APPENDIX: SELF-ADJOINT EXTENSIONS OF THE MOMENTUM OPERATOR

Let us consider the Hilbert space $\mathcal{H}=L^2(a,b)$. The maximal domain on which the operator $P=-i\hbar D$ has a well-defined action has been called $\mathcal{D}_{\max}(a,b)$ in Sec. V. It is the linear space of functions $\psi(x)$ constrained by the following:

(1) $\psi(x)$ is absolutely continuous[18] on $[a,b]$.
(2) $\psi(x)$ and $\psi'(x)$ belong to $L^2(a,b)$.

It is useful to introduce the quantity

$$B(\psi,\phi)\equiv\frac{1}{2i}[(P\psi,\phi)-(\psi,P\phi)]$$
$$=\frac{\hbar}{2}[\overline{\psi}(b)\phi(b)-\overline{\psi}(a)\phi(a)]. \quad (43)$$

1. The operator *P* on the whole real axis

The Hilbert space is $\mathcal{H}=L^2(\mathbb{R})$ and the maximal domain of P is $\mathcal{D}_{\max}(\mathbb{R})$.

One can prove that for any ψ in this maximal domain, one has

$$\lim_{x\to\pm\infty}\psi(x)=0.$$

Note that this statement would not be true under the single hypothesis $\psi\in L^2(\mathbb{R})$. The symmetry of P is then, for ϕ, $\psi\in\mathcal{D}_{\max}(\mathbb{R})$, an obvious consequence of (43). To prove that $(P,\mathcal{D}_{\max}(\mathbb{R}))$ is indeed self-adjoint, one should show that, if $\phi\in L^2(\mathbb{R})$ is such that

$$\forall\psi\in\mathcal{D}_{\max}(\mathbb{R}),$$
$$\left|\int_{-\infty}^{+\infty}\psi'(x)\overline{\phi}(x)dx\right|\leqslant C\left(\int_{-\infty}^{+\infty}|\psi|^2dx\right)^{1/2},$$

then ϕ belongs to $\mathcal{D}_{\max}(\mathbb{R})$. But it is easier to check this using von Neumann's theorem, which was done in Sec. V A. We have proven that the deficiency indices are (0, 0) and concluded that the operator $(P,\mathcal{D}_{\max}(\mathbb{R}))$ is the *unique* self-adjoint extension of D.

2. The operator *P* on the positive semi-axis

The Hilbert space is $\mathcal{H}=L^2(0,+\infty)$ and we take as domain

$$\mathcal{D}_0(P)=\{\psi\in\mathcal{D}_{\max}(0,+\infty)\quad\text{and}\quad\psi(0)=0\}. \quad (44)$$

As in the previous subsection, one can prove that $\lim_{x\to+\infty}\psi(x)=0$. Then the symmetry of the operator P on $\mathcal{D}_0(P)$ follows again from relation (43).

The adjoint of $(P,\mathcal{D}_0(P))$ is given by

$$(P^\dagger=P,\quad\mathcal{D}(P^\dagger)=\mathcal{D}_{\max}(0,+\infty)).$$

The double adjoint is simply

$$P^{\dagger\dagger}=P,\quad\mathcal{D}(P^{\dagger\dagger})=\mathcal{D}_0(P),$$

which shows that $(P,\mathcal{D}_0(P))$ is closed.

However, as we checked in Sec. V B, the deficiency indices are (1, 0) and therefore, by the von Neumann theorem, $(P,\mathcal{D}(P))$ has no self-adjoint extension.

3. The operator *P* on a finite interval

The Hilbert space is now $\mathcal{H}=L^2(0,L)$ and we take

$$P=-i\hbar D,$$
$$\mathcal{D}_0(P)=\{\psi\in\mathcal{D}_{\max}(0,L),\quad\psi(0)=\psi(L)=0\}.$$

The symmetry of P on $\mathcal{D}_0(P)$ follows again from relation (43). Its adjoint is

$$(P^\dagger=P,\quad\mathcal{D}(P^\dagger)=\mathcal{D}_{\max}(0,L)).$$

Let us notice that the adjoint of $(P,\mathcal{D}(P^\dagger))$ is $(P,\mathcal{D}_0(P))$, which implies its closedness.

In Sec. V C, we have obtained the deficiency indices (1, 1) and, from von Neumann's theorem, we know that the self-adjoint extensions are parametrized by $U(1)$, i.e., a phase $e^{i\theta}$.

4. Remarks

(1) In all cases we observe that the adjoint $(P^\dagger,\mathcal{D}(P^\dagger))$ has for domain $\mathcal{D}(P^\dagger)=\mathcal{D}_{\max}$, which is the largest domain in $\mathcal{H}$ in which $-i\hbar D$ is defined. It follows that the actual computation of the deficiency indices is always an easy task.

(2) Let us observe that for symmetric operators one has the hierarchy

$$(P,\mathcal{D}(P))\subset(P^\dagger,\mathcal{D}(P^\dagger)),$$

which means that the adjoint is the ''biggest.'' When self-adjoint extensions $(P,\mathcal{D}_\theta)$ do exist they must lie in the in-between, according to the scheme

$$(P,\mathcal{D}_0(P))\subset(P,\mathcal{D}_\theta)\subset(P^\dagger,\mathcal{D}(P^\dagger)).$$

(3) For further use, let us point out the useful theorem, proved in Ref. 6 (Vol. 2, p. 90), stating that for a differential operator of order n with deficiency indices (n,n) all of its self-adjoint extensions have a discrete spectrum.

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FARADAY'S LAW

Out of the Boulder Dam come a few dozen rods of copper—long, long, long rods of copper perhaps the thickness of your wrist that go for hundreds of miles in all directions. Small rods of copper carrying the power of a giant river. Then the rods are split to make more rods . . . then to more transformers . . . sometimes to great generators which recreate the current in another form . . . sometimes to engines turning for big industrial purposes . . . to more transformers . . . then more splitting and spreading . . . until finally the river is spread throughout the whole city—turning motors, making heat, making light, working gadgetry. The miracle of hot lights from cold water over 600 miles away—all done with specially arranged pieces of copper and iron. Large motors for rolling steel, or tiny motors for a dentist's drill. Thousands of little wheels, turning in response to the turning of the big wheel at Boulder Dam. Stop the big wheel, and all the wheels stop; the lights go out. They really are connected. . . .

All this is possible because of carefully designed arrangements of copper and iron—efficiently created magnetic fields . . . blocks of rotating iron six feet in diameter whirling with clearances of 1/16 of an inch . . . careful proportions of copper for the optimum efficiency . . . strange shapes all serving a purpose, like the curve of the dam.

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