The rigged Hilbert space of the algebra of the one-dimensional rectangular barrier potential

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Abstract. The rigged Hilbert space of the algebra of the one-dimensional rectangular barrier potential is constructed. The one-dimensional rectangular potential provides another opportunity to show that the rigged Hilbert space fully accounts for Dirac's bra-ket formalism. The analogy between Dirac's formalism and Fourier methods is pointed out.

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1. Introduction

One-dimensional (1D) models play a paramount role in Quantum Mechanics, because they enable us to understand a number of properties that also appear in more realistic situations. The simplicity of 1D models facilitates testing new hypothesis, approximation methods and theories without unnecessary and costly complications. In many cases, after proper calculations, it is possible to reduce an intricate problem to a Schrödinger equation in one dimension. For example: three-dimensional (3D) spherically symmetric Schrödinger equations can be reduced to 1D radial equations; time quantities such as tunneling or arrival times have in many cases been studied in 1D models [1, 2]; electrons in strong magnetic fields can be described by 1D potentials [3]; some surface phenomena are described by 1D models [4]; the application of the effective mass approximation to layered semiconductor structures leads to effective 1D systems [5]; the conductance of some semiconductor nanostructures can be obtained by solving 1D Schrödinger equations [6]. One-dimensional potentials have even practical interest, since advances in the microfabrication of semiconductors have allowed to design and control essentially 1D potentials [7, 8].

One-dimensional models are also ideally suited to examine the mathematical foundations of Quantum Mechanics. In this paper, we shall take this foundational route. We shall construct the rigged Hilbert space (RHS) of the one-dimensional rectangular barrier potential, thereby showing that the mathematical setting of quantum mechanical systems with continuous spectrum is the RHS rather than just the Hilbert space.

This paper follows up on Refs. [9, 10, 11], where the RHSs of 3D spherical shell potentials were constructed [12], and on Ref. [13], where the RHS of the 3D free Hamiltonian was constructed. The present paper complements Refs. [9, 10, 11, 13] in the following ways:

- We treat a truly 1D model on the full real line, rather than the radial part of a 3D model.
- We construct the RHS of the algebra generated by the position, momentum and energy observables, rather than just the RHS of the Hamiltonian.
- We construct not only the Dirac kets but also the Dirac bras, thereby showing even more clearly that the RHS fully implements Dirac's bra-ket formalism.

The model we consider in this paper is supposed to represent a spinless particle moving in one dimension and impinging on a barrier. The relevant observables to this system are the position Q, the momentum P and the Hamiltonian H. These observables are represented by the following differential operators:

$$Qf(x) = xf(x)\,, \tag{1.1}$$

$$Pf(x) = -\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}x}f(x)\,, \tag{1.2}$$

$$Hf(x) = -\frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x^2}f(x) + V(x)f(x)\,, \tag{1.3}$$

where

$$V(x) = \begin{cases} 0 & -\infty < x < a \\ V_0 & a < x < b \\ 0 & b < x < \infty \end{cases} \tag{1.4}$$

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

$$[Q, P] = \mathrm{i}\hbar I \,, \tag{1.5}$$

$$[H, Q] = -\frac{\mathrm{i}\hbar}{m} P \,, \tag{1.6}$$

$$[H, P] = \mathrm{i}\hbar \frac{\partial V(x)}{\partial x} \,. \tag{1.7}$$

The finite linear combinations of powers of P, Q and H constitute the algebra of the 1D rectangular barrier potential. This algebra will be denoted by $\mathcal{A}$.

The differential operators (1.1)-(1.3) induce three linear operators on the Hilbert space $L^2(\mathbb{R}, \mathrm{d}x)$. We shall denote their Hilbert space domains by $\mathcal{D}(Q)$, $\mathcal{D}(P)$ and $\mathcal{D}(H)$. A major shortcoming of the Hilbert space is that $\mathcal{D}(P)$, $\mathcal{D}(Q)$ and $\mathcal{D}(H)$ do not remain stable under the action of the operators of $\mathcal{A}$, which prevents algebraic operations (e.g., sums, multiplications and commutation relations) of observables from being well defined on the whole Hilbert space. Further, the operators P, Q and H are unbounded, and hence discontinuous, with respect to the topology of the Hilbert space. Mathematically speaking, these are the reasons why we introduce a subdomain $\mathbf{\Phi}$ of the Hilbert space such that:

(*i*) The subdomain $\mathbf{\Phi}$ remains stable under the action of $\mathcal{A}$. This stability makes, in particular, algebraic operations such as the commutation relations (1.5)-(1.7) well defined on $\mathbf{\Phi}$.

(*ii*) The operators of $\mathcal{A}$ are continuous with respect to a properly chosen topology of $\mathbf{\Phi}$.

As we shall see, the space $\mathbf{\Phi}$ is given by the maximal invariant subspace of $\mathcal{A}$.

The spectrum of P, Q and H is respectively $(-\infty, \infty)$, $(-\infty, \infty)$ and $[0, \infty)$. If $\mathrm{Sp}(A)$ denotes the spectrum of the operator A, where A can denote P, Q or H, then with each element a of $\mathrm{Sp}(A)$ we associate a Dirac ket $|a\rangle$ and a Dirac bra $\langle a|$ such that

(*i*) The ket $|a\rangle$ is a right eigenvector of A with eigenvalue a,

$$A|a\rangle = a|a\rangle \,, \tag{1.8}$$

and the bra $\langle a|$ is a left eigenvector of A with eigenvalue a,

$$\langle a|A = a\langle a| \,. \tag{1.9}$$

(*ii*) The kets and bras are δ-normalized,

$$\langle a|a'\rangle = \delta(a - a') \,. \tag{1.10}$$

(*iii*) The kets and bras form a complete basis system that can be used to expand any wave function φ,

$$\varphi = \sum_{\alpha} \int_{\mathrm{Sp}(A)} \mathrm{d}a \, |a\rangle_{\alpha \, \alpha}\langle a|\varphi\rangle \, , \qquad A = P, Q, H \, , \tag{1.11}$$

where the label α accounts for any possible degeneracy of the spectrum.

