

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

Guy BONNEAU *

Jacques FARAUT †

Galliano VALENT *

Abstract

For the example of the infinitely deep 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 physical situations. Some consequences are worked out, which could lead to experimental checks.

*Laboratoire de Physique Théorique et des Hautes Energies, Unité associée au CNRS UMR 7589, Université Paris 7-Denis Diderot, 2 Place Jussieu, 75251 Paris Cedex 05.

†Laboratoire d'Analyse Algébrique, Université Paris 6-Pierre et Marie Curie, 4 Place Jussieu, 75252 Paris Cedex 05.

1 Introduction

In most 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 such commonly used examples as 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 [2, p. 11] being a notable exception as it includes a discussion of the momentum operator. But there, we find only two references relevant to the subject. The first one [5] 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 [4] mentions the self-adjoint extensions of the Hamiltonian for a particle in a semi-axis and its relevance, first pointed out by Jackiw [9], 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 organised as follows : in Section 2 we discuss some paradoxes met in the study of the infinite potential well. Then, in Section 3, we present a first analysis of the boundary conditions for the self-adjoint extensions of the momentum operator.

In Section 4 we introduce the concept of deficiency indices and state von Neumann’s theorem. In Section 5 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 of easy access. The reader interested in these technical aspects may consult the references [1] and [12].

Then, in section 6, we describe the self-adjoint extensions of the Hamiltonian operator in various settings (on the real axis, on the positive semi-axis and in a box). Several physical implications are analysed, while in section 7, we use different constraints from physics to reduce the set of all possible self-adjoint extensions.

We have gathered in appendix A some technical details on the extensions of the momentum operator and in appendix B we discuss the spectra of the Hamiltonian operator for a particle in a box. A proof for parity preserving self-adjoint extension is given in Appendix C.

2 The infinite potential well : paradoxes

Let us consider the standard problem (see for example [10, p. 299] or [8, p. 109]) of a particule of mass m in a one dimensional, infinitely deep, potential well of width L :

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

Stationary states are obtained through the Schrödinger (eigenvalue) equation

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

and the vanishing of their wave function at both ends. This means that the action of the hamiltonian operator for a free particle, unbounded on the closed interval $[-\frac{L}{2}, +\frac{L}{2}]$, is defined by:

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

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

Two series of normalised eigenfunctions of opposite parity are obtained. They vanish outside the well and for $x \in [-\frac{L}{2}, +\frac{L}{2}]$ they write :

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

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

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

$$\Psi(x) = -\sqrt{\frac{30}{L^5}} \left(x^2 - \frac{L^2}{4}\right), \quad |x| \leq \frac{L}{2}; \quad \Psi(x) = 0, \quad |x| \geq \frac{L}{2}. \quad (4)$$

It may be expanded [17] on the complete basis of eigen functions of H given in (3) :

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

Let us define also, for further use,

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

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

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

but on the other hand

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

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

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

leads to

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

and on the other hand

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

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

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

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

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

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

$$\langle E^2 \rangle = (H\Psi, H\Psi) = (\Psi, H^2\Psi) = 0 \quad (11)$$

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

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

on the contrary, 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 summarise, 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 $-\frac{\hbar^2}{2m}D^2$, question already solved by mathematicians in the thirties. Before explaining this theory in a simple manner, we analyse in the next Section the momentum operator $-i\hbar D$.

3 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

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

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

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

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

Conclusion : A symmetric differential operator acting on a given functional space is not automatically a self-adjoint operator and may have none, a unique or an infinity of self-adjoint extensions. In the next Section, we give some mathematical results on the theory of self-adjoint extensions of a differential operator in a Hilbert space and “deficiency indices”.

4 Deficiency indices and von Neumann’s theorem

Since this Section makes use of mathematical terminology, let us begin with some precise 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

$$\lim_{n \rightarrow \infty} \phi_n = \phi, \quad \lim_{n \rightarrow \infty} A\phi_n = \psi,$$

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

Let us recall the definition of the adjoint operator of a (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

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

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 [1, p. 80, vol. 1].

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

$$\begin{aligned} \mathcal{N}_+ &= \{\psi \in \mathcal{D}(A^\dagger), \quad A^\dagger\psi = z_+\psi, \quad \text{Im } z_+ > 0\}, \\ \mathcal{N}_- &= \{\psi \in \mathcal{D}(A^\dagger), \quad A^\dagger\psi = z_-\psi, \quad \text{Im } z_- < 0\}, \end{aligned}$$

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_+ (resp. n_-) is completely independent of the choice of z_+ (resp. z_-) as far as it lies in the upper (resp. lower) half-plane. It follows that a simple way to determine (n_+, n_-) is to take $z_+ = i\lambda$ and $z_- = -i\lambda$ with an arbitrary strictly positive constant λ needed for dimensional reasons.

