The role of the rigged Hilbert space in Quantum Mechanics

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Abstract. There is compelling evidence that, when continuous spectrum is present, the natural mathematical setting for Quantum Mechanics is the rigged Hilbert space rather than just the Hilbert space. In particular, Dirac's bra-ket formalism is fully implemented by the rigged Hilbert space rather than just by the Hilbert space. In this paper, we provide a pedestrian introduction to the role the rigged Hilbert space plays in Quantum Mechanics, by way of a simple, exactly solvable example. The procedure will be constructive and based on a recent publication. We also provide a thorough discussion on the physical significance of the rigged Hilbert space.

PACS numbers: 03.65.-w, 02.30.Hq

1. Introduction

It has been known for several decades that Dirac's bra-ket formalism is mathematically justified not by the Hilbert space alone, but by the rigged Hilbert space (RHS). This is the reason why there is an increasing number of Quantum Mechanics textbooks that already include the rigged Hilbert space as part of their contents (see, for example, Refs. [1]-[9]). Despite the importance of the RHS, there is still a lack of simple examples for which the corresponding RHS is constructed in a didactical manner. Even worse, there is no pedagogical discussion on the physical significance of the RHS. In this paper, we use the one-dimensional (1D) rectangular barrier potential to introduce the RHS at the graduate student level. As well, we discuss the physical significance of each of the ingredients that form the RHS. The construction of the RHS of such a simple model will unambiguously show that the RHS is needed at the most basic level of Quantum Mechanics.

The present paper is complemented by a previous publication, Ref. [10], to which we shall refer the reader interested in a detailed mathematical account on the construction of the RHS of the 1D rectangular barrier. For a general background on the Hilbert and the rigged Hilbert space methods, the reader may consult Ref. [11] and references therein.

Dirac's bra-ket formalism was introduced by Dirac in his classic monograph [12]. Since its inception, Dirac's abstract algebraic model of *bras* and *kets* (from the bracket notation for the inner product) proved to be of great calculational value, although there were serious difficulties in finding a mathematical justification for the actual calculations within the Hilbert space, as Dirac [12] and von Neumann [13] themselves state in their books [14]. As part of his bra-ket formalism, Dirac introduced the so-called Dirac delta function, a formal entity without a counterpart in the classical theory of functions. It was L. Schwartz who gave a precise meaning to the Dirac delta function as a functional over a space of test functions [15]. This led to the development of a new branch of functional analysis, the theory of distributions. By combining von Neumann's Hilbert space with the theory of distributions, I. Gelfand and collaborators introduced the RHS [16, 17]. It was already clear to the creators of the RHS that their formulation was the mathematical support of Dirac's bra-ket formalism [18]. The RHS made its first appearance in the Physics literature in the 1960s [19, 20, 21], when some physicists also realized that the RHS provides a rigorous mathematical rephrasing of all of the aspects of Dirac's bra-ket formalism. Nowadays, there is a growing consensus that the RHS, rather than the Hilbert space alone, is the natural mathematical setting of Quantum Mechanics [22].

A note on semantics. The word "rigged" in rigged Hilbert space has a nautical connotation, such as the phrase "fully rigged ship;" it has nothing to do with any unsavory practice such as "fixing" or predetermining a result. The phrase "rigged Hilbert space" is a direct translation of the phrase "osnashchyonnoe Hilbertovo prostranstvo" from the original Russian. A more faithful translation would be "equipped Hilbert space." Indeed, the rigged Hilbert space is just the Hilbert space equipped with distribution theory—in Quantum Mechanics, to rig a Hilbert space means simply to equip that Hilbert space with distribution theory. Thus, the RHS is not a replacement but an enlargement of the Hilbert space.

The RHS is *neither* an extension *nor* an interpretation of the physical principles of Quantum Mechanics, but rather the most natural, concise and logic language to formulate Quantum Mechanics. The RHS is simply a mathematical tool to extract and process the information contained in observables that have continuous spectrum. Observables with discrete spectrum and a finite number of eigenvectors (e.g., spin) do not need the RHS. For such observables, the Hilbert space is sufficient. Actually, as we shall explain, in general only unbounded observables with continuous spectrum need the RHS.

The usefulness of the RHS is not simply restricted to accounting for Dirac's bra-ket formalism. The RHS has also proved to be a very useful research tool in the quantum theory of scattering and decay (see Ref. [11] and references therein), and in the construction of generalized spectral decompositions of chaotic maps [23, 24]. In fact, it seems that the RHS is the natural language to deal with problems that involve continuous and resonance spectra.

Loosely speaking, a rigged Hilbert space (also called a Gelfand triplet) is a triad of spaces

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^{\times} \tag{1.1}$$

such that $\mathcal{H}$ is a Hilbert space, $\mathbf{\Phi}$ is a dense subspace of $\mathcal{H}$ [25], and $\mathbf{\Phi}^{\times}$ is the space of antilinear functionals over $\mathbf{\Phi}$ [26]. Mathematically, $\mathbf{\Phi}$ is the space of test functions, and $\mathbf{\Phi}^{\times}$ is the space of distributions. The space $\mathbf{\Phi}^{\times}$ is called the antidual space of $\mathbf{\Phi}$. Associated with the RHS (1.1), there is always another RHS,

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}' \, , \tag{1.2}$$

where $\mathbf{\Phi}'$ is called the dual space of $\mathbf{\Phi}$ and contains the linear functionals over $\mathbf{\Phi}$ [26].

The basic reason why we need the spaces $\mathbf{\Phi}'$ and $\mathbf{\Phi}^{\times}$ is that the bras and kets associated with the elements in the continuous spectrum of an observable belong, respectively, to $\mathbf{\Phi}'$ and $\mathbf{\Phi}^{\times}$ rather than to $\mathcal{H}$. The basic reason reason why we need the space $\mathbf{\Phi}$ is that unbounded operators are not defined on the whole of $\mathcal{H}$ but only on dense subdomains of $\mathcal{H}$ that are not invariant under the action of the observables. Such non-invariance makes expectation values, uncertainties and commutation relations not well defined on the whole of $\mathcal{H}$. The space $\mathbf{\Phi}$ is the largest subspace of the Hilbert space on which such expectation values, uncertainties and commutation relations are well defined.

The original formulation of the RHS [16, 17] does not provide a systematic procedure to construct the RHS generated by the Hamiltonian of the Schrödinger equation, since the space $\mathbf{\Phi}$ is assumed to be given beforehand. Such systematic procedure is important because, after all, claiming that the RHS is the natural setting for Quantum Mechanics is about the same as claiming that, when the Hamiltonian has continuous spectrum, the natural setting for the solutions of the Schrödinger equation is the RHS rather than just the Hilbert space. The task of developing a systematic procedure to construct the RHS generated by the Schrödinger equation was undertaken in Ref. [11]. The method proposed in Ref. [11], which was partly based on Refs. [19, 20, 21], has been applied to two simple three-dimensional potentials, see Refs. [27, 28], to the three-dimensional free Hamiltonian, see Ref. [29], and to the 1D rectangular barrier potential, see Ref. [10]. In this paper, we present the method of Ref. [11] in a didactical manner.

The organization of the paper is as follows. In Sec. 2, we outline the major reasons why the RHS provides the mathematical setting for Quantum Mechanics. In Sec. 3, we recall the basics of the 1D rectangular potential model. Section 4 provides the RHS of this model. In Sec. 5, we discuss the physical meaning of each of the ingredients that form the RHS. In Sec. 6, we discuss the relation of the Hilbert space spectral measures with the bras and kets, as well as the limitations of our method to construct RHSs. Finally, Sec. 7 contains the conclusions to the paper.

2. Motivating the rigged Hilbert space

The *linear superposition principle* and the *probabilistic interpretation* of Quantum Mechanics are two major guiding principles in our understanding of the microscopic world. These two principles suggest that the space of states be a linear space (which accounts for the superposition principle) endowed with a scalar product (which is used to calculate probability amplitudes). A linear space endowed with a scalar product is called a Hilbert space and is usually denoted by $\mathcal{H}$ [30].

In Quantum Mechanics, observable quantities are represented by linear, self-adjoint operators acting on $\mathcal{H}$. The eigenvalues of an operator represent the possible values of the measurement of the corresponding observable. These eigenvalues, which mathematically correspond to the spectrum of the operator, can be discrete (as the energies of a particle in a box), continuous (as the energies of a free, unconstrained particle), or a combination of discrete and continuous (as the energies of the Hydrogen atom).

When the spectrum of an observable A is discrete and A is bounded [31], then A is defined on the whole of $\mathcal{H}$ and the eigenvectors of A belong to $\mathcal{H}$. In this case, A can be essentially seen as a matrix. This means that, as far as discrete spectrum is concerned, there is no need to extend $\mathcal{H}$. However, quantum mechanical observables are in general unbounded [31] and their spectrum has in general a continuous part. In order to deal with continuous spectrum, textbooks usually follow Dirac's bra-ket formalism, which is a heuristic generalization of the linear algebra of Hermitian matrices used for discrete spectrum. As we shall see, the mathematical methods of the Hilbert space are not sufficient to make sense of the prescriptions of Dirac's formalism, the reason for which we shall extend the Hilbert space to the rigged Hilbert space.

For pedagogical reasons, we recall the essentials of the linear algebra of Hermitian matrices before proceeding with Dirac's formalism.

2.1. Hermitian matrices

If the measurement of an observable A (e.g., spin) yields a discrete, finite number N of results a_n, $n = 1, 2, \ldots, N$, then A is realized by a Hermitian matrix on a Hilbert space $\mathcal{H}$ of dimension N. Since $\mathcal{H}$ is an N-dimensional linear space, there are N linearly independent vectors $\{e_n\}_{n=1}^{N}$ that form an orthonormal basis system for $\mathcal{H}$. We denote these basis vectors e_n also by $|e_n\rangle$. The scalar products of the elements of the basis system are written in one of the following ways:

$$e_n \cdot e_m \equiv (e_n, e_m) \equiv \langle e_n | e_m \rangle = \delta_{nm} \, , \qquad n, m = 1, 2, \ldots, N \, , \tag{2.1}$$

where δ_{nm} is the Kronecker delta. As the basis system for the space $\mathcal{H}$, it is always possible to choose the eigenvectors of A. Therefore, one can choose basis vectors $e_n \in \mathcal{H}$ which also fulfill

$$A e_n = a_n e_n \, . \tag{2.2}$$

Since A is Hermitian, the eigenvalues a_n are real. The eigenvectors e_n are often labeled by their eigenvalues a_n and denoted by

$$e_n \equiv |a_n\rangle \, , \tag{2.3}$$

and they are represented by column vectors. For each column eigenvector $e_n \equiv |a_n\rangle$, there also exists a row eigenvector $\tilde{e}_n \equiv \langle a_n|$ that is a left eigenvector of A,

$$\tilde{e}_n A = a_n \tilde{e}_n \, . \tag{2.4}$$

Thus, when A is a Hermitian matrix acting on an N-dimensional Hilbert space $\mathcal{H}$, for each eigenvalue a_n of A there exist a right (i.e., column) eigenvector of A

$$A|a_n\rangle = a_n |a_n\rangle \, , \quad n = 1, 2, \ldots, N \, , \tag{2.5}$$

and also a left (i.e., row) eigenvector of A

$$\langle a_n | A = a_n \langle a_n | \, , \quad n = 1, 2, \ldots, N \, , \tag{2.6}$$

such that these row and column eigenvectors are orthonormal,

$$\langle a_n | a_m \rangle = \delta_{nm} \, , \quad n, m = 1, 2, \ldots, N \, , \tag{2.7}$$

and such that every vector $\varphi \in \mathcal{H}$ can be written as

$$\varphi = \sum_{n=1}^{N} |a_n\rangle \langle a_n | \varphi \rangle \, . \tag{2.8}$$

Equation (2.8) is called the eigenvector expansion of φ with respect to the eigenvectors of A. The complex numbers $\langle a_n|\varphi\rangle$ are the components of the vector φ with respect to the basis of eigenvectors of A. Physically, $\langle a_n|\varphi\rangle$ represents the probability amplitude of obtaining the value a_n in the measurement of the observable A on the state φ. By acting on both sides of Eq. (2.8) with A, and recalling Eq. (2.5), we obtain that

$$A\varphi = \sum_{n=1}^{N} a_n |a_n\rangle \langle a_n | \varphi \rangle \, . \tag{2.9}$$

2.2. Dirac's bra-ket formalism

Dirac's formalism is an elegant, heuristic generalization of the algebra of finite dimensional matrices to the continuous-spectrum, infinite-dimensional case. Four of the most important features of Dirac's formalism are:

(i) To each element of the spectrum of an observable A, there correspond a left and a right eigenvector (for the moment, we assume that the spectrum is non-degenerate). If discrete eigenvalues are denoted by a_n and continuous eigenvalues by a, then the corresponding right eigenvectors, which are denoted by the kets $|a_n\rangle$ and $|a\rangle$, satisfy

$$A|a_n\rangle = a_n|a_n\rangle \, , \tag{2.10a}$$

$$A|a\rangle = a|a\rangle \, , \tag{2.10b}$$

and the corresponding left eigenvectors, which are denoted by the bras $\langle a_n|$ and $\langle a|$, satisfy

$$\langle a_n|A = a_n\langle a_n| \, , \tag{2.11a}$$

$$\langle a|A = a\langle a| \, . \tag{2.11b}$$

The bras $\langle a|$ generalize the notion of row eigenvectors, whereas the kets $|a\rangle$ generalize the notion of column eigenvectors.