However, because the spectra of P, Q and H are continuous, the bras and kets are not in the Hilbert space. Indeed, the Dirac kets $|a\rangle$ belong to the *antidual* space of $\mathbf{\Phi}$, which we shall denote by $\mathbf{\Phi}^{\times}$, whereas the Dirac bras $\langle a|$ belong to the *dual* space of $\mathbf{\Phi}$, which we shall denote by $\mathbf{\Phi}'$. Further, the Dirac basis vector expansions (1.11) do not hold for all the elements of $\mathcal{H}$—Eq. (1.11) holds only when φ belongs to $\mathbf{\Phi}$.

We are thus led to two Gel'fand triplets

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^{\times} \tag{1.12}$$

and

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}' \, . \tag{1.13}$$

The space $\mathbf{\Phi}$ contains those square integrable functions that can be considered as physical, since algebraic operations (e.g., the commutation relations of observables) are well defined on $\mathbf{\Phi}$ but not the whole Hilbert space. The space $\mathbf{\Phi}^{\times}$ contains the Dirac kets, that is, $\mathbf{\Phi}^{\times}$ contains the generalized right eigenvectors of the observables of the algebra. The space $\mathbf{\Phi}'$ contains the Dirac bras, that is, $\mathbf{\Phi}'$ contains the generalized left eigenvectors of the observables of the algebra. Furthermore, the expansions (1.11) hold only when φ is in $\mathbf{\Phi}$. Aside from providing us with mathematical concepts such as unitarity, self-adjointness and so on, the Hilbert space $\mathcal{H}$ singles out the scalar product that is used to calculate probability amplitudes.

We recall that the RHS uses distribution theory to give meaning to the eigenvalue equations (1.8) and (1.9). Within the RHS, Eq. (1.8) means that

$$\langle\varphi|A|a\rangle \equiv \langle A^{\dagger}\varphi|a\rangle = a\langle\varphi|a\rangle \, , \qquad \forall\varphi \in \mathbf{\Phi} \, , \tag{1.14}$$

and Eq. (1.9) means that

$$\langle a|A|\varphi\rangle \equiv \langle a|A^{\dagger}\varphi\rangle = a\langle a|\varphi\rangle \, , \qquad \forall\varphi \in \mathbf{\Phi} \, . \tag{1.15}$$

Sometimes, whenever is necessary to make clear that the operator A in Eqs. (1.14) and (1.15) is acting outside the Hilbert space, we shall write these equations as

$$\langle\varphi|A^{\times}|a\rangle = a\langle\varphi|a\rangle \, , \qquad \forall\varphi \in \mathbf{\Phi} \, , \tag{1.16}$$

$$\langle a|A'|\varphi\rangle = a\langle a|\varphi\rangle \, , \qquad \forall\varphi \in \mathbf{\Phi} \, . \tag{1.17}$$

Here, $A^{\times}$ denotes the *antidual* extension of A acting to the right on the elements of $\mathbf{\Phi}^{\times}$, whereas A' denotes the *dual* extension of A acting to the left on the elements of $\mathbf{\Phi}'$. Nevertheless, we shall normally use A to denote both $A^{\times}$ and A' unless there is a risk of confusion.

The "scalar product" $\langle a|a'\rangle = \delta(a-a')$ in Eq. (1.10) should not be interpreted as an actual scalar product of two functionals $\langle a|$ and $|a'\rangle$. The delta function $\langle a|a'\rangle = \delta(a-a')$ appears as the kernel of the functionals $\langle a|$ and $|a'\rangle$ when we write these functionals as integral operators. As well, the delta function $\delta(a-a')$ is the solution to the eigenvalue equation of the operator A in the representation in which A acts as multiplication by a. In general, given two operators A and B, quantities such as $\langle b|a\rangle$ are distributions that are obtained by solving a differential eigenequation in the b-representation:

$$\langle b|A|a\rangle = A\langle b|a\rangle = a\langle b|a\rangle \,. \tag{1.18}$$

The $\langle b|a\rangle$ can also be seen as transition elements from the a- into the b-representation. Similar to the Dirac delta, $\langle b|a\rangle$ appears as the kernel of the functionals $\langle b|$ and $|a\rangle$ when we write these functionals as integral operators:

$$\langle\varphi|a\rangle = \int \mathrm{d}b\, \langle\varphi|b\rangle\langle b|a\rangle \,, \quad \varphi \in \mathbf{\Phi} \,, \tag{1.19}$$

$$\langle\varphi|b\rangle = \int \mathrm{d}a\, \langle\varphi|a\rangle\langle a|b\rangle \,, \quad \varphi \in \mathbf{\Phi} \,. \tag{1.20}$$

In this paper, we shall encounter a few of these "scalar products" such as $\langle x|p\rangle$, $\langle x|x'\rangle$ and $\langle x|E^{\pm}\rangle_{\mathrm{l,r}}$, which will be respectively obtained as the eigensolution to the eigenvalue equation for the operator P, Q and H.

Fourier methods play a central role in any problem that is both linear and shift invariant, and this includes many wave-related phenomena [14]. Hence, Fourier methods are at the foundations of the modeling of, for example, sound and light. As a result, the notions of frequency decomposition and uncertainty principle (that there is a minimum width to the spectrum that is inversely proportional to the localization of the signal) are widely used. Quantum Mechanics also uses Fourier methods. In Quantum Mechanics, the Fourier transform relates the position and the energy representations, it amounts to a decomposition in plane waves, and it entails an uncertainty principle. The difference between classical wave phenomena and Quantum Mechanics is that, in the quantum case, what is "waving" is the probability amplitude. Other than that, the analogy is very close.

In this paper, we shall push this analogy further and see that Dirac's formalism is, in fact, a generalization of Fourier methods: The classical monochromatic plane waves correspond to the Dirac bras and kets; the classical frequency decomposition corresponds to the Dirac basis vector expansions (1.11); the classical uncertainty principle of Fourier Optics corresponds to the quantum uncertainty principle associated with two non-commuting observables. Thus, in a way, Dirac's formalism is to Quantum Mechanics what Fourier methods are to classical wave-related phenomena.