The following theorem, first discovered by Weyl [16] in 1910 for second order differential operators and generalized by von Neumann [15] in 1929, is of primary 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 $n_+ = n_- = n \geq 1$, 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 application of this theorem to differential operators requires still a lot of work : even if we start from an operator P which is formally self-adjoint, this does not prove that P is truly self-adjoint because the domains $\mathcal{D}(P)$ and $\mathcal{D}(P^\dagger)$ will be different in general.

For a given differential operator P 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^\dagger .
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 and is given in many text-books (for instance [1],[12]). In the next Section we describe the results for the simplest case of the momentum operator $P = -i\hbar D$, referring for the proofs to [1, vol. 1, p. 106-111].

5 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 $\mathcal{D}_{\max}(a, b)$. In this Section, we apply the previous theorem, postponing some mathematical details to the Appendix A.

Let us consider the Hilbert space $\mathcal{H} = L^2(a, b)$ and 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) .

5.1 The operator P on the whole real axis

None of the functions $\psi_\pm(x)$ belong 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.

5.2 The operator P on the positive semi-axis

Among the functions $\psi_\pm(x)$, only ψ_+ belongs to $L^2(0, +\infty)$. We conclude to the deficiency indices $(1, 0)$ and therefore, by the von Neumann theorem, 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 !

5.3 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 section 3. Denoting these extensions by $P_\theta = (P, \mathcal{D}_\theta)$, they are given by

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

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

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

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

$$c_n(\theta) = -\frac{\sqrt{30}}{2\pi^2\nu^2} \left[\cos(\theta/2) - \frac{\sin(\theta/2)}{\pi\nu} \right] e^{-i\theta/2}, \quad \text{for } \theta \neq 0, \quad (16)$$

and

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

So the probability to find the particle with a momentum $\frac{2\pi\nu\hbar}{L}$, 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 ([2] and [6, 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 anti-periodic boundary condition (i.e. $\theta = \pi$) has been considered by Capri in [5].

2. For a particle in a box, it is often argued that the ‘‘physical’’ wave function should continuously vanish on the walls $x = 0$ and $x = L$, ensuring that the presence probability vanishes continuously for $x \leq 0$ and for $x \geq L$. One should realize that the continuity of the measurable quantity

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

is ensured as soon as the integral $\int_0^L |\phi(x)|^2 dx$ does converge 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

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

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

3. The existence of normalisable eigenfunctions of the momentum operator has an important consequence : the Heisenberg inequality $\Delta X \cdot \Delta P \geq \hbar/2$ 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 normalisable 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 $L_z = -i\hbar \frac{d}{d\varphi}$. The previous remark shows that the inequality $\Delta\varphi \cdot \Delta L_z \geq \hbar/2$ can be violated, even by wave functions periodic in the angle φ .

6 Self-adjoint extensions of the Hamiltonian

In the same setting as in the previous section, 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

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

and get

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

6.1 The Hamiltonian on the whole real axis

The physical situation corresponds to 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 understanding of this case.

6.2 The Hamiltonian on the positive semi-axis

The physical problem is that of a free particle in front of an infinitely high wall for $x < 0$. In the Hilbert space $\mathcal{H} = L^2(0, +\infty)$ we have the solutions to equation (18) given by

$$\phi_\pm = b_\pm e^{-k_0 x / \sqrt{2}} e^{\pm i k_0 x / \sqrt{2}},$$

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

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

see [1, vol. 2, p.187, 204]. The boundary condition $\phi'(0) = 0$ corresponds to $\lambda = \infty$. Physicists use the particular extension with $\lambda = 0$, see for instance [10, p. 328] and [14, p. 33].

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

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

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

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

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

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

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 normalised wave function are

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

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

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

In an attempt to lift this degeneracy, we consider the simplified deuteron theory described by the potential

$$V(x) = \begin{cases} \infty & \text{for } x < 0, \\ -V_0 & \text{for } 0 < x < a, \\ 0 & \text{for } x > a. \end{cases} \quad V_0 > 0, \quad (24)$$

The wave function is well known to be

$$\begin{aligned} x < a : \quad \phi_1(x) &= A \sin kx + B \cos kx, & E + V_0 &= \frac{\hbar^2 k^2}{2m}, & k > 0, \\ x > a : \quad \phi_2(x) &= C e^{-\rho x}, & E &= -\frac{\hbar^2 \rho^2}{2m}, & \rho > 0. \end{aligned} \quad (25)$$

We next impose the boundary condition (20) and the usual continuity conditions at $x = a$. Using the notations $X = ka$ and $Y = \rho a$, we get that the bound state energy is given by the solution of the system

$$\lambda \geq 0 \quad \longrightarrow \quad Y = -X \frac{1 - (\lambda/a)X \tan X}{\tan X + (\lambda/a)X}, \quad \text{and} \quad \frac{V_0}{|E|} = 1 + \left(\frac{X}{Y}\right)^2. \quad (26)$$

In the case of the deuteron, the absolute value of the binding energy $|E|$, is roughly equal to 2.2 MeV. Its size is $a = 2$ F and we take $2m = M$ where M is the nucleon mass. It follows that $Y = 0.46$. For a given value of λ , we have to solve for X , and then recover the potential V_0 . Numerical analysis gives the following dependence on V_0 with respect to the parameter λ :

λ/a	0	0.1	0.2	0.5	1	2	5	10	100	∞
V_0 (MeV)	36.8	31.5	27.5	20.5	15.3	11.5	8.59	7.50	6.47	6.34

Let us observe that the parameter λ , describing the different extensions, does indeed have an effect on physical quantities (as already observed for the momentum operator, in subsection 5.3) and in fact experiment, not just theoretical prejudices, should decide which is the “right” value for it.