(ii) In analogy to Eq. (2.8), the eigenbras and eigenkets of an observable form a complete basis, that is, any wave function φ can be expanded in the so-called Dirac basis expansion:

$$\varphi = \sum_n |a_n\rangle\langle a_n|\varphi\rangle + \int \mathrm{d}a \, |a\rangle\langle a|\varphi\rangle \, . \tag{2.12}$$

In addition, the bras and kets furnish a resolution of the identity,

$$I = \sum_n |a_n\rangle\langle a_n| + \int \mathrm{d}a \, |a\rangle\langle a| \, , \tag{2.13}$$

and, in a generalization of Eq. (2.9), the action of A can be written as

$$A = \sum_n a_n|a_n\rangle\langle a_n| + \int \mathrm{d}a \, a|a\rangle\langle a| \, . \tag{2.14}$$

(iii) The bras and kets are normalized according to the following rule:

$$\langle a_n|a_m\rangle = \delta_{nm} \, , \tag{2.15a}$$

$$\langle a|a'\rangle = \delta(a-a') \, , \tag{2.15b}$$

where δ_{nm} is the Kronecker delta and $\delta(a-a')$ is the Dirac delta. The Dirac delta normalization generalizes the orthonormality (2.7) of the eigenvectors of a Hermitian matrix.

(iv) Like in the case of two finite-dimensional matrices, all algebraic operations such as the commutator of two observables A and B,

$$[A,B] = AB - BA \, , \tag{2.16}$$

are always well defined.

2.3. The need of the rigged Hilbert space

In Quantum Mechanics, observables are usually given by differential operators. In the Hilbert space framework, the formal prescription of an observable leads to the definition of a linear operator as follows: One has to find first the Hilbert space $\mathcal{H}$, then one sees on what elements of $\mathcal{H}$ the action of the observable makes sense, and finally one checks whether the action of the observable remains in $\mathcal{H}$. For example, the position observable Q of a 1D particle is given by

$$Qf(x) = xf(x)\,. \tag{2.17}$$

The Hilbert space of a 1D particle is given by the collection of square integrable functions,

$$L^2 = \{f(x) \,|\, \int_{-\infty}^{\infty} \mathrm{d}x\, |f(x)|^2 < \infty\}\,, \tag{2.18}$$

and the action of Q, although in principle well defined on every element of L^2, remains in L^2 only for the elements of the following subspace:

$$\mathcal{D}(Q) = \{f(x) \in L^2 \,|\, \int_{-\infty}^{\infty} \mathrm{d}x\, |xf(x)|^2 < \infty\}\,. \tag{2.19}$$

The space $\mathcal{D}(Q)$ is the domain of the position operator. Domain (2.19) is not the whole of L^2, since the function $g(x) = 1/(x + \mathrm{i})$ belongs to L^2 but not to $\mathcal{D}(Q)$; as well, Q is an unbounded operator, because $\|Qg\| = \infty$; as well, $Q\mathcal{D}(Q)$ is not included in $\mathcal{D}(Q)$, since $h(x) = 1/(x^2 + 1)$ belongs to $\mathcal{D}(Q)$ but Qh does not belong to $\mathcal{D}(Q)$. The denseness and the non-invariance of the domains of unbounded operators create much trouble in the Hilbert space framework, because one has always to be careful whether formal operations are valid. For example, $Q^2 = QQ$ is not defined on the whole of L^2, not even on the whole of $\mathcal{D}(Q)$, but only on those square integrable functions such that $x^2 f \in L^2$. Also, the expectation value of the measurement of Q in the state φ,

$$(\varphi, Q\varphi)\,, \tag{2.20}$$

is not finite for every $\varphi \in L^2$, but only when $\varphi \in \mathcal{D}(Q)$. Similarly, the uncertainty of the measurement of Q in φ,

$$\Delta_\varphi Q = \sqrt{(\varphi, Q^2\varphi) - (\varphi, Q\varphi)^2}\,, \tag{2.21}$$

is not defined on the whole of L^2.

On the other hand, if we denote the momentum observable by

$$Pf(x) = -\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}x} f(x)\,, \tag{2.22}$$

then the product of P and Q, PQ, is not defined everywhere in the Hilbert space, but only on those square integrable functions for which the quantity

$$PQf(x) = -\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}x} xf(x) = -\mathrm{i}\hbar\,(f(x) + xf'(x)) \tag{2.23}$$

makes sense and is square integrable. Obviously, PQf makes sense only when f is differentiable, and PQf remains in L^2 only when f, f' and xf' are also in L^2; thus,

PQ is not defined everywhere in L^2 but only on those square integrable functions that satisfy the aforementioned conditions. Similar domain concerns arise in calculating the commutator of P with Q.

As in the case of the position operator, the domain $\mathcal{D}(A)$ of an unbounded operator A does not coincide with the whole of $\mathcal{H}$ [32], but is just a dense subspace of $\mathcal{H}$ [25]; also, in general $\mathcal{D}(A)$ does not remain invariant under the action of A, that is, $A\mathcal{D}(A)$ is not included in $\mathcal{D}(A)$. Such non-invariance makes expectation values,

$$(\varphi, A\varphi)\,, \tag{2.24}$$

uncertainties,

$$\Delta_{\varphi}A = \sqrt{(\varphi, A^2\varphi) - (\varphi, A\varphi)^2}\,, \tag{2.25}$$

and algebraic operations such as commutation relations not well defined on the whole of the Hilbert space $\mathcal{H}$ [34]. Thus, when the position, momentum and energy operators Q, P, H are unbounded, it is natural to seek a subspace $\mathbf{\Phi}$ of $\mathcal{H}$ on which all of these physical quantities can be calculated and yield meaningful, finite values. Because the reason why these quantities may not be well defined is that the domains of Q, P and H are not invariant under the action of these operators, the subspace $\mathbf{\Phi}$ must be such that it remains invariant under the actions of Q, P and H. This is why we take as $\mathbf{\Phi}$ the intersection of the domains of all the powers of Q, P and H [19]:

$$\mathbf{\Phi} = \bigcap_{\substack{n,m=0 \\ A,B=Q,P,H}}^{\infty} \mathcal{D}(A^n B^m)\,. \tag{2.26}$$

This space is known as the maximal invariant subspace of the algebra generated by Q, P and H, because it is the largest subdomain of the Hilbert space that remains invariant under the action of any power of Q, P or H,

$$A\mathbf{\Phi} \subset \mathbf{\Phi}\,, \qquad A = Q, P, H\,. \tag{2.27}$$

On $\mathbf{\Phi}$, all physical quantities such as expectation values and uncertainties can be associated well-defined, finite values, and algebraic operations such as the commutation relation (2.16) are well defined. In addition, the elements of $\mathbf{\Phi}$ are represented by smooth, continuous functions that have a definitive value at each point, in contrast to the elements of $\mathcal{H}$, which are represented by classes of functions which can vary arbitrarily on sets of zero Lebesgue measure.

Not only there are compelling reasons to shrink the Hilbert space $\mathcal{H}$ to $\mathbf{\Phi}$, but, as we are going to explain now, there are also reasons to enlarge $\mathcal{H}$ to the spaces $\mathbf{\Phi}^{\times}$ and $\mathbf{\Phi}'$ of Eqs. (1.1) and (1.2). When the spectrum of A has a continuous part, prescriptions (2.11*b*) and (2.10*b*) associate a bra $\langle a|$ and a ket $|a\rangle$ to each element a of the continuous spectrum of A. Obviously, the bras $\langle a|$ and kets $|a\rangle$ are not in the Hilbert space [35], and therefore we need two linear spaces larger than the Hilbert space to accommodate them. It turns out that the bras and kets acquire mathematical meaning as distributions. More specifically, the bras $\langle a|$ are *linear* functionals over the space

$\mathbf{\Phi}$, and the kets $|a\rangle$ are *antilinear* functionals over the space $\mathbf{\Phi}$. That is, $\langle a| \in \mathbf{\Phi}'$ and $|a\rangle \in \mathbf{\Phi}^{\times}$.

In this way, the Gelfand triplets of Eqs. (1.1) and (1.2) arise in a natural way. The Hilbert space $\mathcal{H}$ arises from the requirement that the wave functions be square normalizable. Aside from providing mathematical concepts such as self-adjointness or unitarity, the Hilbert space plays a very important physical role, namely $\mathcal{H}$ selects the scalar product that is used to calculate probability amplitudes. The subspace $\mathbf{\Phi}$ contains those square integrable functions that should be considered as physical, because any expectation value, any uncertainty and any algebraic operation can be calculated for its elements, whereas this is not possible for the rest of the elements of the Hilbert space. The dual space $\mathbf{\Phi}'$ and the antidual space $\mathbf{\Phi}^{\times}$ contain respectively the bras and the kets associated with the continuous spectrum of the observables. These bras and kets can be used to expand any $\varphi \in \mathbf{\Phi}$ as in Eq. (2.12). Thus, the rigged Hilbert space, rather than the Hilbert space alone, can accommodate prescriptions (2.10a)-(2.16) of Dirac's formalism.

It should be clear that the rigged Hilbert space is just a combination of the Hilbert space with distribution theory. This combination enables us to deal with singular objects such as bras, kets, or Dirac's delta function, something that is impossible if we only use the Hilbert space.

Even though it is apparent that the rigged Hilbert space should be an essential part of the mathematical methods for Quantum Mechanics, one may still wonder if the rigged Hilbert space is a helpful tool in teaching Quantum Mechanics, or rather is a technical nuance. Because basic quantum mechanical operators such as P and Q are in general unbounded operators with continuous spectrum [36], and because this kind of operators necessitates the rigged Hilbert space, it seems pertinent to introduce the rigged Hilbert space in graduate courses on Quantum Mechanics.

From a pedagogical standpoint, however, this section's introduction to the rigged Hilbert space is not sufficient. In the classroom, new concepts are better introduced by way of a simple, exactly solvable example. This is why we shall construct the RHS of the 1D rectangular barrier system. We note that this system does not have bound states, and therefore in what follows we shall not deal with discrete spectrum.

2.4. Representations

In working out specific examples, the prescriptions of Dirac's formalism have to be written in a particular representation. Thus, before constructing the RHS of the 1D rectangular barrier, it is convenient to recall some of the basics of representations.

In Quantum Mechanics, the most common of all representations is the position representation, sometimes called the x-representation. In the x-representation, the position operator Q acts as multiplication by x. Since the spectrum of Q is $(-\infty, \infty)$, the x-representation of the Hilbert space $\mathcal{H}$ is given by the space L^2. In this paper, we shall mainly work in the position representation.

In general, given an observable B, the b-representation is that in which the operator B acts as multiplication by b, where the b's denote the eigenvalues of B. If we denote the spectrum of B by $\mathrm{Sp}(B)$, then the b-representation of the Hilbert space $\mathcal{H}$ is given by the space $L^2(\mathrm{Sp}(B), \mathrm{d}b)$, which is the space of square integrable functions $f(b)$ with b running over $\mathrm{Sp}(B)$. In the b-representation, the restrictions to purely continuous spectrum of prescriptions (2.10a)-(2.13) become

$$\langle b|A|a\rangle = a\langle b|a\rangle \,, \tag{2.28a}$$

$$\langle a|A|b\rangle = a\langle a|b\rangle \,, \tag{2.28b}$$

$$\langle b|\varphi\rangle = \int \mathrm{d}a \, \langle b|a\rangle\langle a|\varphi\rangle \,, \tag{2.28c}$$

$$\delta(b-b') = \langle b|b'\rangle = \int \mathrm{d}a \, \langle b|a\rangle\langle a|b'\rangle \,. \tag{2.28d}$$

The "scalar product" $\langle b|a\rangle$ is obtained from Eq. (2.28a) as the solution of a differential eigenequation in the b-representation. The $\langle b|a\rangle$ can also be seen as transition elements from the a- to the b-representation. Mathematically, the $\langle b|a\rangle$ are to be treated as distributions, and therefore they often appear as kernels of integrals. In this paper, we shall encounter a few of these "scalar products" such as $\langle x|p\rangle$, $\langle x|x'\rangle$ and $\langle x|E^{\pm}\rangle_{\mathrm{l,r}}$.