The structure of the paper is the same as that in Refs. [9, 10, 11, 13]: In Sections 2–5, we shall use the Sturm-Liouville theory to obtain the self-adjoint extension of H (in Section 2), the resolvent and the Green function of H (in Section 3), the spectrum of H (in Section 4), and the diagonalizations and eigenfunction expansions associated to H (in Section 5). In Section 6, we shall construct the RHS, the bras, the kets and the

Dirac basis vector expansion of the 1D rectangular barrier. The results of Section 6 will essentially follow from those in Refs. [15, 16, 9]. At the end of Section 6, we shall construct the energy, the momentum and the wave-number representations of the RHS of the 1D rectangular potential. Finally, the conclusions of the paper will be inserted in Section 7. Throughout the paper, we shall recall the well-known results for Q, P and the Fourier transform, in order to show that Dirac's formalism can be viewed as a Fourier-like formalism.

Before proceeding with the main body of the paper, we recall that the RHS is becoming a standard research tool in many areas of theoretical physics, especially in Quantum Mechanics. The RHS is widely used in the quantum theory of scattering and decay (see Refs. [9, 17, 18] and references therein), in the ongoing effort to construct quantum time operators [19], and in the construction of generalized spectral decompositions of chaotic maps [20, 21]. We note, however, that the use some authors make of the RHS differs from ours in many fundamental ways. For example, in Ref. [22], the authors claim that the Hilbert space is "only of pedagogical or historical importance" and therefore, according to A. Bohm *et al.*, only the dual pair $\mathbf{\Phi}$, $\mathbf{\Phi}^{\times}$ should matter (see Ref. [22], page 443). However, from the results of this paper, it should be clear that the RHS is an extension (rather than a replacement) of the Hilbert space, and that the RHS arises when we equip the Hilbert space with distribution theory. In particular, the Hilbert space is at the core of the RHS.

2. Domains of self-adjointness and deficiency indexes

In order to make the paper self-contained, we recall in this section the domains of the Hilbert space $L^2(\mathbb{R}, \mathrm{d}x)$ on which Q, P and H are self-adjoint. In what follows, it will be convenient to distinguish between the formal differential operator (which can act inside and outside the Hilbert space) and the self-adjoint operator (which is defined by the formal differential operator and by the Hilbert space domain on which it acts).

The formal differential operator corresponding to the energy observable will be denoted by h:

$$h \equiv -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\,. \tag{2.1}$$

In order to obtain the domain on which h induces the self-adjoint operator H, we need first some definitions (cf. [23]):

Definition 1. By $AC(\mathbb{R})$ we denote the space of all functions f which are not only continuous but also absolutely continuous over each compact subinterval of $\mathbb{R}$. Thus, f' exists almost everywhere and is integrable over any compact subinterval of $\mathbb{R}$.

By $AC^2(\mathbb{R})$ we denote the space of all functions f which have a continuous derivative in $\mathbb{R}$, and for which f' is not only continuous but also absolutely continuous over each compact subinterval of $\mathbb{R}$. Thus, $f^{(2)}$ exists almost everywhere and is integrable over any compact subinterval of $\mathbb{R}$.

The space $AC(\mathbb{R})$ is the largest space of functions on which the differential operator $-\mathrm{i}\hbar \mathrm{d}/\mathrm{d}x$ can be defined. The space $AC^2(\mathbb{R})$ is the largest space of functions on which the differential operator h can be defined.

Definition 2. We define the spaces

$$\mathcal{H}_h^2(\mathbb{R}) \equiv \{f \in AC^2(\mathbb{R}) \ : \ f, hf \in L^2(\mathbb{R}, \mathrm{d}x)\} \tag{2.2}$$

$$\mathcal{H}^2(\mathbb{R}) \equiv \{f \in AC^2(\mathbb{R}) \ : \ f, f^{(2)} \in L^2(\mathbb{R}, \mathrm{d}x)\} \tag{2.3}$$

$$\mathcal{H}_{\rm min}^2(\mathbb{R}) \equiv \{f \in \mathcal{H}^2(\mathbb{R}) \ : \ f \text{ vanishes outside some compact subset of } \mathbb{R}\} . \tag{2.4}$$

By using these spaces, we can define the necessary operators to obtain the self-adjoint extensions associated to h.

Definition 3. Let h be the formal differential operator (2.1). The operators $H_{\rm min}$ and $H_{\rm max}$ are defined on $L^2(\mathbb{R}, \mathrm{d}x)$ by the formulas

$$\mathcal{D}(H_{\rm min}) = \mathcal{H}_{\rm min}^2(\mathbb{R}), \quad H_{\rm min} f := hf, \quad f \in \mathcal{D}(H_{\rm min}) . \tag{2.5}$$

$$\mathcal{D}(H_{\rm max}) = \mathcal{H}_h^2(\mathbb{R}), \quad H_{\rm max} f := hf, \quad f \in \mathcal{D}(H_{\rm max}) . \tag{2.6}$$

The operators $H_{\rm min}$ and $H_{\rm max}$ are sometimes called the *minimal* and the *maximal* operators associated to the differential operator h, respectively. The domain $\mathcal{D}(H_{\rm max})$ is the largest domain of $L^2(\mathbb{R}, \mathrm{d}x)$ on which the action of h can be defined and remains inside $L^2(\mathbb{R}, \mathrm{d}x)$. Further, $H_{\rm min}^\dagger = H_{\rm max}$.