6.3 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 the previous section, but up 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 equation (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 $\mathcal{D}_{\max}(0, L)$,

$$B(\phi, \psi) = \frac{1}{2i} \left((H^\dagger \phi, \psi) - (\phi, H^\dagger \psi) \right) \quad (27)$$

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

$$B(\phi, \phi) = \frac{1}{2i} \left(\phi'(L) \overline{\phi(L)} - \phi(L) \overline{\phi'(L)} - \phi'(0) \overline{\phi(0)} + \phi(0) \overline{\phi'(0)} \right). \quad (28)$$

The identity

$$\frac{1}{2i} (x\bar{y} - \bar{x}y) = \frac{1}{4} (|x + iy|^2 - |x - iy|^2), \quad (29)$$

applied to $x = L\phi'(L)$, $y = \phi(L)$ and $x = L\phi'(0)$, $y = \phi(0)$ brings relation (28) to

$$4LB(\phi, \phi) = |L\phi'(0) - i\phi(0)|^2 + |L\phi'(L) + i\phi(L)|^2 - |L\phi'(0) + i\phi(0)|^2 - |L\phi'(L) - i\phi(L)|^2. \quad (30)$$

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

$$\begin{pmatrix} L\phi'(0) - i\phi(0) \\ L\phi'(L) + i\phi(L) \end{pmatrix} = U \begin{pmatrix} L\phi'(0) + i\phi(0) \\ L\phi'(L) - i\phi(L) \end{pmatrix}. \quad (31)$$

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 [12, 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 of these spectra to the Appendix B, we only give the results.

Let us parametrize the unitary matrix U as :

$$U = e^{i\psi} M, \quad \det M = 1, \quad \Rightarrow \quad \det U = e^{2i\psi}, \quad \psi \in [0, \pi] \quad (32)$$

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.

To parametrize the matrix M , we used 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 : $\vec{n} \cdot \vec{\tau} = n_1 \tau_1 + n_2 \tau_2 + n_3 \tau_3$. With coordinates $m = (m_0, \vec{m})$ constrained by

$$m_0^2 + \vec{m} \cdot \vec{m} = 1 \quad \Longleftrightarrow \quad m \in \mathbb{S}^3, \quad (33)$$

M writes :

$$M = \begin{pmatrix} m_0 - im_3 & -m_2 - im_1 \\ m_2 - im_1 & m_0 + im_3 \end{pmatrix} = m_0 I - i \vec{m} \cdot \vec{\tau}. \quad (34)$$

Then, starting from the boundary conditions (31), we obtain the spectra for the Hamiltonian

in a box (see details in Appendix B) :

$$\begin{aligned}
a) \ E = \frac{s^2}{L^2} > 0 : & & 2s[\sin \psi \cos s - m_1] &= \sin s[\cos \psi(s^2 + 1) - m_0(s^2 - 1)], \\
b) \ E = 0 : & & s \rightarrow 0 \text{ in result (35 - a)} &\Leftrightarrow \\
& & 2 \sin \psi - \cos \psi &= 2m_1 + m_0, \\
c) \ E = -\frac{r^2}{L^2} < 0 : & & s = ir \text{ in result (35 - a)} &\Leftrightarrow \\
& & 2r[\sin \psi \cosh r - m_1] &= \sinh r[-\cos \psi(r^2 - 1) + m_0(r^2 + 1)].
\end{aligned} \tag{35}$$

Remarks :

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

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

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, then the spectrum will be positive, an issue which depends on the extension H_U considered (see section 7.3).

7 Restrictions from physics on the self-adjoint extensions

In the previous section 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.

7.1 Extensions preserving time reversal

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

$$i\hbar \frac{\partial \Psi}{\partial t}(x, t) = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}(x, t) \tag{36}$$

inside the box. The time reversal invariance of this equation means that if $\Psi(x, t)$ is a solution of (36), then $\bar{\Psi}(x, t)$ is also a solution. If we consider a stationary state of definite energy E with the wave function

$$\Psi(x, t) = \phi_E(x) e^{-i\frac{Et}{\hbar}},$$

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

The shortcoming in this argument is that the boundary conditions (31) 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 $\bar{\psi}_{\pm}(x) = \psi_{\mp}(x)$. Taking the complex conjugate of relation (31) gives

$$\begin{pmatrix} \psi_+(0) \\ \psi_-(L) \end{pmatrix} = \bar{U} \begin{pmatrix} \psi_-(0) \\ \psi_+(L) \end{pmatrix} = \bar{U}U \begin{pmatrix} \psi_+(0) \\ \psi_-(L) \end{pmatrix}. \quad (37)$$