3. Example: The one-dimensional rectangular barrier potential

The example we consider in this paper is supposed to represent a spinless particle moving in one dimension and impinging on a rectangular barrier. The observables relevant to this system are the position Q, the momentum P, and the Hamiltonian H. In the position representation, Q and P are respectively realized by the differential operators (2.17) and (2.22), whereas H is realized by

$$Hf(x) = \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \right) f(x) \,, \tag{3.1}$$

where

$$V(x) = \begin{cases} 0 & -\infty < x < a \\ V_0 & a < x < b \\ 0 & b < x < \infty \end{cases} \tag{3.2}$$

is the 1D rectangular barrier potential. Formally, these observables satisfy the following commutation relations:

$$[Q,P] = \mathrm{i}\hbar I \,, \tag{3.3a}$$

$$[H,Q] = -\frac{\mathrm{i}\hbar}{m}P \,, \tag{3.3b}$$

$$[H,P] = \mathrm{i}\hbar\frac{\partial V}{\partial x} \,. \tag{3.3c}$$

Since our particle can move in the full real line, the Hilbert space on which the differential operators (2.17), (2.22) and (3.1) should act is L^2 of Eq. (2.18). The corresponding scalar product is

$$(f,g)=\int_{-\infty}^{\infty}\mathrm{d}x\,\overline{f(x)}g(x)\,,\qquad f,g\in L^2\,, \tag{3.4}$$

where $\overline{f(x)}$ denotes the complex conjugate of $f(x)$.

The differential operators (2.17), (2.22) and (3.1) induce three linear operators on the Hilbert space L^2. These operators are unbounded [10], and therefore they cannot be defined on the whole of L^2, but only on the following subdomains of L^2 [10]:

$$\mathcal{D}(Q)=\left\{f\in L^2\mid xf\in L^2\right\}\,, \tag{3.5a}$$

$$\mathcal{D}(P)=\left\{f\in L^2\mid f\in AC,\ Pf\in L^2\right\}\,, \tag{3.5b}$$

$$\mathcal{D}(H)=\left\{f\in L^2\mid f\in AC^2,\ Hf\in L^2\right\}\,, \tag{3.5c}$$

where, essentially, AC is the space of functions whose derivative exists, and AC^2 is the space of functions whose second derivative exists (see Ref. [10] for more details). On these domains, the operators Q, P and H are self-adjoint [10].

In our example, the eigenvalues (i.e., the spectrum) and the eigenfunctions of the observables are provided by the Sturm-Liouville theory. Mathematically, the eigenvalues and eigenfunctions of operators extend the notions of eigenvalues and eigenvectors of a matrix to the infinite-dimensional case. The Sturm-Liouville theory tells us that these operators have the following spectra [10]:

$$\mathrm{Sp}(Q)=(-\infty,\infty)\,, \tag{3.6a}$$

$$\mathrm{Sp}(P)=(-\infty,\infty)\,, \tag{3.6b}$$

$$\mathrm{Sp}(H)=[0,\infty)\,. \tag{3.6c}$$

These spectra coincide with those we would expect on physical grounds. We expect the possible measurements of Q to be the full real line, because the particle can in principle reach any point of the real line. We also expect the possible measurements of P to be the full real line, since the momentum of the particle is not restricted in magnitude or direction. The possible measurements of H have the same range as that of the kinetic energy, because the potential does not have any wells of negative energy, and therefore we expect the spectrum of H to be the positive real line.

To obtain the eigenfunction corresponding to each eigenvalue, we have to solve the eigenvalue equation (2.10b) for each observable. Since we are working in the position representation, we have to write Eq. (2.10b) in the position representation for each observable:

$$\langle x|Q|x'\rangle=x'\langle x|x'\rangle\,, \tag{3.7a}$$

$$\langle x|P|p\rangle=p\langle x|p\rangle\,, \tag{3.7b}$$

$$\langle x|H|E\rangle = E\langle x|E\rangle \, . \tag{3.7c}$$

By recalling Eqs. (2.17), (2.22) and (3.1), we can write Eqs. (3.7a)-(3.7c) as

$$x\langle x|x'\rangle = x'\langle x|x'\rangle \, , \tag{3.8a}$$

$$-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}\langle x|p\rangle = p\langle x|p\rangle \, , \tag{3.8b}$$

$$\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right)\langle x|E\rangle = E\langle x|E\rangle \, . \tag{3.8c}$$

For each position x', Eq. (3.8a) yields the corresponding eigenfunction of Q as a delta function,

$$\langle x|x'\rangle = \delta(x - x') \, . \tag{3.9}$$

For each momentum p, Eq. (3.8b) yields the corresponding eigenfunction of P as a plane wave,

$$\langle x|p\rangle = \frac{\mathrm{e}^{\mathrm{i}px/\hbar}}{\sqrt{2\pi\hbar}} \, . \tag{3.10}$$

For each energy E, Eq. (3.8c) yields the following two linearly independent eigenfunctions [10]:

$$\langle x|E^+\rangle_{\mathrm{r}} = \left(\frac{m}{2\pi k\hbar^2}\right)^{1/2} \times \begin{cases} T(k)\mathrm{e}^{-\mathrm{i}kx} & -\infty < x < a \\ A_{\mathrm{r}}(k)\mathrm{e}^{\mathrm{i}\kappa x} + B_{\mathrm{r}}(k)\mathrm{e}^{-\mathrm{i}\kappa x} & a < x < b \\ R_{\mathrm{r}}(k)\mathrm{e}^{\mathrm{i}kx} + \mathrm{e}^{-\mathrm{i}kx} & b < x < \infty \, , \end{cases} \tag{3.11a}$$

$$\langle x|E^+\rangle_{\mathrm{l}} = \left(\frac{m}{2\pi k\hbar^2}\right)^{1/2} \times \begin{cases} \mathrm{e}^{\mathrm{i}kx} + R_{\mathrm{l}}(k)\mathrm{e}^{-\mathrm{i}kx} & -\infty < x < a \\ A_{\mathrm{l}}(k)\mathrm{e}^{\mathrm{i}\kappa x} + B_{\mathrm{l}}(k)\mathrm{e}^{-\mathrm{i}\kappa x} & a < x < b \\ T(k)\mathrm{e}^{\mathrm{i}kx} & b < x < \infty \, , \end{cases} \tag{3.11b}$$

where

$$k = \sqrt{\frac{2m}{\hbar^2}E} \, , \quad \kappa = \sqrt{\frac{2m}{\hbar^2}(E - V_0)} \, , \tag{3.12}$$

and where the coefficients that appear in Eqs. (3.11a)-(3.11b) can be easily found by the standard matching conditions at the discontinuities of the potential [10]. Thus, in contrast to the spectra of Q and P, the spectrum of H is doubly degenerate.

Physically, the eigenfunction $\langle x|E^+\rangle_{\mathrm{r}}$ represents a particle of energy E that impinges on the barrier from the right (hence the subscript r) and gets reflected to the right with probability amplitude $R_{\mathrm{r}}(k)$ and transmitted to the left with probability amplitude $T(k)$, see Fig. 1a. The eigenfunction $\langle x|E^+\rangle_{\mathrm{l}}$ represents a particle of energy E that impinges on the barrier from the left (hence the subscript l) and gets reflected to the left with probability amplitude $R_{\mathrm{l}}(k)$ and transmitted to the right with probability amplitude $T(k)$, see Fig. 1b.

Note that, instead of (3.11*a*)-(3.11*b*), we could choose another pair of linearly independent solutions of Eq. (3.8*c*) as follows [10]:

$$\langle x|E^-\rangle_{\rm r} = \left(\frac{m}{2\pi k\hbar^2}\right)^{1/2} \times \begin{cases} T^*(k)\mathrm{e}^{\mathrm{i}kx} & -\infty < x < a \\ A_{\rm r}^*(k)\mathrm{e}^{-\mathrm{i}\kappa x} + B_{\rm r}^*(k)\mathrm{e}^{\mathrm{i}\kappa x} & a < x < b \\ R_{\rm r}^*(k)\mathrm{e}^{-\mathrm{i}kx} + \mathrm{e}^{\mathrm{i}kx} & b < x < \infty\,, \end{cases} \tag{3.13a}$$

$$\langle x|E^-\rangle_{\rm l} = \left(\frac{m}{2\pi k\hbar^2}\right)^{1/2} \times \begin{cases} \mathrm{e}^{-\mathrm{i}kx} + R_{\rm l}^*(k)\mathrm{e}^{\mathrm{i}kx} & -\infty < x < a \\ A_{\rm l}^*(k)\mathrm{e}^{-\mathrm{i}\kappa x} + B_{\rm l}^*(k)\mathrm{e}^{\mathrm{i}\kappa x} & a < x < b \\ T^*(k)\mathrm{e}^{-\mathrm{i}kx} & b < x < \infty\,, \end{cases} \tag{3.13b}$$

where the coefficients of these eigenfunctions can also be calculating by means of the standard matching conditions at $x = a, b$ [10]. The eigenfunction $\langle x|E^-\rangle_{\rm r}$ represents two plane waves—one impinging on the barrier from the left with probability amplitude $T^*(k)$ and another impinging on the barrier from the right with probability amplitude $R_{\rm r}^*(k)$—that combine in such a way as to produce an outgoing plane wave to the right, see Fig. 2a. The eigenfunction $\langle x|E^-\rangle_{\rm l}$ represents two other planes waves—one impinging on the barrier from left with probability amplitude $R_{\rm l}^*(k)$ and another impinging on the barrier from the right with probability amplitude $T^*(k)$—that combine in such a way as to produce an outgoing wave to the left, see Fig. 2b. The eigensolutions $\langle x|E^-\rangle_{\rm r,l}$ correspond to the *final* condition of an outgoing plane wave propagating away from the barrier respectively to the right and to the left, as opposed to $\langle x|E^+\rangle_{\rm r,l}$, which correspond to the *initial* condition of a plane wave that propagates towards the barrier respectively from the right and from the left.

The eigenfunctions (3.9), (3.10), (3.11*a*)-(3.11*b*) and (3.13*a*)-(3.13*b*) are not square integrable, that is, they do not belong to L^2. Mathematically speaking, this is the reason why they are to be dealt with as distributions (note that all of them except for the delta function are also proper functions). Physically speaking, they are to be interpreted in analogy to electromagnetic plane waves, as we shall see in Section 5.

4. Construction of the rigged Hilbert space

In the previous section, we saw that the observables of our system are implemented by unbounded operators with continuous spectrum. We also saw that the eigenfunctions of the observables do not belong to L^2. Thus, as we explained in Sec. 2, we need to construct the rigged Hilbert spaces of Eqs. (1.1) and (1.2) [see Eqs. (4.8) and (4.21) below]. We start by constructing $\mathbf{\Phi}$.

4.1. Construction of $\mathbf{\Phi} \equiv \mathcal{S}(\mathbb{R}\text{-}\{a,b\})$

The subspace $\mathbf{\Phi}$ is given by Eq. (2.26). In view of expressions (2.17), (2.22) and (3.1), the elements of $\mathbf{\Phi}$ must fulfill the following conditions:

- they are infinitely differentiable, so the differentiation operation can be applied as many times as wished,

- they vanish at $x = a$ and $x = b$, so differentiation is meaningful at the discontinuities of the potential [37],
- the action of all powers of Q, P and H remains square integrable.