The self-adjoint extensions we are looking for are operators H such that

$$H_{\rm min} \subset H \subset H_{\rm max} . \tag{2.7}$$

In order to obtain these self-adjoint extensions, we need to calculate the deficiency indexes $n_\pm(H)$, which are the number of linearly independent solutions of the equations

$$H_{\rm min}^\dagger f = \pm \mathrm{i}\lambda f , \quad f \in \mathcal{D}(H_{\rm min}^\dagger) , \tag{2.8}$$

where $\lambda > 0$ has been introduced on dimensional grounds. It is straightforward to see that the only solution of Eq. (2.8) that belongs to $\mathcal{D}(H_{\rm min}^\dagger)$ is the zero solution, that is, $n_\pm(H) = 0$. Thus, the only domain $\mathcal{D}(H)$ of $L^2(\mathbb{R}, \mathrm{d}x)$ on which h induces a self-adjoint operator coincides with the maximal domain:

$$\mathcal{D}(H) = \left\{ f \in L^2(\mathbb{R}, \mathrm{d}x) \ : \ f \in AC^2(\mathbb{R}, \mathrm{d}x), \ hf \in L^2(\mathbb{R}, \mathrm{d}x) \right\} . \tag{2.9}$$

By similar arguments, it can be shown that the only domain on which the multiplication operator induces a self-adjoint operator is given by

$$\mathcal{D}(Q) = \left\{ f \in L^2(\mathbb{R}, \mathrm{d}x) \ : xf \in L^2(\mathbb{R}, \mathrm{d}x) \right\} , \tag{2.10}$$

and that the only domain on which the differential operator $-\mathrm{i}\hbar \mathrm{d}/\mathrm{d}x$ induces a self-adjoint operator is given by

$$\mathcal{D}(P) = \left\{ f \in L^2(\mathbb{R}, \mathrm{d}x) \ : \ f \in AC(\mathbb{R}, \mathrm{d}x), \ f' \in L^2(\mathbb{R}, \mathrm{d}x) \right\} . \tag{2.11}$$

3. The resolvent operator and the Green function

In this section, we obtain the resolvent and the Green function of H, which can be easily calculated by way of the following theorem (cf. Theorem XIII.3.16 of Ref. [23]):

Theorem 1. *Let H be the self-adjoint Hamiltonian operator derived from the real formal differential operator (2.1) and the domain (2.9). Let $\mathrm{Im}(E) \neq 0$. Then there is exactly one solution $\chi_{\rm r}(x;E)$ of $(h-E)\sigma = 0$ square integrable at $-\infty$, and exactly one solution $\chi_{\rm l}(x;E)$ of $(h-E)\sigma = 0$ square-integrable at $+\infty$. The resolvent $(E-H)^{-1}$ is an integral operator whose kernel $G(x,x';E)$ is given by*

$$G(x,x';E) = \left\{ \begin{array}{ll} \frac{2m}{\hbar^2} \frac{\chi_{\rm r}(x;E)\,\chi_{\rm l}(x';E)}{W(\chi_{\rm r},\chi_{\rm l})} & x<x' \\ \frac{2m}{\hbar^2} \frac{\chi_{\rm r}(x';E)\,\chi_{\rm l}(x;E)}{W(\chi_{\rm r},\chi_{\rm l})} & x>x' \, , \end{array} \right. \tag{3.1}$$

where $W(\chi_{\rm r},\chi_{\rm l})$ is the Wronskian of $\chi_{\rm r}$ and $\chi_{\rm l}$:

$$W(\chi_{\rm r},\chi_{\rm l}) = \chi_{\rm r}\chi_{\rm l}' - \chi_{\rm r}'\chi_{\rm l} \, . \tag{3.2}$$

To obtain $G(x,x';E)$, we divide the complex E-plane in three regions (left half-plane, first quadrant, and fourth quadrant) and apply Theorem 1 to each of these regions separately. In our calculations, we shall use the following branch of the square root function:

$$\sqrt{\cdot} : \{E \in \mathbb{C} \, : \, -\pi < \arg(E) \leq \pi\} \longmapsto \{E \in \mathbb{C} \, : \, -\pi/2 < \arg(E) \leq \pi/2\} \, . \tag{3.3}$$

This branch is chosen because it grants the following relation:

$$\overline{\sqrt{\overline{z}}} = z \, , \quad z \in \mathbb{C} \, . \tag{3.4}$$

It is important to keep in mind that $\chi_{\rm r}(x;E)$ and $\chi_{\rm l}(x;E)$ of Theorem 1 are well defined for real as well as for complex energies. More precisely, the functions $\chi_{\rm r}(x;E)$ and $\chi_{\rm l}(x;E)$, which are derived for complex E of nonzero imaginary part, have a well-defined limiting value when E approaches the real line. The values of $\chi_{\rm r}(x;E)$ and $\chi_{\rm l}(x;E)$ for complex E will be used in this section to calculate $G(x,x';E)$. The values of $\chi_{\rm r}(x;E)$ and $\chi_{\rm l}(x;E)$ for real E will be used in Sec. 6 to construct the bras and kets associated to the energies in the spectrum of the Hamiltonian.

3.1. Left half-plane: $\mathrm{Re}(E) < 0$, $\mathrm{Im}(E) \neq 0$

According Theorem 1, we need to obtain the eigensolutions $\widetilde{\chi}_{\rm r}$ and $\widetilde{\chi}_{\rm l}$ of the Schrödinger equation

$$\left(-\frac{\hbar^2}{2m}\frac{{\rm d}^2}{{\rm d}x^2} + V(x) \right) \sigma(x;E) = E\sigma(x;E) \tag{3.5}$$

that are square integrable at $-\infty$ and at ∞, respectively. Thus, the eigensolution $\widetilde{\chi}_{\rm r}(x;E)$ satisfies

$$\widetilde{\chi}_{\rm r}(x;E) \in AC^2(\mathbb{R}) \, , \tag{3.6a}$$

$$\widetilde{\chi}_{\rm r}(x;E) \text{ is square integrable at } -\infty \, , \tag{3.6b}$$

whereas the eigensolution $\widetilde{\chi}_{\rm l}(x;E)$ satisfies

$$\widetilde{\chi}_{\rm l}(x;E) \in AC^2(\mathbb{R})\,, \tag{3.7a}$$

$$\widetilde{\chi}_{\rm l}(x;E) \text{ is square integrable at } +\infty\,. \tag{3.7b}$$