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

$$\det(\mathbb{I} - \bar{U}U) = 0. \quad (38)$$

Using for U the coordinates given by (34), easy computations give $m_2 = 0$ and, correspondingly, the matrix

$$U = e^{i\psi} \begin{pmatrix} m_0 - im_3 & -im_1 \\ -im_1 & m_0 + im_3 \end{pmatrix} \quad \text{with } \psi \in [0, \pi] \quad \text{and} \quad m_0^2 + m_1^2 + m_3^2 = 1, \quad (39)$$

7.2 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 (31) 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 Schrodinger 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 condition $\int |\phi(x)|^2 dx < \infty$. 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 $x \rightarrow -\infty$, while for $x \rightarrow +\infty$ 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

$$|\tilde{\phi}_E(-u)|^2 = |\tilde{\phi}_E(u)|^2. \quad (40)$$

Here one finds (Appendix C) that all parity preserving extensions are given by $m_3 = 0$ and so correspond to the matrix

$$U = e^{i\psi} \begin{pmatrix} m_0 & -m_2 - im_1 \\ m_2 - im_1 & m_0 \end{pmatrix}, \quad \psi \in [0, \pi], \quad m_0^2 + m_1^2 + m_2^2 = 1. \quad (41)$$

7.3 Extensions preserving positivity

One of the most surprising facts, for a physicist, is the appearance of extensions with negative energies (these can be determined explicitly in some particular cases, see appendix B).

From a theorem proved in [12, 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 equation (35), which are fairly tedious.

A partial answer to this problem is offered by an interesting theorem due to von Neumann (see [1, 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 Subsection 5.3, whose adjoint was $(P, \mathcal{D}_{\max}(0, L))$. It follows that the operator

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

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

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

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

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

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

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

corresponding to the matrix

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

As shown in the appendix B.2., for this choice of matrix U , the operators (P^2, \mathcal{D}_U) and (P, \mathcal{D}_θ) have the same eigenfunctions. These extensions, (P^2, \mathcal{D}_U) are really the square of the ones of the momentum operator (P, \mathcal{D}_θ) .

7.4 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 :

$$V(x) = 0, \quad x \in]0, L[; \quad V(x) = V_0 > 0, \quad x \notin]0, L[. \quad (42)$$

A standard computation gives the bound states wave function

$$\begin{aligned} x \leq 0 & : \quad \phi_n(x) = d_n e^{\rho x} & \rho^2 &= \frac{2m(V_0 - E)}{\hbar^2} \\ x \geq L & : \quad \phi_n(x) = \pm d_n e^{-\rho(x-L)} & & \\ 0 \leq x \leq L & : \quad \phi_n(x) = d_n \left[\cos kx + \frac{\rho}{k} \sin kx \right] & k^2 &= \frac{2mE}{\hbar^2} \end{aligned} \quad (43)$$

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 the relation

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

When V_0 is large, one finds for the spectrum ($\rho \simeq \infty$, $v_0 = \sqrt{\frac{2mV_0L^2}{\hbar^2}} \gg 1$, k fixed) :

$$k_n L \simeq n\pi(1 - 2/v_0), \quad E_n \simeq E_n^\infty(1 - 4/v_0) \quad (44)$$

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

$$\begin{aligned} \phi_n(x \leq 0) & \sim \sqrt{\frac{2}{L}} \left(\frac{n\pi}{v_0} \right) \exp -v_0|x/L| \sim 0 \\ \phi_n(x \geq L) & \sim \pm \sqrt{\frac{2}{L}} \left(\frac{n\pi}{v_0} \right) \exp -v_0(x/L - 1) \sim 0 \\ \phi_n(0 \leq x \leq L) & \sim \sqrt{2/L} \left[\sin n\pi \frac{x}{L} + \left(\frac{n\pi}{v_0} \right) \left[\cos n\pi \frac{x}{L} - \frac{1}{n\pi} \sin n\pi \frac{x}{L} \right] \right], \end{aligned} \quad (45)$$

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 non-symmetric 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 $V_0 \rightarrow \infty$ and $V_1 \rightarrow \infty$ 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 off to zero in the $V_0 \rightarrow \infty$ 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 [6, vol. 1, p. 78], [10, 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 $\phi(0) = 0$ (Subsection 6.2). 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 Subsection 5.2)!

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

8 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 point out some physical consequences which could be checked by experiment.

For example the new spectra for a particle in a box should lead to different low temperature behaviours of the specific heat, following the lines of [13], [7]. Similarly, the boundary effects computed in [3] should be examined anew.

Certainly the examples considered here are too simple, and are of questionable practical feasibility. Our hope is that people will extend our analysis to the differential operators acting in three dimensional space which could lead to more realistic physical situations and put 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 by 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.