Hence,

$$\begin{aligned}\mathbf{\Phi} = \{\varphi \in L^2 \mid \varphi \in C^\infty(\mathbb{R}),\ \varphi^{(n)}(a) = \varphi^{(n)}(b) = 0\,,\ n = 0, 1, \dots\,,\\ P^n Q^m H^l \varphi(x) \in L^2\,,\ n, m, l = 0, 1, \dots\}\,,\end{aligned} \tag{4.1}$$

where $C^\infty(\mathbb{R})$ is the collection of infinite differentiable functions, and $\varphi^{(n)}$ denotes the nth derivative of φ. From the last condition in Eq. (4.1), we deduce that the elements of $\mathbf{\Phi}$ satisfy the following estimates:

$$\|\varphi\|_{n,m,l} \equiv \sqrt{\int_{-\infty}^{\infty} \mathrm{d}x\ |P^n Q^m H^l \varphi(x)|^2} < \infty\,, \quad n, m, l = 0, 1, \dots\,. \tag{4.2}$$

These estimates mean that the action of any combination of any power of the observables remains square integrable. For this to happen, the functions $\varphi(x)$ must be infinitely differentiable and must fall off at infinity faster than any polynomial. The estimates (4.2) induce a topology on $\mathbf{\Phi}$, that is, they induce a meaning of convergence of sequences, in the following way. A sequence $\{\varphi_\alpha\}$ $\mathbf{\Phi}$-converges to φ when $\{\varphi_\alpha\}$ converges to φ with respect to all the estimates (4.2),

$$\varphi_\alpha \xrightarrow[\alpha\to\infty]{\tau_{\mathbf{\Phi}}} \varphi \quad \text{if} \quad \|\varphi_\alpha - \varphi\|_{n,m,l} \xrightarrow[\alpha\to\infty]{} 0\,, \quad n, m, l = 0, 1, \dots\,. \tag{4.3}$$

Intuitively, a sequence φ_α converges to φ if whenever we follow the terms of the sequence, we get closer and closer to the limit point φ with respect to a certain sense of closeness. In our system, the notion of closeness is determined by the estimates $\|\ \|_{n,m,l}$, which originate from the physical requirements that led us to construct $\mathbf{\Phi}$.

From Eqs. (4.1) and (4.2), we can see that $\mathbf{\Phi}$ is very similar to the Schwartz space $\mathcal{S}(\mathbb{R})$, the major differences being that the derivatives of the elements of $\mathbf{\Phi}$ vanish at $x = a, b$ and that $\mathbf{\Phi}$ is not only invariant under P and Q but also under H. This is why we shall write

$$\mathbf{\Phi} \equiv \mathcal{S}(\mathbb{R}\text{-}\{a, b\})\,. \tag{4.4}$$

It is always a good, though lengthy exercise to check that $\mathcal{S}(\mathbb{R}\text{-}\{a, b\})$ is indeed invariant under the action of the observables,

$$A\,\mathcal{S}(\mathbb{R}\text{-}\{a, b\}) \subset \mathcal{S}(\mathbb{R}\text{-}\{a, b\})\,, \qquad A = P, Q, H\,. \tag{4.5}$$

This invariance guarantees that the expectation values

$$(\varphi, A^n \varphi)\,, \quad \varphi \in \mathcal{S}(\mathbb{R}\text{-}\{a, b\})\,,\ A = P, Q, H,\ n = 0, 1, \dots \tag{4.6}$$

are finite, and that the commutation relations (3.3a)-(3.3c) are well defined [38]. It can also be checked that P, Q and H, which are not continuous with respect the topology of the Hilbert space L^2, are now continuous with respect to the topology $\tau_{\mathbf{\Phi}}$ of $\mathcal{S}(\mathbb{R}\text{-}\{a, b\})$ [10, 11].

4.2. Construction of $\mathbf{\Phi}^\times \equiv \mathcal{S}^\times(\mathbb{R}\text{-}\{a,b\})$. The Dirac kets

The space $\mathbf{\Phi}^\times$ is simply the collection of $\tau_{\mathbf{\Phi}}$-continuous *antilinear* functionals over $\mathbf{\Phi}$ [26]. By combining the spaces $\mathbf{\Phi}$, $\mathcal{H}$ and $\mathbf{\Phi}^\times$, we obtain the RHS of our system,

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times \, , \tag{4.7}$$

which we denote in the position representation by

$$\mathcal{S}(\mathbb{R}\text{-}\{a,b\}) \subset L^2 \subset \mathcal{S}^\times(\mathbb{R}\text{-}\{a,b\}) \, . \tag{4.8}$$

The space $\mathcal{S}^\times(\mathbb{R}\text{-}\{a,b\})$ is meant to accommodate the eigenkets $|p\rangle$, $|x\rangle$ and $|E^\pm\rangle_{\rm l,r}$ of P, Q and H. In the remainder of this subsection, we construct these eigenkets explicitly and see that they indeed belong to $\mathcal{S}^\times(\mathbb{R}\text{-}\{a,b\})$. We shall also see that $|p\rangle$, $|x\rangle$ and $|E^\pm\rangle_{\rm l,r}$ are indeed eigenvectors of the observables.

The definition of a ket is borrowed from the theory of distributions as follows [16]. Given a function $f(x)$ and a space of test functions $\mathbf{\Phi}$, the antilinear functional F that corresponds to the function $f(x)$ is an integral operator whose kernel is precisely $f(x)$:

$$F(\varphi) = \int {\rm d}x \, \overline{\varphi(x)} f(x) \, , \tag{4.9a}$$

which in Dirac's notation becomes

$$\langle \varphi | F \rangle = \int {\rm d}x \, \langle \varphi | x \rangle \langle x | f \rangle \, . \tag{4.9b}$$

It is important to keep in mind that, though related, the function $f(x)$ and the functional F are two different things, the relation between them being that $f(x)$ is the kernel of F when we write F as an integral operator. In the physics literature, the term *distribution* is usually reserved for $f(x)$.

Definition (4.9a) provides the link between the quantum mechanical formalism and the theory of distributions. In practical applications, what one obtains from the quantum mechanical formalism is the distribution $f(x)$ (in this paper, the plane waves $\frac{1}{\sqrt{2\pi\hbar}}{\rm e}^{{\rm i}px/\hbar}$, the delta function $\delta(x-x')$ and the eigenfunctions $\langle x|E^\pm\rangle_{\rm l,r}$). Once $f(x)$ is given, one can use definition (4.9a) to generate the functional $|F\rangle$. Then, the theory of distributions can be used to obtain the properties of the functional $|F\rangle$, which in turn yield the properties of the distribution $f(x)$.

By using prescription (4.9a), we can define for each eigenvalue p the eigenket $|p\rangle$ associated with the eigenfunction (3.10):

$$\langle \varphi | p \rangle \equiv \int_{-\infty}^{\infty} {\rm d}x \, \overline{\varphi(x)} \frac{1}{\sqrt{2\pi\hbar}} {\rm e}^{{\rm i}px/\hbar} \, , \tag{4.10a}$$

which, using Dirac's notation for the integrand, becomes

$$\langle \varphi | p \rangle \equiv \int_{-\infty}^{\infty} {\rm d}x \, \langle \varphi | x \rangle \langle x | p \rangle \, . \tag{4.10b}$$

Similarly, for each x, we can define the ket $|x\rangle$ associated with the eigenfunction (3.9) of the position operator as

$$\langle \varphi | x \rangle \equiv \int_{-\infty}^{\infty} {\rm d}x' \, \overline{\varphi(x')} \delta(x-x') \, , \tag{4.11a}$$

which, using Dirac's notation for the integrand, becomes

$$\langle\varphi|x\rangle \equiv \int_{-\infty}^{\infty} \mathrm{d}x' \, \langle\varphi|x'\rangle\langle x'|x\rangle \, . \tag{4.11b}$$

The definition of the kets $|E^{\pm}\rangle_{\mathrm{l,r}}$ that correspond to the Hamiltonian's eigenfunctions (3.11a)-(3.11b) and (3.13a)-(3.13b) follows the same prescription:

$$\langle\varphi|E^{\pm}\rangle_{\mathrm{l,r}} \equiv \int_{-\infty}^{\infty} \mathrm{d}x \, \overline{\varphi(x)}\langle x|E^{\pm}\rangle_{\mathrm{l,r}} \, , \tag{4.12a}$$

that is,

$$\langle\varphi|E^{\pm}\rangle_{\mathrm{l,r}} \equiv \int_{-\infty}^{\infty} \mathrm{d}x \, \langle\varphi|x\rangle\langle x|E^{\pm}\rangle_{\mathrm{l,r}} \, . \tag{4.12b}$$

(Note that this equation defines four different kets.) One can now show that the definition of the kets $|p\rangle$, $|x\rangle$ and $|E^{\pm}\rangle_{\mathrm{l,r}}$ makes sense, and that these kets indeed belong to the space of distributions $\mathcal{S}^{\times}(\mathbb{R}\text{-}\{a,b\})$ [10].

As in the general case of Eqs. (4.9a)-(4.9b), it is important to keep in mind the difference between eigenfunctions and kets. For instance, $\langle x|p\rangle$ is an eigenfunction of a differential equation, Eq. (3.8b), whereas $|p\rangle$ is a functional, the relation between them being given by Eq. (4.10b). A similar relation holds between $\langle x'|x\rangle$ and $|x\rangle$, and between $\langle x|E^{\pm}\rangle_{\mathrm{l,r}}$ and $|E^{\pm}\rangle_{\mathrm{l,r}}$. It is also important to keep in mind that "scalar products" like $\langle x|p\rangle$, $\langle x'|x\rangle$ or $\langle x|E^{\pm}\rangle_{\mathrm{l,r}}$ do not represent an actual scalar product of two functionals; these "scalar products" are simply solutions to differential equations.

We now turn to the question of whether the kets $|p\rangle$, $|x\rangle$ and $|E^{\pm}\rangle_{\mathrm{l,r}}$ are eigenvectors of the corresponding observable [see Eqs. (4.17)-(4.19) below]. Since the observables act in principle only on their Hilbert space domains, and since the kets lie outside the Hilbert space, we need to extend the definition of the observables from $\mathbf{\Phi}$ into $\mathbf{\Phi}^{\times}$, in order to specify how the observables act on the kets. The theory of distributions provides us with a precise prescription of how an observable acts on $\mathbf{\Phi}^{\times}$, and therefore of how it acts on the kets, as follows [16]. The action of a self-adjoint operator A on a functional $|F\rangle \in \mathbf{\Phi}^{\times}$ is defined as

$$\langle\varphi|A|F\rangle \equiv \langle A\varphi|F\rangle \, , \quad \text{for all } \varphi \text{ in } \mathbf{\Phi} \, . \tag{4.13}$$

Note that this definition extends the Hilbert space definition of a self-adjoint operator,

$$(f, Ag) = (Af, g) \, , \tag{4.14}$$

which is valid only when f and g belong to the domain of A. In turn, Eq. (4.13) can be used to define the notion of eigenket of an observable: A functional $|a\rangle$ in $\mathbf{\Phi}^{\times}$ is an eigenket of A with eigenvalue a if

$$\langle\varphi|A|a\rangle = \langle A\varphi|a\rangle = a\langle\varphi|a\rangle \, , \quad \text{for all } \varphi \text{ in } \mathbf{\Phi} \, . \tag{4.15}$$

When the "left sandwiching" of this equation with the elements of $\mathbf{\Phi}$ is understood and therefore omitted, we shall simply write

$$A|a\rangle = a|a\rangle \, , \tag{4.16}$$

which is just Dirac's eigenket equation (2.10*b*). Thus, Dirac's eigenket equation acquires a precise meaning through Eq. (4.15), in the sense that it has to be understood as "left sandwiched" with the wave functions φ of $\mathbf{\Phi}$.

By using definition (4.15), one can show that $|p\rangle$, $|x\rangle$ and $|E^{\pm}\rangle_{\mathrm{l,r}}$ are indeed eigenvectors of P, Q and H, respectively [10]:

$$P|p\rangle = p|p\rangle\,, \quad p \in \mathbb{R}\,, \tag{4.17}$$

$$Q|x\rangle = x|x\rangle\,, \quad x \in \mathbb{R}\,, \tag{4.18}$$

$$H|E^{\pm}\rangle_{\mathrm{l,r}} = E|E^{\pm}\rangle_{\mathrm{l,r}}\,, \quad E \in [0,\infty)\,. \tag{4.19}$$

4.3. Construction of $\mathbf{\Phi}' \equiv \mathcal{S}'(\mathbb{R}\text{-}\{a,b\})$. *The Dirac bras*

In complete analogy with the construction of the Dirac kets, we construct in this subsection the Dirac bras $\langle p|$, $\langle x|$ and ${}_{\mathrm{l,r}}\langle^{\pm}E|$ of P, Q and H. Mathematically, the Dirac bras are distributions that belong to the space $\mathbf{\Phi}'$, which is the space of *linear* functionals over $\mathbf{\Phi}$ [26]. The corresponding RHS is

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}'\,, \tag{4.20}$$

which we denote in the position representation by

$$\mathcal{S}(\mathbb{R}\text{-}\{a,b\}) \subset L^2 \subset \mathcal{S}'(\mathbb{R}\text{-}\{a,b\})\,. \tag{4.21}$$

Likewise the definition of a ket, the definition of a bra is borrowed from the theory of distributions [16]. Given a function $f(x)$ and a space of test functions $\mathbf{\Phi}$, the linear functional $\tilde{F}$ generated by the function $f(x)$ is an integral operator whose kernel is the complex conjugate of $f(x)$:

$$\tilde{F}(\varphi) = \int \mathrm{d}x\, \varphi(x)\overline{f(x)}\,, \tag{4.22a}$$

which in Dirac's notation becomes

$$\langle F|\varphi\rangle = \int \mathrm{d}x\, \langle f|x\rangle\langle x|\varphi\rangle\,. \tag{4.22b}$$

Note that this definition is very similar to that of a linear functional, Eq. (4.9*a*), except that the complex conjugation affects $f(x)$ rather than $\varphi(x)$, which makes $\tilde{F}$ linear rather than antilinear. Likewise the antilinear case (4.9*a*), it is important to keep in mind that, though related, the function $f(x)$ and the functional $\tilde{F}$ are two different objects, the relation between them being that $\overline{f(x)}$ is the kernel of $\tilde{F}$ when we write $\tilde{F}$ as an integral operator.