Solving Eq. (3.5) subjected to (3.6a)-(3.6b) yields

$$\widetilde{\chi}_{\rm r}(x;E) = \left(\frac{m}{2\pi\widetilde{k}\hbar^2}\right)^{1/2} \times \left\{ \begin{array}{ll} \widetilde{T}(\widetilde{k}){\rm e}^{\widetilde{k}x} & -\infty < x < a \\ \widetilde{A}_{\rm r}(\widetilde{k}){\rm e}^{-\widetilde{Q}x} + \widetilde{B}_{\rm r}(\widetilde{k}){\rm e}^{\widetilde{Q}x} & a < x < b \\ \widetilde{R}_{\rm r}(\widetilde{k}){\rm e}^{-\widetilde{k}x} + {\rm e}^{\widetilde{k}x} & b < x < \infty\,, \end{array} \right. \tag{3.8}$$

where

$$\widetilde{k} = \sqrt{-\frac{2m}{\hbar^2}E}\,, \quad \widetilde{Q} = \sqrt{-\frac{2m}{\hbar^2}(E-V_0)}\,, \tag{3.9}$$

where the coefficients $\widetilde{T}(\widetilde{k})$, $\widetilde{A}_{\rm r}(\widetilde{k})$, $\widetilde{B}_{\rm r}(\widetilde{k})$ and $\widetilde{R}_{\rm r}(\widetilde{k})$ can be found in Appendix A, and where $\left(\frac{m}{2\pi\widetilde{k}\hbar^2}\right)^{1/2}$ is a normalization factor.

Solving Eq. (3.5) subjected to (3.7a)-(3.7b) yields

$$\widetilde{\chi}_{\rm l}(x;E) = \left(\frac{m}{2\pi\widetilde{k}\hbar^2}\right)^{1/2} \times \left\{ \begin{array}{ll} {\rm e}^{-\widetilde{k}x} + \widetilde{R}_{\rm l}(\widetilde{k}){\rm e}^{\widetilde{k}x} & -\infty < x < a \\ \widetilde{A}_{\rm l}(\widetilde{k}){\rm e}^{-\widetilde{Q}x} + \widetilde{B}_{\rm l}(\widetilde{k}){\rm e}^{\widetilde{Q}x} & a < x < b \\ \widetilde{T}(\widetilde{k}){\rm e}^{-\widetilde{k}x} & b < x < \infty\,, \end{array} \right. \tag{3.10}$$

where the coefficients $\widetilde{R}_{\rm l}(\widetilde{k})$, $\widetilde{A}_{\rm l}(\widetilde{k})$, $\widetilde{B}_{\rm l}(\widetilde{k})$ and $\widetilde{T}(\widetilde{k})$ can be found in Appendix A.

The Wronskian of $\widetilde{\chi}_{\rm r}$ and $\widetilde{\chi}_{\rm l}$ is given by

$$W(\widetilde{\chi}_{\rm r},\widetilde{\chi}_{\rm l}) = -\frac{m}{\pi\hbar^2}\,\widetilde{T}(\widetilde{k})\,. \tag{3.11}$$

From Eqs. (3.1), (3.8), (3.10) and (3.11), it follows that, when E belongs to the left half-plane, the expression of the Green function reads as

$$G(x,x';E) = \left\{ \begin{array}{ll} -2\pi\,\frac{\widetilde{\chi}_{\rm r}(x;E)\,\widetilde{\chi}_{\rm l}(x';E)}{\widetilde{T}(E)} & x < x' \\ -2\pi\,\frac{\widetilde{\chi}_{\rm r}(x';E)\,\widetilde{\chi}_{\rm l}(x;E)}{\widetilde{T}(E)} & x > x' \end{array} \right. \quad {\rm Re}(E) < 0\,,\ {\rm Im}(E) \neq 0\,. \tag{3.12}$$

3.2. First quadrant: Re$(E) > 0$, Im$(E) > 0$

When E belongs to the first quadrant, the eigensolution $\chi_{\rm r}^+$ that satisfies Eq. (3.5) subjected to the boundary conditions (3.6a)-(3.6b) is given by

$$\chi_{\rm r}^+(x;E) = \left(\frac{m}{2\pi k\hbar^2}\right)^{1/2} \times \left\{ \begin{array}{ll} T(k){\rm e}^{-{\rm i}kx} & -\infty < x < a \\ A_{\rm r}(k){\rm e}^{{\rm i}Qx} + B_{\rm r}(k){\rm e}^{-{\rm i}Qx} & a < x < b \\ R_{\rm r}(k){\rm e}^{{\rm i}kx} + {\rm e}^{-{\rm i}kx} & b < x < \infty\,, \end{array} \right. \tag{3.13}$$

where

$$k = \sqrt{\frac{2m}{\hbar^2}E}\,, \quad Q = \sqrt{\frac{2m}{\hbar^2}(E-V_0)}\,, \tag{3.14}$$

where the coefficients $T(k)$, $A_{\rm r}(k)$, $B_{\rm r}(k)$ and $R_{\rm r}(k)$ can be found in Appendix A, and where $\left(\frac{m}{2\pi k\hbar^2}\right)^{1/2}$ is a normalization factor. We recall that $\chi_{\rm r}^+(x;E)$ corresponds to a plane wave that impinges the barrier from the right (hence the subscript r) and gets reflected to the right with probability amplitude $R_{\rm r}(k)$ and transmitted to the left with probability amplitude $T(k)$.