We have also emphasized in the previous Section the role of the symmetry properties (resp. reality properties) of the boundary conditions when the potential has some symmetry properties (resp. reality properties). Moreover, in subsection (5.3) we show that, in presence of an infinite discontinuity of the potential, the continuity of the wave function does not result from 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 Section 2, where it was observed that H^2 is not the square of the operator H . On the contrary, in subsection 7.3, we have exhibited a specific extension of P^2 which is really the square of the extension P_θ of P .

A 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 in Section.5 $\mathcal{D}_{\max}(a, b)$. It is the linear space of functions $\psi(x)$ constrained by :

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

$$B(\psi, \phi) \equiv \frac{1}{2i} [(P\psi, \phi) - (\psi, P\phi)] = \frac{\hbar}{2} [\overline{\psi}(b)\phi(b) - \overline{\psi}(a)\phi(a)]. \quad (46)$$

A.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 :

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

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 $\phi, \psi \in \mathcal{D}_{\max}(\mathbb{R})$, an obvious consequence of (46). 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

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

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 Subsection 5.1. 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 .

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

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

$$\mathcal{D}_0(P) = \{\psi \in \mathcal{D}_{\max}(0, +\infty) \text{ and } \psi(0) = 0\}. \quad (47)$$

As in the previous subsection one can prove that $\lim_{x \rightarrow +\infty} \psi(x) = 0$. Then the symmetry of the operator P on $\mathcal{D}_0(P)$ follows again from relation (46).

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 Subsection 5.2, the deficiency indices are $(1, 0)$ and therefore, by von Neumann's theorem, $(P, \mathcal{D}(P))$ has no self-adjoint extension.

A.3 The operator P on a finite interval

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

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

The symmetry of P on $\mathcal{D}_0(P)$ follows again from relation (46). 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 Subsection 5.3, 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 $e^{i\theta}$.

A.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}_θ) 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 [12, 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.

B The spectra of the Hamiltonian in a box

Starting from the boundary conditions (31) we now derive the equations giving the eigenvalues for all the extensions H_U .

Let us consider the positive spectrum, the zero and negative ones being obtained in the same way and, as a matter of fact, obtained by substitutions as indicated in (35).

Denoting by $E = \frac{s^2}{L^2}$, with $s > 0$, the eigenvalues of H_U , and its eigenfunctions by

$$\phi(s, x) = A e^{isx/L} + B e^{-isx/L}, \quad \Phi = \begin{pmatrix} A \\ B \end{pmatrix}, \quad (48)$$

one can easily check the relations

$$\begin{pmatrix} L\phi'(0) - i\phi(0) \\ L\phi'(L) + i\phi(L) \end{pmatrix} = i\mathcal{L}(s)\Phi, \quad \begin{pmatrix} L\phi'(0) + i\phi(0) \\ L\phi'(L) - i\phi(L) \end{pmatrix} = i\mathcal{M}(s)\Phi, \quad (49)$$

with the matrices

$$\mathcal{L}(s) = \begin{pmatrix} s-1 & -s-1 \\ (s+1)e^{is} & -(s-1)e^{-is} \end{pmatrix}, \quad \mathcal{M}(s) = \begin{pmatrix} s+1 & -s+1 \\ (s-1)e^{is} & -(s+1)e^{-is} \end{pmatrix}. \quad (50)$$

The determinants of these matrices are given by

$$\det \mathcal{M}(s) = 2[i(s^2 + 1) \sin s - 2s \cos s], \quad \det \mathcal{L}(s) = -\overline{\det \mathcal{M}(s)},$$

from which it follows that $\mathcal{L}(s)$ and $\mathcal{M}(s)$ have vanishing determinant if and only if $s = 0$.

Using these notations the equations for the eigenfunctions become

$$(\mathcal{L}(s) - U\mathcal{M}(s))\Phi = 0, \quad (51)$$

and for the spectra

$$\det(\mathcal{L}(s) - U\mathcal{M}(s)) = 0. \quad (52)$$

To get a more explicit form of the eigenvalue equation let us use some simple relations valid for arbitrary 2×2 matrices

$$2 \det A = (\operatorname{tr} A)^2 - \operatorname{tr}(A^2) \quad \Rightarrow \quad \det(A - B) = \det A + \det B + \operatorname{tr}(AB) - \operatorname{tr} A \cdot \operatorname{tr} B. \quad (53)$$

For $s \neq 0$ we can write relation (52) as

$$\det(\mathcal{L}(s)\mathcal{M}^{-1}(s) - U) = 0, \quad (54)$$

where the matrix $\mathcal{L}\mathcal{M}^{-1}$ has the simple form

$$\mathcal{L}(s)\mathcal{M}^{-1}(s) = \frac{2}{\det \mathcal{M}(s)} \begin{pmatrix} i(s^2 - 1) \sin s & -2s \\ -2s & i(s^2 - 1) \sin s \end{pmatrix}.$$

Subsequent use of (53) in relation (54) and simple computations lead to

$$2s [\cos s(1 - \det U) - \operatorname{tr}(U\tau_1)] + i \sin s [(s^2 + 1)(1 + \det U) - (s^2 - 1) \operatorname{tr} U] = 0, \quad (55)$$

valid for the positive non-zero spectrum.