By using prescription (4.22*a*), we can now define for each eigenvalue p the eigenbra $\langle p|$ associated with the eigenfunction (3.10):

$$\langle p|\varphi\rangle \equiv \int_{-\infty}^{\infty} \mathrm{d}x\, \varphi(x)\frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{-\mathrm{i}px/\hbar}\,, \tag{4.23a}$$

which, using Dirac's notation for the integrand, becomes

$$\langle p|\varphi\rangle \equiv \int_{-\infty}^{\infty} \mathrm{d}x\, \langle p|x\rangle\langle x|\varphi\rangle\,. \tag{4.23b}$$

Comparison with Eq. (4.10a) shows that the action of $\langle p|$ is the complex conjugate of the action of $|p\rangle$,

$$\langle p|\varphi\rangle = \overline{\langle \varphi|p\rangle}\,, \tag{4.24}$$

and that

$$\langle p|x\rangle = \overline{\langle x|p\rangle} = \frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{-\mathrm{i}px/\hbar}\,. \tag{4.25}$$

The bra $\langle x|$ is defined as

$$\langle x|\varphi\rangle \equiv \int_{-\infty}^{\infty} \mathrm{d}x'\,\varphi(x')\delta(x-x')\,, \tag{4.26a}$$

which, using Dirac's notation for the integrand, becomes

$$\langle x|\varphi\rangle \equiv \int_{-\infty}^{\infty} \mathrm{d}x'\,\langle x|x'\rangle\langle x'|\varphi\rangle\,. \tag{4.26b}$$

Comparison with Eq. (4.11a) shows that the action of $\langle x|$ is complex conjugated to the action of $|x\rangle$,

$$\langle x|\varphi\rangle = \overline{\langle \varphi|x\rangle}\,, \tag{4.27}$$

and that

$$\langle x|x'\rangle = \langle x'|x\rangle = \delta(x-x')\,. \tag{4.28}$$

Analogously, the eigenbras of the Hamiltonian are defined as

$${}_{\mathrm{l,r}}\langle^{\pm}E|\varphi\rangle \equiv \int_{-\infty}^{\infty} \mathrm{d}x\;\varphi(x)\;{}_{\mathrm{l,r}}\langle^{\pm}E|x\rangle\,, \tag{4.29a}$$

that is,

$${}_{\mathrm{l,r}}\langle^{\pm}E|\varphi\rangle \equiv \int_{-\infty}^{\infty} \mathrm{d}x\;{}_{\mathrm{l,r}}\langle^{\pm}E|x\rangle\langle x|\varphi\rangle\,, \tag{4.29b}$$

where

$${}_{\mathrm{l,r}}\langle^{\pm}E|x\rangle = \overline{\langle x|E^{\pm}\rangle_{\mathrm{l,r}}}\,. \tag{4.30}$$

(Note that in Eq. (4.29a) we have defined four different bras.) Comparison of Eq. (4.29a) with Eq. (4.12a) shows that the actions of the bras ${}_{\mathrm{l,r}}\langle^{\pm}E|$ are the complex conjugates of the actions of the kets $|E^{\pm}\rangle_{\mathrm{l,r}}$:

$${}_{\mathrm{l,r}}\langle^{\pm}E|\varphi\rangle = \overline{\langle \varphi|E^{\pm}\rangle_{\mathrm{l,r}}}\,. \tag{4.31}$$

Now, by using the RHS mathematics, one can show that the definitions of $\langle p|$, $\langle x|$ and ${}_{\mathrm{l,r}}\langle^{\pm}E|$ make sense and that $\langle p|$, $\langle x|$ and ${}_{\mathrm{l,r}}\langle^{\pm}E|$ belong to $\mathcal{S}'(\mathbb{R}\text{-}\{a,b\})$ [10].

Our next task is to see that the bras we just defined are left eigenvectors of the corresponding observable [see Eqs. (4.35)-(4.37) below]. For this purpose, we need to specify how the observables act on the bras, that is, how they act on the dual space $\mathcal{S}'(\mathbb{R}\text{-}\{a,b\})$. We shall do so in analogy to the definition of their action on the kets, by means of the theory of distributions [16]. The action to the left of a self-adjoint operator A on a linear functional $\langle F| \in \mathbf{\Phi}'$ is defined as

$$\langle F|A|\varphi\rangle \equiv \langle F|A\varphi\rangle\,, \quad \text{for all } \varphi \text{ in } \mathbf{\Phi}\,. \tag{4.32}$$

Likewise definition (4.13), this definition generalizes Eq. (4.14). In turn, Eq. (4.32) can be used to define the notion of eigenbra of an observable: A functional $\langle a|$ in $\mathbf{\Phi}'$ is an eigenbra of A with eigenvalue a if

$$\langle a|A|\varphi\rangle = \langle a|A\varphi\rangle = a\langle a|\varphi\rangle\,, \quad \text{for all } \varphi \text{ in } \mathbf{\Phi}\,. \tag{4.33}$$

When the "right sandwiching" of this equation with the elements of $\mathbf{\Phi}$ is understood and therefore omitted, we shall simply write

$$\langle a|A = a\langle a|\,, \tag{4.34}$$

which is just Dirac's eigenbra equation (2.11*b*). Thus, Dirac's eigenbra equation acquires a precise meaning through Eq. (4.33), in the sense that it has to be understood as "right sandwiched" with the wave functions φ of $\mathbf{\Phi}$.

By using definition (4.33), one can show that $\langle p|$, $\langle x|$ and ${}_{\rm l,r}\langle^{\pm}E|$ are indeed left eigenvectors of P, Q and H, respectively [10]:

$$\langle p|P = p\langle p|\,, \quad p \in \mathbb{R}\,, \tag{4.35}$$

$$\langle x|Q = x\langle x|\,, \quad x \in \mathbb{R}\,, \tag{4.36}$$

$${}_{\rm l,r}\langle^{\pm}E|H = E\;{}_{\rm l,r}\langle^{\pm}E|\,, \quad E \in [0,\infty)\,. \tag{4.37}$$

It is worthwhile noting that, in accordance with Dirac's formalism, there is a one-to-one correspondence between bras and kets [39]; that is, given an observable A, to each element a in the spectrum of A there correspond a bra $\langle a|$ that is a left eigenvector of A and also a ket $|a\rangle$ that is a right eigenvector of A. The bra $\langle a|$ belongs to $\mathbf{\Phi}'$, whereas the ket $|a\rangle$ belongs to $\mathbf{\Phi}^{\times}$.

4.4. The Dirac basis expansions

A crucial ingredient of Dirac's formalism is that the bras and kets of an observable form a complete basis system, see Eqs. (2.12) and (2.13). When applied to P, Q and H, Eq. (2.13) yields

$$\int_{-\infty}^{\infty} {\rm d}p\, |p\rangle\langle p| = I\,, \tag{4.38}$$

$$\int_{-\infty}^{\infty} {\rm d}x'\, |x'\rangle\langle x'| = I\,, \tag{4.39}$$

$$\int_0^{\infty} {\rm d}E\, |E^{\pm}\rangle_{\rm l\,l}\langle^{\pm}E| + \int_0^{\infty} {\rm d}E\, |E^{\pm}\rangle_{\rm r\,r}\langle^{\pm}E| = I\,, \tag{4.40}$$

In the present subsection, we derive various Dirac basis expansions for the algebra of the 1D rectangular barrier potential. We will do so by formally sandwiching Eqs. (4.38)-(4.40) in between different vectors.

If we sandwich Eqs. (4.38)-(4.40) in between $\langle x|$ and φ, we obtain

$$\langle x|\varphi\rangle = \int_{-\infty}^{\infty} {\rm d}p\, \langle x|p\rangle\langle p|\varphi\rangle\,, \tag{4.41}$$

$$\langle x|\varphi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x' \, \langle x|x'\rangle\langle x'|\varphi\rangle \, , \tag{4.42}$$

$$\langle x|\varphi\rangle = \int_{0}^{\infty} \mathrm{d}E \, \langle x|E^{\pm}\rangle_{\mathrm{l}\,\mathrm{l}}\langle^{\pm}E|\varphi\rangle + \int_{0}^{\infty} \mathrm{d}E \, \langle x|E^{\pm}\rangle_{\mathrm{r}\,\mathrm{r}}\langle^{\pm}E|\varphi\rangle \, . \tag{4.43}$$

Equations (4.41)-(4.43) can be rigorously proved by way of the RHS [10]. In proving these equations, we give meaning to Eqs. (4.38)-(4.40), which are just formal equations: Equations (4.38)-(4.40) have always to be understood as part of a "sandwich." Note that Eqs. (4.41)-(4.43) are not valid for every element of the Hilbert space but only for those φ that belong to $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, because the action of the bras and kets is well defined only on $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ [40]. Thus, the RHS, rather than just the Hilbert space, fully justifies the Dirac basis expansions. Physically, the Dirac basis expansions provide the means to visualize wave packet formation out of a continuous linear superposition of bras and kets.

We can obtain similar expansions to Eqs. (4.41)-(4.43) by sandwiching Eqs. (4.38)-(4.40) in between other vectors. For example, sandwiching Eq. (4.39) in between $\langle p|$ and φ yields [10]

$$\langle p|\varphi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x \, \langle p|x\rangle\langle x|\varphi\rangle \, , \tag{4.44}$$

and sandwiching Eq. (4.39) in between ${}_{\mathrm{l,r}}\langle^{\pm}E|$ and φ yields [10]

$${}_{\mathrm{l,r}}\langle^{\pm}E|\varphi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x \; {}_{\mathrm{l,r}}\langle^{\pm}E|x\rangle\langle x|\varphi\rangle \, . \tag{4.45}$$

It is worthwhile noting the parallel between the Dirac basis expansions and the Fourier expansions (4.41) and (4.44) [10]. This parallel will be used in Sec. 5 to physically interpret the Dirac bras and kets.

We can also sandwich Eqs. (4.38)-(4.40) in between two elements ψ and φ of $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, and obtain [10]

$$(\varphi,\psi) = \int_{-\infty}^{\infty} \mathrm{d}p \, \langle\varphi|p\rangle\langle p|\psi\rangle \, , \tag{4.46}$$

$$(\varphi,\psi) = \int_{-\infty}^{\infty} \mathrm{d}x \, \langle\varphi|x\rangle\langle x|\psi\rangle \, , \tag{4.47}$$

$$(\varphi,\psi) = \int_{0}^{\infty} \mathrm{d}E \, \langle\varphi|E^{\pm}\rangle_{\mathrm{l}\,\mathrm{l}}\langle^{\pm}E|\psi\rangle + \int_{0}^{\infty} \mathrm{d}E \, \langle\varphi|E^{\pm}\rangle_{\mathrm{r}\,\mathrm{r}}\langle^{\pm}E|\psi\rangle \, . \tag{4.48}$$

Equations (4.46)-(4.48) allow us to calculate the overlap of two wave functions φ and ψ by way of the action of the bras and kets on those wave functions.