The eigensolution of (3.5) subjected to (3.7a)-(3.7b) is

$$\chi_{\rm l}^{+}(x;E)=\left(\frac{m}{2\pi k\hbar^2}\right)^{1/2}\times\begin{cases} {\rm e}^{{\rm i}kx}+R_{\rm l}(k){\rm e}^{-{\rm i}kx} & -\infty<x<a \\ A_{\rm l}(k){\rm e}^{{\rm i}Qx}+B_{\rm l}(k){\rm e}^{-{\rm i}Qx} & a<x<b \\ T(k){\rm e}^{{\rm i}kx} & b<x<\infty\,, \end{cases} \tag{3.15}$$

where the coefficients $R_{\rm l}(k)$, $A_{\rm l}(k)$, $B_{\rm l}(k)$ and $T(k)$ can be found in Appendix A. We recall that $\chi_{\rm l}^{+}(x;E)$ corresponds to a plane wave that impinges the barrier from the left (hence the subscript l) and gets reflected to the left with probability amplitude $R_{\rm l}(k)$ and transmitted to the right with probability amplitude $T(k)$.

The Wronskian of $\chi_{\rm r}^{+}$ and $\chi_{\rm l}^{+}$ is given by

$$W(\chi_{\rm r}^{+},\chi_{\rm l}^{+})=\frac{{\rm i}m}{\pi\hbar^2}\,T(k)\,. \tag{3.16}$$

Thus, when E belongs to the first quadrant, the expression of the Green function is given by

$$G(x,x';E)=\begin{cases} \frac{2\pi}{\rm i}\,\frac{\chi_{\rm r}^{+}(x;E)\,\chi_{\rm l}^{+}(x';E)}{T(k)} & x<x' \\ \frac{2\pi}{\rm i}\,\frac{\chi_{\rm r}^{+}(x';E)\,\chi_{\rm l}^{+}(x;E)}{T(k)} & x>x' \end{cases} \qquad {\rm Re}(E)>0\,,\ {\rm Im}(E)>0\,. \tag{3.17}$$

3.3. Fourth quadrant: ${\rm Re}(E)>0$, ${\rm Im}(E)<0$

When E belongs to the fourth quadrant, the eigensolution $\chi_{\rm r}^{-}$ that satisfies Eq. (3.5) subjected to the boundary conditions (3.6a)-(3.6b) is given by

$$\chi_{\rm r}^{-}(x;E)=\left(\frac{m}{2\pi k\hbar^2}\right)^{1/2}\times\begin{cases} T^{*}(k){\rm e}^{{\rm i}kx} & -\infty<x<a \\ A_{\rm r}^{*}(k){\rm e}^{-{\rm i}Qx}+B_{\rm r}^{*}(k){\rm e}^{{\rm i}Qx} & a<x<b \\ R_{\rm r}^{*}(k){\rm e}^{-{\rm i}kx}+{\rm e}^{{\rm i}kx} & b<x<\infty\,, \end{cases} \tag{3.18}$$

where the coefficients $T^{*}(k)$, $A_{\rm r}^{*}(k)$, $B_{\rm r}^{*}(k)$ and $R_{\rm r}^{*}(k)$ can be found in Appendix A. This eigensolution corresponds to two plane waves—one impinging the barrier from the left with probability amplitude $T^{*}(k)$ and another impinging 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.

The eigensolution of (3.5) subjected to (3.7a)-(3.7b) reads as

$$\chi_{\rm l}^{-}(x;E)=\left(\frac{m}{2\pi k\hbar^2}\right)^{1/2}\times\begin{cases} {\rm e}^{-{\rm i}kx}+R_{\rm l}^{*}(k){\rm e}^{{\rm i}kx} & -\infty<x<a \\ A_{\rm l}^{*}(k){\rm e}^{-{\rm i}Qx}+B_{\rm l}^{*}(k){\rm e}^{{\rm i}Qx} & a<x<b \\ T^{*}(k){\rm e}^{-{\rm i}kx} & b<x<\infty\,, \end{cases} \tag{3.19}$$

where the functions $R_{\rm l}^{*}(k)$, $A_{\rm l}^{*}(k)$, $B_{\rm l}^{*}(k)$ and $T^{*}(k)$ can be found in Appendix A. This eigensolution corresponds to two plane waves—one impinging the barrier from left with probability amplitude $R_{\rm l}^{*}(k)$ and another impinging 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. Clearly, both $\chi_{\rm r}^-(x;E)$ and $\chi_{\rm l}^-(x;E)$ correspond to the *final* condition of an outgoing plane wave propagating respectively to the right and to the left, as opposed to $\chi_{\rm r}^+(x;E)$ and $\chi_{\rm l}^+(x;E)$, which correspond to the *initial* condition of a plane wave that impinges the barrier respectively from the left and from the right.

The Wronskian of $\chi_{\rm r}^-$ and $\chi_{\rm l}^-$ is given by

$$W(\chi_{\rm r}^-,\chi_{\rm l}^-) = -\frac{{\rm i}m}{\pi\hbar^2}\, T^*(k)\,. \tag{3.20}$$

Thus, when E belongs to the fourth quadrant, the expression of the Green function is given by

$$G(x,x';E) = \left\{ \begin{array}{ll} -\frac{2\pi}{\rm i}\,\frac{\chi_{\rm r}^-(x;E)\,\chi_{\rm l}^-(x';E)}{T^*(k)} & x<x' \\ -\frac{2\pi}{\rm i}\,\frac{\chi_{\rm r}^-(x';E)\,\chi_{\rm l}^-(x;E)}{T^*(k)} & x>x' \end{array} \right. \qquad {\rm Re}(E)>0\,,\ {\rm Im}(E)<0\,. \tag{3.21}$$

To finish this section, we recall the resolvents of Q and P, which are well known and can be calculated by similar arguments. The resolvent of Q is an integral operator whose kernel is

$$\langle x|\frac{1}{z-Q}|x'\rangle = \frac{1}{z-x}\delta(x-x')\,, \quad z\in\mathbb{C}/\mathbb{R}\,,\ x,x'\in\mathbb{R}\,. \tag{3.22}$$