The parametrization of the matrix U given by (32), (34) simplifies relation (55) to

$$2s \left[\sin \psi \cos s + \frac{1}{2i} \operatorname{tr}(M\tau_1) \right] = \sin s \left[(s^2 + 1) \cos \psi - \frac{1}{2}(s^2 - 1) \operatorname{tr}(M) \right], \quad (56)$$

a writing which exhibits the reality of the eigenvalue equation. It also displays a nice invariance under the transformation

$$M \rightarrow M' = e^{-\theta\tau_1/2i} M e^{+\theta\tau_1/2i}, \quad \theta \in [0, 2\pi], \quad (57)$$

as it leaves $\operatorname{tr} M$ and $\operatorname{tr}(M\tau_1)$ unchanged. Let us point out that this invariance is specific of the spectra, not of the eigenfunctions.

The strictly positive spectrum is then given by

$$2s [\sin \psi \cos s - m_1] = \sin s [\cos \psi (s^2 + 1) - m_0 (s^2 - 1)], \quad E = \frac{s^2}{L^2}. \quad (58)$$

The invariance (57) explains why the spectrum does not depend either of m_2 or of m_3 .

An explicit solution of the eigenvalue equation (58) is clearly hopeless for the most general unitary matrix U . Nevertheless there are many special cases for which this can be achieved explicitly. We therefore classify the spectra as :

1. “Simple” if the eigenvalue equation can be solved explicitly. This happens for two families :

$$m_1 = \sin \psi = 0, \quad \text{or} \quad m_0 = \cos \psi = 0.$$

2. “Generic” if this is not the case. Typically the “generic” spectra are solutions of at least one transcendental equation and only their large n behaviour can be obtained explicitly.

B.1 First family of “simple” spectra

This first family corresponds to $\psi = 0$ and $m_1 = 0$ and its matrix U has the form

$$U = \begin{pmatrix} m_0 - im_3 & -m_2 \\ m_2 & m_0 + im_3 \end{pmatrix} \quad \text{with} \quad m_0^2 + m_2^2 + m_3^2 = 1 \quad \Leftrightarrow \quad m \in S^2. \quad (59)$$

The eigenvalue equation reduces to

$$\sin s [(1 - m_0)s^2 + 1 + m_0] = 0.$$

Since $m_0 \in [-1, +1]$ the factor in front of the sine never vanishes, so we get for spectrum

$$s_n = n\pi, \quad n = 1, 2, \dots$$

Note that the zero spectrum is easily checked to appear only for the extension with $U = -\mathbb{I}$, while the strictly negative spectrum is given by

$$\sinh r [(m_0 - 1)r^2 + m_0 + 1] = 0,$$

which has always a solution, except for $m_0 = \pm 1$. We conclude to the negative energy

$$r^2 = \frac{1 + m_0}{1 - m_0}, \quad \longrightarrow \quad E = -\frac{1}{L^2} \frac{1 + m_0}{1 - m_0}, \quad m_0 \in] -1, +1[.$$

Remark : In this family two and only two extensions (with $m_0 = \pm 1$) are therefore distinguished by the absence of negative energies in their spectra. The first one is

$$\left\{ \begin{array}{l} U = \mathbb{I} \\ \phi(0) = \phi(L) = 0 \end{array} \right. \longrightarrow \left\{ \begin{array}{l} s_n = n\pi, \quad n = 1, 2, \dots, \\ \phi_n(x) = \sqrt{\frac{2}{L}} \sin \left(n\pi \frac{x}{L} \right). \end{array} \right.$$

This is the “standard” self-adjoint extension considered in the textbooks on quantum mechanics [8, p. 109],[10, p. 300].

The second one is

$$\left\{ \begin{array}{l} U = -\mathbb{I} \\ \phi'(0) = \phi'(L) = 0 \end{array} \right. \longrightarrow \left\{ \begin{array}{l} s_n = n\pi, \quad n = 0, 1, \dots, \\ \phi_n(x) = \sqrt{\frac{2}{L}} \cos \left(n\pi \frac{x}{L} \right). \end{array} \right. \quad (60)$$

A different understanding of the absence of negative energies for these two extensions is given, using von Neumann theorem, in Subsection 7.3.

B.2 Second family of “simple” spectra.

This second family corresponds to $\cos \psi = 0$, or equivalently $\psi = \pi/2$, and $m_0 = 0$. The corresponding matrix U is

$$U = \begin{pmatrix} m_3 & m_1 - im_2 \\ m_1 + im_2 & -m_3 \end{pmatrix}, \quad \text{with} \quad m_1^2 + m_2^2 + m_3^2 = 1. \quad (61)$$

Relation (58) reduces to

$$\cos s = m_1.$$

From (61) we know that $m_1 \in [-1, +1]$. Excluding the values $m_1 = \pm 1$, discussed in the final remark, the positive spectrum is

$$s_n = \begin{cases} +\cos^{-1}(m_1) + 2n\pi, & n = 0, 1, \dots \\ -\cos^{-1}(m_1) + 2n\pi, & n = 1, 2, \dots \end{cases} \quad \cos^{-1}(1) = \pi/2.$$

As already observed, these eigenvalues are independent of m_2 and m_3 , but this degeneracy affects only the spectra, not the eigenfunctions.