The last aspect of Dirac's formalism we need to implement is prescription (2.14), which expresses the action of an observable A in terms of the action of its bras and kets. When applied to P, Q and H, prescription (2.14) yields

$$P = \int_{-\infty}^{\infty} \mathrm{d}p \, p|p\rangle\langle p| \, , \tag{4.49}$$

$$Q = \int_{-\infty}^{\infty} \mathrm{d}x \, x|x\rangle\langle x| \, , \tag{4.50}$$

$$H = \int_0^{\infty} \mathrm{d}E \, E|E^{\pm}\rangle_{\mathrm{l}\,\mathrm{l}}\langle^{\pm}E| + \int_0^{\infty} \mathrm{d}E \, E|E^{\pm}\rangle_{\mathrm{r}\,\mathrm{r}}\langle^{\pm}E| \, . \tag{4.51}$$

Needless to say, these equations are formal expressions that acquire meaning when properly sandwiched. For example, sandwiching them in between $\langle x|$ and φ yields [10]

$$\langle x|P\varphi\rangle = \int_{-\infty}^{\infty} \mathrm{d}p \, p\langle x|p\rangle\langle p|\varphi\rangle \, , \tag{4.52}$$

$$\langle x|Q\varphi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x' \, x'\langle x|x'\rangle\langle x'|\varphi\rangle \, , \tag{4.53}$$

$$\langle x|H\varphi\rangle = \int_0^{\infty} \mathrm{d}E \, E\langle x|E^{\pm}\rangle_{\mathrm{l}\,\mathrm{l}}\langle^{\pm}E|\varphi\rangle + \int_0^{\infty} \mathrm{d}E \, E\langle x|E^{\pm}\rangle_{\mathrm{r}\,\mathrm{r}}\langle^{\pm}E|\varphi\rangle \, , \tag{4.54}$$

and sandwiching them in between two elements φ and ψ of $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ yields [10]

$$(\varphi, P\psi) = \int_{-\infty}^{\infty} \mathrm{d}p \, p\langle\varphi|p\rangle\langle p|\psi\rangle \, , \tag{4.55}$$

$$(\varphi, Q\psi) = \int_{-\infty}^{\infty} \mathrm{d}x \, x\langle\varphi|x\rangle\langle x|\psi\rangle \, , \tag{4.56}$$

$$(\varphi, H\psi) = \int_0^{\infty} \mathrm{d}E \, E\langle\varphi|E^{\pm}\rangle_{\mathrm{l}\,\mathrm{l}}\langle^{\pm}E|\psi\rangle + \int_0^{\infty} \mathrm{d}E \, E\langle\varphi|E^{\pm}\rangle_{\mathrm{r}\,\mathrm{r}}\langle^{\pm}E|\psi\rangle \, . \tag{4.57}$$

Note that, in particular, the operational definition of an observable—according to which an observable is simply an operator whose eigenvectors form a complete basis such that Eqs. (2.12), (2.13) and (2.14) hold, see for example Ref. [41]—acquires meaning within the RHS.

The sandwiches we have made so far always involved at least a wave function φ of $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$. When the sandwiches do not involve elements of $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ at all, we obtain expressions that are simply formal. These formal expressions are often useful though, because they help us understand the meaning of concepts such as the delta normalization or the "matrix elements" of an operator. Let us start with the meaning of the delta normalization. When we sandwich Eq. (4.39) in between $\langle p'|$ and $|p\rangle$, we get

$$\int_{-\infty}^{\infty} \mathrm{d}x \, \langle p'|x\rangle\langle x|p\rangle = \langle p'|p\rangle \, . \tag{4.58}$$

This equation is a formal expression that is to be understood in a distributional sense, that is, both sides must appear smeared out by a smooth function $\varphi(p) = \langle p|\varphi\rangle$ in an integral over p:

$$\int_{-\infty}^{\infty} \mathrm{d}p \, \varphi(p) \int_{-\infty}^{\infty} \mathrm{d}x \, \langle p'|x\rangle\langle x|p\rangle = \int_{-\infty}^{\infty} \mathrm{d}p \, \varphi(p)\langle p'|p\rangle \, . \tag{4.59}$$

The left-hand side of Eq. (4.59) can be written as

$$\begin{aligned}\int_{-\infty}^{\infty} \mathrm{d}x \, \langle p'|x\rangle \int_{-\infty}^{\infty} \mathrm{d}p \, \varphi(p)\langle x|p\rangle &= \int_{-\infty}^{\infty} \mathrm{d}x \, \langle p'|x\rangle \int_{-\infty}^{\infty} \mathrm{d}p \, \langle x|p\rangle\langle p|\varphi\rangle \\ &= \int_{-\infty}^{\infty} \mathrm{d}x \, \langle p'|x\rangle\langle x|\varphi\rangle \\ &= \varphi(p') \end{aligned} \tag{4.60}$$

Plugging Eq. (4.60) into Eq. (4.59) leads to

$$\int_{-\infty}^{\infty} \mathrm{d}p \, \varphi(p)\langle p'|p\rangle = \varphi(p') \, . \tag{4.61}$$

By recalling the definition of the delta function, we see that Eq. (4.61) leads to

$$\langle p'|p\rangle = \delta(p-p') \, , \tag{4.62}$$

and to

$$\int_{-\infty}^{\infty} \mathrm{d}x \, \langle p'|x\rangle\langle x|p\rangle = \delta(p-p') \, . \tag{4.63}$$

By using Eq. (4.25), we can write Eq. (4.63) in a well-known form:

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} \mathrm{d}x \, \mathrm{e}^{\mathrm{i}(p-p')x/\hbar} = \delta(p-p') \, . \tag{4.64}$$

This formal equation is interpreted by saying that the bras and kets of the momentum operator are delta normalized. That the energy bras and kets are also delta normalized can be seen in a similar, though slightly more involved way [28]:

$${}_{\alpha}\langle {}^{\pm}E'|E^{\pm}\rangle_{\beta} = \delta(E-E') \, \delta_{\alpha\beta} \, , \tag{4.65a}$$

$$\int_{-\infty}^{\infty} \mathrm{d}x \; {}_{\alpha}\langle {}^{\pm}E'|x\rangle\langle x|E^{\pm}\rangle_{\beta} = \delta(E-E') \, \delta_{\alpha\beta} \, , \tag{4.65b}$$

where α, β stand for the labels l, r that respectively denote left and right incidence. The derivation of expressions involving the Dirac delta function such as Eqs. (4.62), (4.64) or (4.65a)-(4.65b) shows that these formal expressions must be understood in a distributional sense, that is, as kernels of integrals that include the wave functions φ of $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, like in Eq. (4.59).

In a similar way, we can also understand the meaning of the "matrix elements" of the observables in a particular representation, e.g.:

$$\langle x|Q|x'\rangle = x' \, \delta(x-x') \, , \tag{4.66}$$

$$\langle x|P|x'\rangle = -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x} \, \delta(x-x') \, , \tag{4.67}$$

$$\langle x|H|x'\rangle = \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right) \delta(x-x') \, . \tag{4.68}$$

Equations (4.66)-(4.68) can be obtained by formally inserting Eq. (4.39) into respectively Eq. (2.17), (2.22) and (3.1).

It is illuminating to realize that the expressions (4.66)-(4.68) generalize the matrix representation of an observable A in a finite-dimensional Hilbert space. If $a_1, \dots, a_N$ are the eigenvalues of A, then, in the basis $\{|a_1\rangle, \dots, |a_N\rangle\}$, A is represented as

$$A \equiv \begin{pmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & \cdots & a_N \end{pmatrix} , \tag{4.69}$$

which in Dirac's notation reads as

$$\langle a_i|A|a_j\rangle = a_i \delta_{ij} \, . \tag{4.70}$$

Clearly, expressions (4.66)-(4.68) are the infinite-dimensional extension of expression (4.70).

5. Physical meaning of the Dirac bras and kets

The bras and kets associated with eigenvalues in the continuous spectrum are not normalizable. Hence, the standard probabilistic interpretation does not apply to them straightforwardly. In this section, we are going to generalize the probabilistic interpretation of normalizable states to the non-normalizable bras and kets. As well, in order to gain further insight into the physical meaning of bras and kets, we shall present the analogy between classical plane waves and the bras and kets.

In Quantum Mechanics, the scalar product of the Hilbert space is employed to calculate probability amplitudes. In our example, the Hilbert space is L^2, and the corresponding scalar product is given by Eq. (3.4). That an eigenvalue of an observable A lies in the discrete or in the continuous part of the spectrum is determined by this scalar product. An eigenvalue a_n belongs to the discrete part of the spectrum when its corresponding eigenfunction $f_n(x) \equiv \langle x|a_n\rangle$ is square normalizable:

$$(f_n, f_n) = \int_{-\infty}^{\infty} \mathrm{d}x \, |f_n(x)|^2 < \infty \, . \tag{5.1}$$

An eigenvalue a belongs to the continuous part of the spectrum when its corresponding eigenfunction $f_a(x) \equiv \langle x|a\rangle$ is *not* square normalizable:

$$(f_a, f_a) = \int_{-\infty}^{\infty} \mathrm{d}x \, |f_a(x)|^2 = \infty \, . \tag{5.2}$$

In the latter case, one has to use the theory of distributions to "normalize" these states, e.g., delta function normalization:

$$(f_a, f_{a'}) = \int_{-\infty}^{\infty} \mathrm{d}x \, \overline{f_a(x)} f_{a'}(x) = \delta(a - a') \, . \tag{5.3}$$

This Dirac delta normalization generalizes the Kronecker delta normalization of "discrete" states:

$$(f_n, f_{n'}) = \int_{-\infty}^{\infty} \mathrm{d}x \, \overline{f_n(x)} f_{n'}(x) = \delta_{nn'} \, . \tag{5.4}$$

Because they are square integrable, the "discrete" eigenvectors $f_n(x) \equiv \langle x|a_n\rangle$ can be interpreted in the usual way as probability amplitudes. But because they are *not* square integrable, the "continuous" eigenvectors $f_a(x) \equiv \langle x|a\rangle$ must be interpreted as "kernels" of probability amplitudes, in the sense that when we multiply $\langle x|a\rangle$ by $\langle \varphi|x\rangle$ and then integrate, we obtain the density of probability amplitude $\langle \varphi|a\rangle$:

$$\langle \varphi|a\rangle = \int_{-\infty}^{\infty} \mathrm{d}x \, \langle \varphi|x\rangle\langle x|a\rangle \, . \tag{5.5}$$

Thus, in particular, $\langle x|p\rangle$, $\langle x|x'\rangle$ and $\langle x|E^{\pm}\rangle_{\mathrm{l,r}}$ represent "kernels" of probability amplitudes.

Another way to interpret the bras and kets is in analogy to the plane waves of classical optics and classical electromagnetism. Plane waves $\mathrm{e}^{\mathrm{i}kx}$ represent monochromatic light pulses of wave number k and frequency (in vacuum) $w = kc$. Monochromatic light pulses are impossible to prepare experimentally; all that can be prepared are light pulses $\varphi(k)$ that have some wave-number spread. The corresponding pulse in the position representation, $\varphi(x)$, can be "Fourier decomposed" in terms of the monochromatic plane waves as

$$\varphi(x) = \frac{1}{\sqrt{2\pi}} \int \mathrm{d}k \, \mathrm{e}^{\mathrm{i}kx} \varphi(k) \, , \tag{5.6a}$$

which in Dirac's notation becomes

$$\langle x|\varphi\rangle = \int \mathrm{d}k \, \langle x|k\rangle\langle k|\varphi\rangle \, . \tag{5.6b}$$

Thus, physically preparable pulses can be expanded in a Fourier integral by the unpreparable plane waves, the weights of the expansion being $\varphi(k)$. When $\varphi(k)$ is highly peaked around a particular wave number k_0, then the pulse can in general be represented for all practical purposes by a monochromatic plane wave $\mathrm{e}^{\mathrm{i}k_0x}$. Also, in finding out how a light pulse behaves under given conditions (e.g., reflection and refraction at a plane interface between two different media), we only have to find out how plane waves behave and, after that, by means of the Fourier expansion (5.6a), we know how the light pulse $\varphi(x)$ behaves. Because obtaining the behavior of plane waves is somewhat easy, it is advantageous to use them to obtain the behavior of the whole pulse [42].