In the upper complex p-plane, the kernel of the resolvent of P is given by [23]

$$\langle x|\frac{1}{p-P}|x'\rangle = \left\{ \begin{array}{ll} 0 & x<x' \\ \frac{1}{{\rm i}\hbar}\,{\rm e}^{{\rm i}p(x-x')/\hbar} & x>x' \end{array} \right. \qquad {\rm Im}(p)>0\,, \tag{3.23}$$

whereas in the lower complex p-plane it is given by [23]

$$\langle x|\frac{1}{p-P}|x'\rangle = \left\{ \begin{array}{ll} -\frac{1}{{\rm i}\hbar}\,{\rm e}^{{\rm i}p(x-x')/\hbar} & x<x' \\ 0 & x>x' \end{array} \right. \qquad {\rm Im}(p)<0\,. \tag{3.24}$$

4. Spectrum

In this section, we obtain the spectrum of H, which we shall denote by ${\rm Sp}(H)$. In order to obtain ${\rm Sp}(H)$, we shall apply Theorem 3 below. Before stating Theorem 3, we need to state Theorem 2, which provides the unitary operators that diagonalize H (cf. Theorem XIII.5.13 of Ref. [23]):

Theorem 2. *(Weyl-Kodaira) Let h be the formally self-adjoint differential operator (2.1). Let H be the corresponding self-adjoint Hamiltonian. Let Λ be an open interval of the real axis, and suppose that there is given a set $\{\sigma_1(x;E),\, \sigma_2(x;E)\}$ of functions, defined and continuous on $\mathbb{R}\times\Lambda$, such that for each fixed E in Λ, $\{\sigma_1(x;E),\, \sigma_2(x;E)\}$ forms a basis for the space of solutions of $h\sigma=E\sigma$. Then there exists a positive 2×2 matrix measure $\{\varrho_{ij}\}$ defined on Λ, such that the limit*

$$(Uf)_i(E) = \lim_{c\to 0}\lim_{d\to\infty}\left[\int_c^d f(x)\overline{\sigma_i(x;E)}{\rm d}x\right] \tag{4.1}$$

exists in the topology of $L^2(\Lambda,\{\varrho_{ij}\})$ for each f in $L^2(\mathbb{R},{\rm d}x)$ and defines an isometric isomorphism U of $\mathsf{E}(\Lambda)L^2(\mathbb{R},{\rm d}x)$ onto $L^2(\Lambda,\{\varrho_{ij}\})$, where $\mathsf{E}(\Lambda)$ is the spectral projection associated with Λ.

The spectral measures $\{\rho_{ij}\}$ are provided by the following theorem (cf. Theorem XIII.5.18 of Ref. [23]):

Theorem 3. *(Titchmarsh-Kodaira) Let Λ be an open interval of the real axis and O be an open set in the complex plane containing Λ. Let $\mathrm{re}(H)$ be the resolvent set of H. Let $\{\sigma_1(x;E),\, \sigma_2(x;E)\}$ be a set of functions which form a basis for the solutions of the equation $h\sigma = E\sigma$, $E \in O$, and which are continuous on $\mathbb{R}\times O$ and analytically dependent on E for E in O. Suppose that the kernel $G(x,x';E)$ for the resolvent $(E-H)^{-1}$ has a representation*

$$G(x,x';E) = \left\{ \begin{array}{ll} \sum_{i,j=1}^2 \theta_{ij}^-(E)\sigma_i(x;E)\overline{\sigma_j(x';\overline{E})}\, , & x<x'\, , \\ \sum_{i,j=1}^2 \theta_{ij}^+(E)\sigma_i(x;E)\overline{\sigma_j(x';\overline{E})}\, , & x>x'\, , \end{array} \right. \tag{4.2}$$

for all E in $\mathrm{re}(H)\cap O$, and that $\{\varrho_{ij}\}$ is a positive matrix measure on Λ associated with H as in Theorem 2. Then the functions $\theta_{ij}^{\pm}$ are analytic in $\mathrm{re}(H)\cap O$, and given any bounded open interval $(E_1,E_2)\subset\Lambda$, we have for $1\le i,j\le 2$,

$$\begin{array}{rcl} \varrho_{ij}((E_1,E_2)) & = & \lim_{\delta\to 0}\lim_{\varepsilon\to 0+}\frac{1}{2\pi \mathrm{i}}\int_{E_1+\delta}^{E_2-\delta}[\theta_{ij}^-(E-\mathrm{i}\varepsilon)-\theta_{ij}^-(E+\mathrm{i}\varepsilon)]\mathrm{d}E \\ & = & \lim_{\delta\to 0}\lim_{\varepsilon\to 0+}\frac{1}{2\pi \mathrm{i}}\int_{E_1+\delta}^{E_2-\delta}[\theta_{ij}^+(E-\mathrm{i}\varepsilon)-\theta_{ij}^+(E+\mathrm{i}\varepsilon)]\mathrm{d}E\, . \end{array} \tag{4.3}$$

From Eq. (4.3), it is clear that in order to obtain $\mathrm{Sp}(H)$ and ϱ_{ij}, we need to see on what real E's the functions $\theta_{ij}^{\pm}(E)$ fail to be analytic. We shall do so by taking Λ in Theorem 3 to be $(-\infty,0)$ and $(0,\infty)$.

4.1. Negative Energy Real Line: $\Lambda=(-\infty,0)$

On the negative real line, we choose the basis $\{\sigma_1,\sigma_2\}$ of Theorem 3 as

$$\sigma_1(x;E) = \widetilde{\chi}_{\mathrm{l}}(x;E)\, , \tag{4.4a}$$

$$\sigma_2(x;E) = \widetilde{\chi}_{\mathrm{r}}(x;E)\, . \tag{4.4b}$$

From Eqs. (3.4) and (3.10) it follows that

$$\overline{\widetilde{\chi}_l(x';\overline{E})} = \widetilde{\chi}_l(x';E)\, . \tag{4.5}$$

Now, by taking advantage of Eqs. (4.4a), (4.4b) and (4.5), we write Eq. (3.12) as

$$G(x,x';E) = -2\pi\,\frac{\sigma_2(x;E)\overline{\sigma_1(x';\overline{E})}}{\widetilde{T}(E)}\, , \quad x<x'\, ,\ \mathrm{Re}(E)<0\, , \mathrm{Im}(E)\neq 0\, . \tag{4.6}$$