Let us observe that for the particular case

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

we have the full spectrum and eigenfunctions

$$\begin{aligned} s_n &= \theta + 2n\pi, & \phi_n(x) &= \frac{1}{L} e^{2\pi i(n+\theta/2\pi)x/L}, & n &= 1, 2, \dots \\ s_n &= -\theta + 2n\pi, & \phi_n(x) &= \frac{1}{L} e^{2\pi i(-n+\theta/2\pi)x/L}, & n &= 0, 1, \dots \end{aligned}$$

The exceptional cases $\theta = 0$ and $\theta = \pi$ are discussed in the next remark. The important point is that these eigenfunctions of P^2 are the same as for (P, \mathcal{D}_θ) given in Section 5.4

Note that the zero spectrum is easily checked to appear only for the extension with $U = \tau_1$, while the strictly negative spectrum given by

$$\cosh r = m_1$$

is absent because from (61) we know that $m_1 \in [-1, +1]$.

Remark : two extensions are distinguished by their doubly degenerate spectra. The first one corresponds to the periodic boundary conditions (the degeneracy of the energy s_n is denoted by g_n .)

$$\begin{cases} U = \tau_1 \\ \phi(0) = \phi(L), \phi'(0) = \phi'(L) \end{cases} \longrightarrow \begin{cases} s_n = 2n\pi, & n = 1, 2, \dots & g_n = 2, \\ s_0 = 0, & & g_0 = 1, \end{cases}$$

and the second one to the antiperiodic boundary conditions

$$\begin{cases} U = -\tau_1 \\ \phi(0) = -\phi(L), \phi'(0) = -\phi'(L) \end{cases} \longrightarrow s_n = (2n+1)\pi, \quad n = 0, 1, 2, \dots \quad g_n = 2.$$

The periodic boundary conditions may have a physical interpretation for rotational degrees of freedom of molecules [6, vol. 2, p. 1202].

B.3 The “generic” spectra

We now exclude from our analysis the extensions with “simple” spectra. Switching to the variable $t = \tan \frac{s}{2}$, the eigenvalue equation (58) becomes

$$\frac{s}{t^2 + 1} \left\{ (m_1 + \sin \psi)t^2 + \frac{t}{s} [\cos \psi(s^2 + 1) - m_0(s^2 - 1)] + m_1 - \sin \psi \right\} = 0. \quad (62)$$

The overall factor $\frac{1}{1+t^2}$ should not be overlooked since it may vanish for $t = \infty$.

We organise the discussion of the “generic” spectra by distinguishing three different cases :

- $m_1 = -\sin \psi \neq 0$.

In this case the spectrum is

$$\begin{cases} \cot \frac{s}{2} = 0 & \longrightarrow & s = (2n + 1)\pi, & n = 0, 1, 2, \dots, \\ \cot \frac{s}{2} = -\frac{(m_0 - \cos \psi)s^2 - (m_0 + \cos \psi)}{2s \sin \psi}, & & s > 0. \end{cases} \quad (63)$$

Notice that $\sin \psi$ cannot vanish (because then $m_1 = 0$ and we are back to the first family of “simple” spectra). The numerator vanishes identically only for the second family of “simple” spectra, so we conclude that equation (63) gives only “generic” spectra.

- $m_1 = \sin \psi \neq 0$,

in which case we have

$$\begin{cases} \tan \frac{s}{2} = 0 & \longrightarrow & s = 2n\pi, & n = 1, 2, \dots, \\ \tan \frac{s}{2} = \frac{(m_0 - \cos \psi)s^2 - (m_0 + \cos \psi)}{2s \sin \psi}, & & s > 0. \end{cases} \quad (64)$$

By the same argument as before neither the numerator nor the denominator can vanish, therefore equation (64) does give “generic” spectra.

- $m_1 \pm \sin \psi \neq 0$,

in which case the discriminant of equation (62) can be written

$$\Delta(s) = [(m_0 - \cos \psi)s^2 - (m_0 + \cos \psi)]^2 + 4s^2(m_2^2 + m_3^2),$$

and is strictly positive because of the first term squared (otherwise we are back to the second family of “simple” spectra).

The roots of

$$\tan \frac{s}{2} = \frac{1}{2s(m_1 + \sin \psi)} \left\{ (m_0 - \cos \psi)s^2 - (m_0 + \cos \psi) \pm \sqrt{\Delta(s)} \right\}, \quad (65)$$

give spectra which are certainly “generic”.