The quantum mechanical bras and kets can be interpreted in analogy to the classical plane waves. The eigenfunction $\langle x|p\rangle = \mathrm{e}^{\mathrm{i}px/\hbar}/\sqrt{2\pi\hbar}$ represents a particle of sharp momentum p; the eigenfunction $\langle x|x'\rangle = \delta(x-x')$ represents a particle sharply localized at x'; the monoenergetic eigenfunction $\langle x|E^{\pm}\rangle_{\mathrm{l,r}}$ represents a particle with well-defined energy E (and with additional boundary conditions determined by the labels $\pm$ and $\mathrm{l,r}$). In complete analogy to the Fourier expansion of a light pulse by classical plane waves, Eq. (5.6a), the eigenfunctions $\langle x|p\rangle$, $\langle x|x'\rangle$ and $\langle x|E^{\pm}\rangle_{\mathrm{l,r}}$ expand a wave function φ, see Eqs. (4.41)-(4.43). When the wave packet $\varphi(p)$ is highly peaked around a particular momentum p_0, then in general the approximation $\varphi(x) \sim \mathrm{e}^{\mathrm{i}p_0x/\hbar}/\sqrt{2\pi\hbar}$ holds for all practical purposes; when the wave packet $\varphi(x)$ is highly peaked around a particular position x_0, then in general the approximation $\varphi(x) \sim \delta(x-x_0)$ holds for all practical purposes; and when $\varphi(E)$ is highly peaked around a particular energy E_0, then in general the approximation $\varphi(x) \sim \langle x|E_0^{\pm}\rangle_{\mathrm{l,r}}$ holds for all practical purposes (up to the boundary conditions determined by the labels $\pm$ and $\mathrm{l,r}$). Thus, although in principle $\langle x|p\rangle$, $\langle x|x'\rangle$ and $\langle x|E^{\pm}\rangle_{\mathrm{l,r}}$ are impossible to prepare, in many practical situations they can give good approximations when the wave packet is well peaked around some particular values p_0, x_0, E_0 of the momentum, position and energy. Also, in finding out how a wave function behaves under given conditions (e.g., reflection and transmission off a potential barrier), all we have to find out is how the bras and kets behave and, after that, by means of the Dirac basis expansions, we know how the wave function $\varphi(x)$ behaves. Because obtaining the behavior of the bras and kets is somewhat easy, it is advantageous to use them to obtain the behavior of the whole wave function [43].

From the above discussion, it should be clear that there is a close analogy between classical Fourier methods and Dirac's formalism. In fact, one can say that Dirac's formalism is the extension of Fourier methods to Quantum Mechanics: Classical monochromatic plane waves correspond to the Dirac bras and kets; the light pulses correspond to the wave functions φ; the classical Fourier expansion corresponds to the Dirac basis expansions; the classical Fourier expansion provides the means to form light pulses out of a continuous linear superposition of monochromatic plane waves, and the Dirac basis expansions provide the means to form wave functions out of a continuous linear superposition of bras and kets; the classical uncertainty principle of Fourier Optics corresponds to the quantum uncertainty generated by the non-commutativity of two observables [44]. However, although this analogy is very close from a formal point of view, there is a crucial difference from a conceptual point of view. To wit, whereas in the classical domain the solutions of the wave equations represent a physical wave, in Quantum Mechanics the solutions of the equations do *not* represent a physical object, but rather a probability amplitude—In Quantum Mechanics what is "waving" is probability.

6. Further considerations

In Quantum Mechanics, the main objective is to obtain the probability of measuring an observable A in a state φ. Within the Hilbert space setting, such probability can be obtained by means of the spectral measures E_a of A (see, for example, Ref. [8]). These spectral measures satisfy

$$I = \int_{\mathrm{Sp}(A)} \mathrm{d}\mathsf{E}_a \tag{6.1}$$

and

$$A = \int_{\mathrm{Sp}(A)} a \, \mathrm{d}\mathsf{E}_a \tag{6.2}$$

Comparison of these equations with Eqs. (2.13) and (2.14) yields

$$\mathrm{d}\mathsf{E}_a = |a\rangle\langle a| \, \mathrm{d}a \, . \tag{6.3}$$

Thus, the RHS is able to "factor out" the Hilbert space spectral measures in terms of the bras and kets [45]. For the position, momentum and energy observables, Eq. (6.3) reads as

$$\mathrm{d}\mathsf{E}_x = |x\rangle\langle x|\,\mathrm{d}x\,, \tag{6.4}$$

$$\mathrm{d}\mathsf{E}_p = |p\rangle\langle p|\,\mathrm{d}p\,, \tag{6.5}$$

$$\mathrm{d}\mathsf{E}_E = |E^{\pm}\rangle_{\mathrm{l}\,\mathrm{l}}\langle{}^{\pm}E|\,\mathrm{d}E + |E^{\pm}\rangle_{\mathrm{r}\,\mathrm{r}}\langle{}^{\pm}E|\,\mathrm{d}E\,. \tag{6.6}$$

Although the spectral measures $\mathrm{d}\mathsf{E}_a$ associated with a given self-adjoint operator A are unique, the factorization in terms of bras and kets is not. For example, as we can see from Eq. (6.6), the spectral measures of our Hamiltonian can be written in terms of the basis $\{|E^+\rangle_{\mathrm{l,r}}\}$ or the basis $\{|E^-\rangle_{\mathrm{l,r}}\}$. From a physical point of view, those two basis are very different. As we saw in Sec. 3, the basis $\{|E^+\rangle_{\mathrm{l,r}}\}$ represents the initial condition of an incoming particle, whereas the basis $\{|E^-\rangle_{\mathrm{l,r}}\}$ represents the final condition of an outgoing particle. However, the spectral measures of the Hilbert space are insensitive to such difference, in contrast to the RHS, which can differentiate both cases. Therefore, when computing probability amplitudes, the RHS gives more precise information on how those probabilities are physically produced than the Hilbert space.

In this paper, we have restricted our discussion to the simple, straightforward algebra of the 1D rectangular barrier. But, what about more complicated potentials? In general, the situation is not as easy. First, the theory of rigged Hilbert spaces as constructed by Gelfand and collaborators is based on the assumption that the space $\mathbf{\Phi}$ has a property called *nuclearity* [16, 17]. However, it is not clear that one can always find a nuclear space $\mathbf{\Phi}$ that remains invariant under the action of the observables. Nevertheless, Roberts has shown that such $\mathbf{\Phi}$ exists when the potential is infinitely often differentiable except for a closed set of zero Lebesgue measure [19]. Second, the problem of constructing the RHS becomes more involved when the observable A is not cyclic [16]. And third, solving the eigenvalue equation of an arbitrary self-adjoint operator is rarely as easy as in our example.

7. Summary and conclusions

We have used the 1D rectangular barrier model to see that, when the spectra of the observables have a continuous part, the natural setting for Quantum Mechanics is the rigged Hilbert space rather than just the Hilbert space. In particular, Dirac's bra-ket formalism is fully implemented by the rigged Hilbert space rather than just by the Hilbert space.

We have explained the physical and mathematical meanings of each of the ingredients that form the rigged Hilbert space. Physically, the space $\mathbf{\Phi} \equiv \mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ is interpreted as the space of wave functions, since its elements can be associated well-defined, finite physical quantities, and algebraic operations such as commutation relations are well defined on $\mathbf{\Phi}$. Mathematically, $\mathbf{\Phi}$ is the space of test functions. The spaces $\mathbf{\Phi}' \equiv \mathcal{S}'(\mathbb{R}\text{-}\{a,b\})$ and $\mathbf{\Phi}^\times \equiv \mathcal{S}^\times(\mathbb{R}\text{-}\{a,b\})$ contain respectively the bras and kets associated with the eigenvalues that lie in the continuous spectrum. Physically, the bras and kets are interpreted as "kernels" of probability amplitudes. Mathematically, the bras and kets are distributions. The following table summarizes the meanings of each space:

Space	Physical Meaning	Mathematical Meaning
$\mathbf{\Phi}$	Space of wave functions φ	Space of test functions φ
$\mathcal{H}$	Probability amplitudes	Hilbert space
$\mathbf{\Phi}^\times$	Space of kets $\lvert a\rangle$	Antidual space
$\mathbf{\Phi}'$	Space of bras $\langle a\rvert$	Dual space

We have seen that, from a physical point of view, the rigged Hilbert space does not entail an extension of Quantum Mechanics, whereas, from a mathematical point of view, the rigged Hilbert space is an extension of the Hilbert space. Mathematically, the rigged Hilbert space arises when we equip the Hilbert space with distribution theory. Such equipment enables us to cope with singular objects such as bras and kets.

We have also seen that formal expressions involving bras and kets must be understood as "sandwiched" by wave functions φ. Such "sandwiching" by φ's is what controls the singular behavior of bras and kets. This is why mathematically the sandwiching by φ's is so important and must always be implicitly assumed. In practice, we can freely apply the formal manipulations of Dirac's formalism with confidence, since such formal manipulations are justified by the rigged Hilbert space.

We hope that this paper can serve as a pedagogical, enticing introduction to the rigged Hilbert space.

Acknowledgments

Research supported by the Basque Government through reintegration fellowship No. BCI03.96, and by the University of the Basque Country through research project No. 9/UPV00039.310-15968/2004.

References

[1] D. Atkinson, P. W. Johnson, *Quantum Field Theory – a Self-Contained Introduction*, Rinton Press, Princeton (2002).

[2] N. N. Bogolubov, A. A. Logunov, I. T. Todorov, *Introduction to Axiomatic Quantum Field Theory*, Benjamin, Reading, Massachusetts (1975).

[3] L. E. Ballentine, *Quantum Mechanics*, Prentice-Hall International, Inc., Englewood Cliffs, New Jersey (1990).

[4] A. Bohm, *Quantum Mechanics: Foundations and Applications*, Springer-Verlag, New York (1994).

[5] A. Bohm and M. Gadella, *Dirac kets, Gamow Vectors, and Gelfand Triplets*, Springer Lectures Notes in Physics Vol. 348, Springer, Berlin (1989).

[6] A. Z. Capri, *Nonrelativistic Quantum Mechanics*, Benjamin, Menlo Park, California (1985).

[7] D. A. Dubin, M. A. Hennings, *Quantum Mechanics, Algebras and Distributions*, Longman, Harlow (1990).

[8] A. Galindo, P. Pascual, *Quantum Mechanics I*, Springer-Verlag, Berlin (1990).
[9] V. I. Kukulin, V. M. Krasnopol'sky, and J. Horacek, *Theory of resonances*, Kluwer Academic Publishers, Dordrecht (1989).
[10] R. de la Madrid, J. Phys. A: Math. Gen. **37**, 8129-8157 (2004); quant-ph/0407195.
[11] R. de la Madrid, "Quantum mechanics in rigged Hilbert space language," Ph.D. thesis, Universidad de Valladolid (2001). Available at `http://www.ehu.es/~wtbdemor/`.
[12] P. A. M. Dirac, *The principles of Quantum Mechanics*, 3rd ed., Clarendon Press, Oxford (1947).
[13] J. von Neumann, *Mathematische Grundlagen der Quantentheorie*, Springer, Berlin (1931); English translation by R. T. Beyer, *Mathematical Foundations of Quantum Mechanics*, Princeton University Press, Princeton (1955).
[14] In Ref. [12], page 40, Dirac states that "*the bra and ket vectors that we now use form a more general space than a Hilbert space.*"
In Ref. [13], page viii, von Neumann states that "*Dirac has given a representation of quantum mechanics which is scarcely to be surpassed in brevity and elegance,* [...]." On pages viii-ix, von Neumann says that "*The method of Dirac, mentioned above, (and this is overlooked today in a great part of quantum mechanical literature, because of the clarity and elegance of the theory) in no way satisfies the requirements of mathematical rigor – not even if these are reduced in a natural and proper fashion to the extent common elsewhere in theoretical physics.*" On page ix, von Neumann says that "[...],*this requires the introduction of 'improper' functions with self-contradictory properties. The insertion of such mathematical 'fiction' is frequently necessary in Dirac's approach,*[...]." Thus, essentially, although von Neumann recognizes the clarity and beauty of Dirac's formalism, he states very clearly that such formalism cannot be implemented within the framework of the Hilbert space.
[15] L. Schwartz, *Théory de Distributions*, Hermann, Paris (1950).
[16] I. M. Gelfand, N. Y. Vilenkin, *Generalized Functions*, Vol. IV, Academic Press, New York (1964).
[17] K. Maurin, *Generalized Eigenfunction Expansions and Unitary Representations of Topological Groups*, Polish Scientific Publishers, Warsaw (1968).
[18] In Ref. [17], page 7, Maurin states that "*It seems to us that this is the formulation which was anticipated by Dirac in his classic monograph.*"
[19] J. E. Roberts, J. Math. Phys. **7**, 1097–1104 (1966); J. E. Roberts, Commun. Math. Phys. **3**, 98–119 (1966).
[20] J.-P. Antoine, J. Math. Phys. **10**, 53–69 (1969); J.-P. Antoine, J. Math. Phys. **10**, 2276–2290 (1969).
[21] A. Bohm, "The Rigged Hilbert Space in Quantum Mechanics," *Boulder Lectures in Theoretical Physics, 1966*, Vol. 9A (Gordon and Breach, New York, 1967).
[22] The following quotation, extracted from Ref. [3], page 19, gives a clear idea of the status the RHS is achieving: "*...rigged Hilbert space seems to be a more natural mathematical setting for quantum mechanics than Hilbert space.*"
[23] I. Antoniou, S. Tasaki, Int. J. Quant. Chem. **44**, 425–474 (1993).
[24] Z. Suchanecki, I. Antoniou, S. Tasaki, O. F. Brandtlow, J. Math. Phys. **37**, 5837–5847 (1996).
[25] A subspace S of $\mathcal{H}$ is dense in $\mathcal{H}$ if we can approximate any element of $\mathcal{H}$ by an element of S as well as we wish. Thus, for any f of $\mathcal{H}$ and for any small $\epsilon > 0$, we can find a φ in S such that $\|f - \varphi\| < \epsilon$. In physical terms, this inequality means that we can replace f by φ within an accuracy ϵ.
[26] A function $F : \mathbf{\Phi} \to \mathbb{C}$ is called a linear [respectively antilinear] functional over $\mathbf{\Phi}$ if for any complex numbers α, β and for any $\varphi, \psi \in \mathbf{\Phi}$, it holds that $F(\alpha\varphi + \beta\psi) = \alpha F(\varphi) + \beta F(\psi)$ [respectively $F(\alpha\varphi + \beta\psi) = \alpha^* F(\varphi) + \beta^* F(\psi)$].
[27] R. de la Madrid, J. Phys. A: Math. Gen. **35**, 319–342 (2002); quant-ph/0110165.
[28] R. de la Madrid, A. Bohm, and M. Gadella, Fortsch. Phys. **50**, 185–216 (2002); quant-ph/0109154.
[29] R. de la Madrid, Int. J. Theor. Phys. **42**, 2441–2460 (2003); quant-ph/0210167.
[30] Strictly speaking, a Hilbert space possesses additional properties (e.g., it must be complete with

respect to the topology induced by the scalar product). For a more technical definition of the Hilbert space, see for example Ref. [11].