The equations giving the zero and the strictly negative spectrum can also be deduced as already explained in Section 6.

Let us conclude with a simple choice for the eigenfunctions

$$\begin{aligned} A(s) &= \alpha (s - 1) + [\gamma e^{-is} - 1](s + 1), \\ B(s) &= \alpha (s + 1) + [\gamma e^{is} - 1](s - 1) = -A(-s), \end{aligned} \quad U = \begin{pmatrix} \alpha & \gamma \\ \beta & \delta \end{pmatrix}. \quad (66)$$

This gives the relations

$$\phi(s; x) = A(s) e^{isx/L} - A(-s) e^{-isx/L}, \quad \phi(-s; x) = -\phi(s; x). \quad (67)$$

The simultaneous vanishing of A and B signals a doubly degenerate spectrum.

C Extensions preserving parity

The eigenfunctions (67) write in u variable :

$$\tilde{\phi}_E(u) = \phi_E(x) = A(s) e^{is/2} e^{isu} + B(s) e^{-is/2} e^{-isu}.$$

Imposing the constraint (40) gives

$$\text{Im} (A(s) \overline{B}(s) e^{is}) = 0. \quad (68)$$

It is important to observe that this relation should hold only when we take for s the actual spectrum given by relation (58).

Using for $A(s)$ and $B(s)$ the expressions given by (66), and after some algebra, one reduces the constraint (68) to

$$\begin{aligned} 2s [(\sin \psi m_0 - \cos \psi m_3) \cos s - m_0 m_1 - m_2 m_3] = \\ \sin s [(\cos \psi m_0 + \sin \psi m_3)(s^2 + 1) - (m_0^2 + m_3^2)(s^2 - 1)]. \end{aligned} \quad (69)$$

The m_0 dependent terms disappear, thanks to relation (58), and we are left with

$$m_3 \sin \psi \{ 2s [\cos \psi \cos s + m_2] + \sin s [\sin \psi (s^2 + 1) - m_3 (s^2 - 1)] \} = 0. \quad (70)$$

One can check, by enumeration of all the cases, that the coefficient between braces never vanishes for $m_3 \neq 0$.

We conclude that all the parity preserving extensions are given by $m_3 = 0$. Q.E.D

References

- [1] N. I. Akhiezer and I. M. Glazman, Theory of linear operators in Hilbert space, Frederick Ungar Publishing Company, New-York (1961).
- [2] L. E. Ballentine, *Quantum Mechanics*, Prentice Hall, Englewood Cliffs, New Jersey (1990).
- [3] D.H. Berman, "Boundary effects in quantum mechanics", Am. J. Phys. **59**, 937-941 (1991).

- [4] A. Cabo, J. L. Lucio and H. Mercado, “On scale invariance and anomalies in quantum mechanics”, *Am. J. Phys.* **66**, 240-246, (1998).
- [5] A. Z. Capri, “Self-adjointness and spontaneously broken symmetry”, *Am. J. Phys.* **45**, 823-825, (1977).
- [6] C. Cohen-Tannoudji, B. Diu and F. Laloë, *Quantum Mechanics*, John Wiley and Sons, New-York (1977).
- [7] V. Granados and N. Aquino, “Comment on specific heat revisited”, *Am. J. Phys.* **67**, 450-451, (1999).
- [8] W. Greiner, *Quantum Mechanics*, Springer-Verlag, Berlin (1989).
- [9] R. Jackiw, “Delta function potentials in two and three dimensional quantum mechanics”, in *M. A. Bég Memorial Volume*, edited by A. Ali and P. Hoodbhoy (World Scientific, 1991) 1-16.
- [10] J. M. Lévy-Leblond and F. Balibar, *Quantics*, North-Holland (1990).
- [11] A. Kolmogorov and S. Fomine, *Eléments de la théorie des fonctions et de l'analyse fonctionnelle*, Mir-Ellipses, Paris (1994).
- [12] M. A. Naimark, *Linear differential operators*, vol 2, Frederick Ungar Publishing Company, New-York (1968).
- [13] H. B. Rosentock, “Specific heat of a particle in a box”, *Am. J. Phys.* **30**, 38-40 (1962).
- [14] L. Schiff, *Quantum Mechanics*, 3rd edition, Mac-Graw-Hill, New-York (1965).
- [15] J. von Neumann, *Math. Ann.* **102**, 49-131, (1929).
- [16] H. Weyl, *Math. Ann.* **68**, 220-269, (1910).
- [17] Notice that the positive function (4) is nearly equal to the eigenfunction Ψ_1 as $b_1 = 0.99\dots$, $b_2 = -b_1/27$, $b_3 = b_1/125\dots$
- [18] To make things simple we say that a function is absolutely continuous for $x \in [b, c]$ if it can be written in the form $\phi(x) = \int_a^x \psi(u) du$, where $\psi(x)$ is absolutely integrable for any $x \in [b, c]$. Absolute continuity in a finite interval implies uniform continuity, whereas the converse is not true. The interested reader is referred to [11, p.337].