[31] An operator A is bounded if there is some finite K such that $\|Af\| < K\|f\|$ for all $f \in \mathcal{H}$, where $\| \ \|$ denotes the Hilbert space norm. When such K does not exist, A is said to be unbounded. For a detailed account of the properties of bounded and unbounded operators, see for example Ref. [11].

[32] The mathematical reason why quantum mechanical unbounded operators cannot be defined on all the vectors of the Hilbert space can be found, for example, in Ref. [33], page 84.

[33] M. Reed, B. Simon, "Methods of modern mathematical physics," vol. I, Academic Press, Inc., New York (1972).

[34] If we nevertheless insisted in for example calculating the expectation value (2.24) for elements of $\mathcal{H}$ that are not in $\mathcal{D}(A)$, we would obtain an unphysical infinity value. For instance, if A represents an unbounded Hamiltonian H, then the expectation value (2.24) would be infinite for those φ of $\mathcal{H}$ that lie outside of $\mathcal{D}(H)$. Because they have infinite energy, those states do not represent physically preparable wave packets.

[35] If they were in the Hilbert space, $|a\rangle$ and $\langle a|$ would be square integrable, and a would belong to the discrete spectrum.

[36] It is well known that Heisenberg's commutation relation necessarily implies that either P or Q is unbounded. See, for example, Ref. [33], page 274.

[37] The reason why the derivatives of $\varphi(x)$ must vanish at $x = a, b$ is that we want to be able to apply the Hamiltonian H as many times as we wish. Since repeated applications of H to $\varphi(x)$ involve the derivatives of $V(x)\varphi(x)$, and since $V(x)$ is discontinuous at $x = a, b$, the function $V(x)\varphi(x)$ is infinitely differentiable at $x = a, b$ only when the derivatives of $\varphi(x)$ vanish at $x = a, b$. For more details, see Ref. [19]. The vanishing of the derivatives of $\varphi(x)$ at $x = a, b$ must be viewed as a mathematical consequence of the unphysical sharpness of the discontinuities of the potential, rather than as a physical consequence of Quantum Mechanics. Note also that in standard numerical simulations, for example, Gaussian wave packets impinging on a rectangular barrier, one never sees that the wave packet vanishes at $x = a, b$. This is due to the fact that on a Gaussian wave packet, the Hamiltonian (3.1) can only be applied once.

[38] We note that, when acting on elements φ of $\mathcal{S}(\mathbb{R}\text{-}\{a, b\})$, the commutator $[H, P] = \mathrm{i}\hbar\frac{\partial V}{\partial x}$ reduces to $[H, P] = 0$, due to the vanishing of the derivatives of φ at $x = a, b$.

[39] We recall that some authors have erroneously claimed that "there are more kets than bras" [19], and that therefore such one-to-one correspondence between bras and kets does not hold.

[40] We can nevertheless extend Eqs. (4.41) and (4.43) to the whole Hilbert space L^2 by a limiting procedure, although the resulting expansions do not involve the Dirac bras and kets any more, but simply the eigenfunctions of the differential operators.

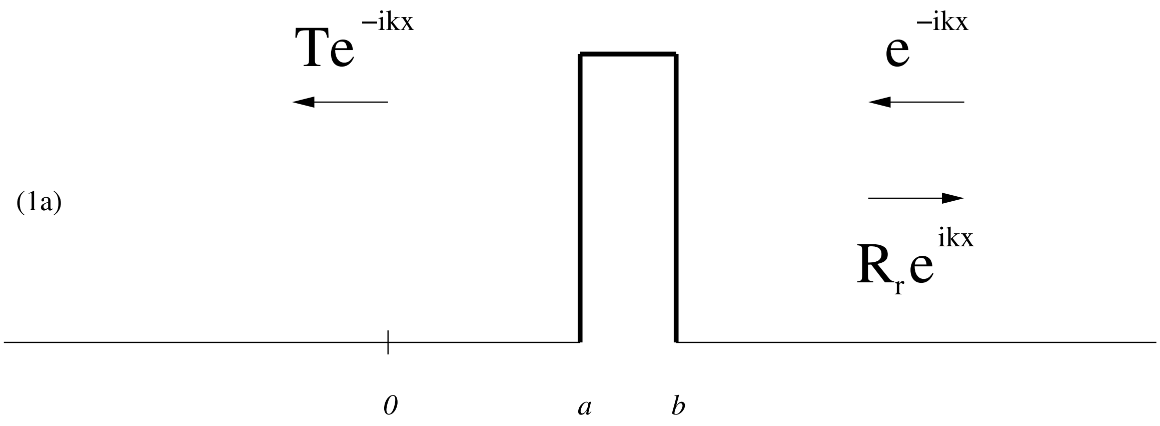
[41] C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum Mechanics*, Wiley, New York (1977).

[42] This is one of the major reasons why plane waves are so useful in practical calculations.

[43] This is one of the major reasons why bras and kets are so useful in practical calculations.

[44] There are many other links between the classical and the quantum worlds, such as for example the de Broglie relation $p = \hbar k$, which entails a formal identity between the classical $\mathrm{e}^{\mathrm{i}kx}$ and the quantum $\mathrm{e}^{\mathrm{i}px/\hbar}$ plane waves.

[45] We recall that the direct integral decomposition of the Hilbert space falls short of such factorization, see Ref. [20].



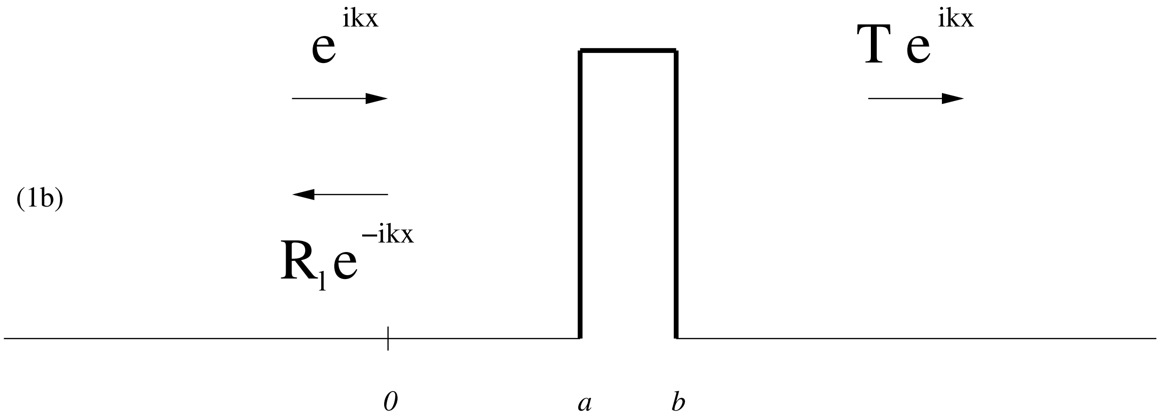


Figure 1. Schematic representation of the eigenfunctions $\langle x|E^+\rangle_{\rm r}$, Fig. 1a, and $\langle x|E^+\rangle_{\rm l}$, Fig. 1b.

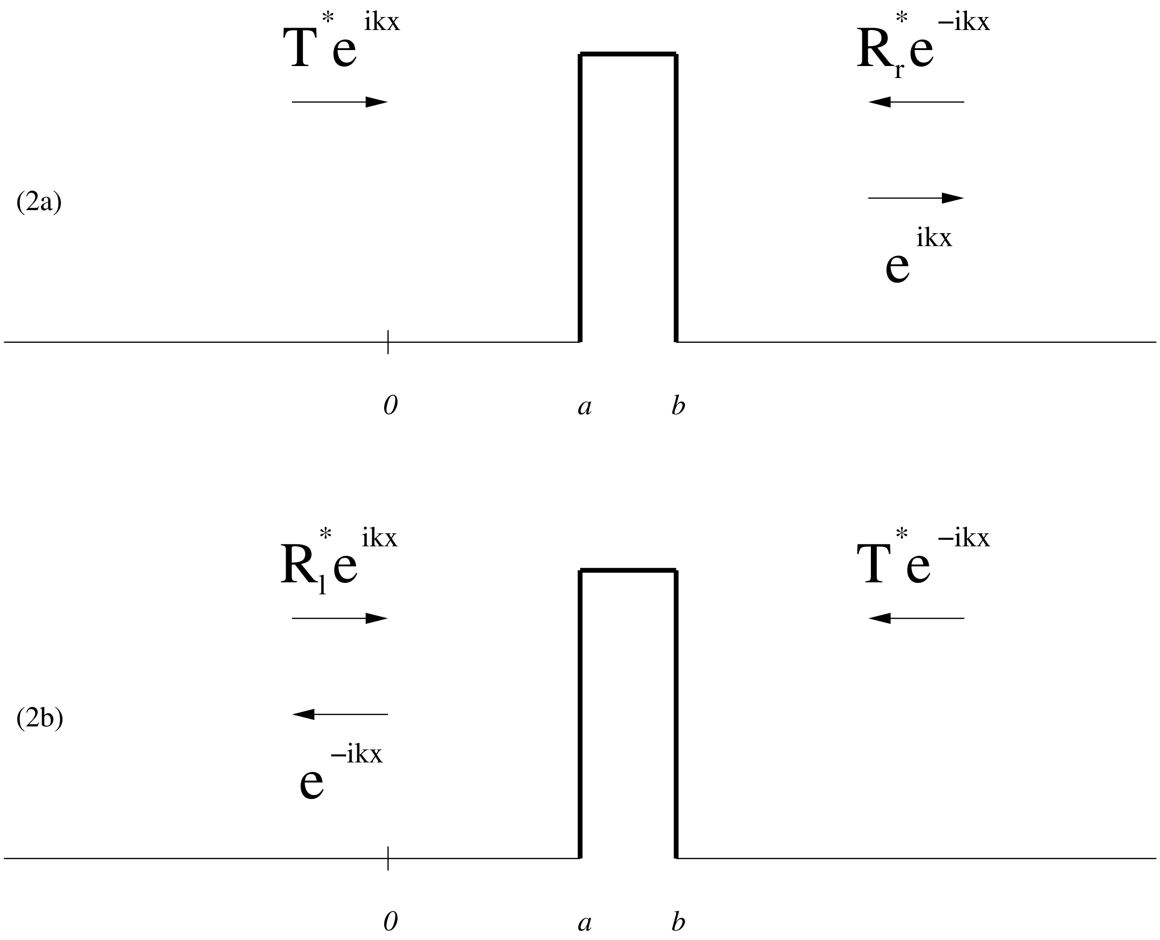


Figure 2. Schematic representation of the eigenfunctions $\langle x|E^-\rangle_{\rm r}$, Fig. 2a, and $\langle x|E^-\rangle_{\rm l}$, Fig. 2b.