By comparing Eqs. (4.2) and (4.6) we see that

$$\theta_{ij}^-(E) = \left(\begin{array}{cc} 0 & 0 \\ -\frac{2\pi}{\widetilde{T}(E)} & 0 \end{array} \right)\, , \quad \mathrm{Re}(E)<0\, ,\ \mathrm{Im}(E)\neq 0\, . \tag{4.7}$$

The functions $\theta_{ij}^-(E)$ are analytic in a neighborhood of $\Lambda=(-\infty,0)$ except at the energies for which $\widetilde{T}(E)$ vanishes. Because for the potential (1.4) the function

$$\widetilde{T}(\widetilde{k}) = \widetilde{T}(-\mathrm{i}k) = T(k) \tag{4.8}$$

does not vanish on the positive k-imaginary axis (i.e., on the negative real axis), the segment $(-\infty, 0)$ belongs to the resolvent of H.

We note in passing that if there had been bound states, the basis (4.4a) and (4.4b) would not had been analytic, and we would have had to multiply $\widetilde{\chi}_{\mathrm{l,r}}$ by the denominator of $\widetilde{T}$ in order to have an analytic basis.

4.2. Positive Energy Real Line: $\Lambda = (0, \infty)$

On the positive real line, we choose the basis $\{\sigma_1, \sigma_2\}$ of Theorem 3 as

$$\sigma_1(x;E) = \chi_{\mathrm{l}}^{+}(x;E)\,, \tag{4.9a}$$

$$\sigma_2(x;E) = \chi_{\mathrm{r}}^{+}(x;E)\,. \tag{4.9b}$$

It is easy to see that Eqs. (3.4), (3.13), (3.15), (3.18) and (3.19) imply that

$$\overline{\chi_{\mathrm{l}}^{+}(x;\overline{E})} = \chi_{\mathrm{l}}^{-}(x;E)\,, \tag{4.10a}$$

$$\overline{\chi_{\mathrm{r}}^{+}(x;\overline{E})} = \chi_{\mathrm{r}}^{-}(x;E)\,. \tag{4.10b}$$

Then, Eqs. (3.13), (3.19) and (4.9a)-(4.10b) lead to

$$\chi_{\mathrm{r}}^{+}(x';E) = T(E)\overline{\sigma_1(x';\overline{E})} - \frac{T(E)R_{\mathrm{l}}^{*}(E)}{T^{*}(E)}\overline{\sigma_2(x';\overline{E})}\,, \tag{4.11a}$$

$$\chi_{\mathrm{l}}^{-}(x;E) = -\frac{T^{*}(E)R_{\mathrm{r}}(E)}{T(E)}\sigma_1(x;E) + T^{*}(E)\sigma_2(x;E)\,, \tag{4.11b}$$

After substituting Eq. (4.11a) into Eq. (3.17) and after some calculations, we get to

$$G(x,x';E) = \frac{2\pi}{\mathrm{i}}\left[\sigma_1(x;E)\overline{\sigma_1(x';\overline{E})} - \frac{R_{\mathrm{l}}^{*}(E)}{T^{*}(E)}\sigma_1(x;E)\overline{\sigma_2(x';\overline{E})}\right]\,,$$
$$\mathrm{Re}(E)>0, \mathrm{Im}(E)>0\,,\ x>x'\,. \tag{4.12}$$

After substituting Eq. (4.11b) into Eq. (3.21) and after some calculations, we get to

$$G(x,x';E) = \frac{2\pi}{\mathrm{i}}\left[\frac{R_{\mathrm{r}}(E)}{T(E)}\sigma_1(x;E)\overline{\sigma_2(x';\overline{E})} - \sigma_2(x;E)\overline{\sigma_2(x';\overline{E})}\right]\,,$$
$$\mathrm{Re}(E)>0, \mathrm{Im}(E)<0\,,\ x>x'\,. \tag{4.13}$$

By comparing (4.2) to (4.12) we obtain

$$\theta_{ij}^{+}(E) = \begin{pmatrix} \frac{2\pi}{\mathrm{i}} & -\frac{2\pi}{\mathrm{i}}\frac{R_{\mathrm{l}}^{*}(E)}{T^{*}(E)} \\ 0 & 0 \end{pmatrix}, \quad \mathrm{Re}(E)>0\,,\ \mathrm{Im}(E)>0\,. \tag{4.14}$$

By comparing (4.2) to (4.13) we obtain

$$\theta_{ij}^{+}(E) = \begin{pmatrix} 0 & \frac{2\pi}{\mathrm{i}}\frac{R_{\mathrm{r}}(E)}{T(E)} \\ 0 & -\frac{2\pi}{\mathrm{i}} \end{pmatrix}, \quad \mathrm{Re}(E)>0\,,\ \mathrm{Im}(E)<0\,. \tag{4.15}$$

Substitution of Eqs. (4.14) and (4.15) into Eq. (4.3) yield the spectral measures ϱ_{ij} of Theorem 3. The measure ϱ_{21} is clearly zero. So is the measure ϱ_{12}, since

$$\varrho_{12}((E_1,E_2)) = \lim_{\delta\to 0}\lim_{\varepsilon\to 0+}\frac{1}{2\pi\mathrm{i}}\int_{E_1+\delta}^{E_2-\delta}\left[\theta_{12}^{+}(E-\mathrm{i}\varepsilon) - \theta_{12}^{+}(E+\mathrm{i}\varepsilon)\right]\mathrm{d}E$$

$$= \int_{E_1}^{E_2} - \left(\frac{R_{\rm r}(E)}{T(E)} + \frac{R_{\rm l}^*(E)}{T^*(E)} \right) {\rm d}E$$
$$= 0 \, , \tag{4.16}$$

where in the last step we have used the relation

$$R_{\rm r}(E)T^*(E) + T(E)R_{\rm l}^*(E) = 0 \, . \tag{4.17}$$

The measures ϱ_{11} and ϱ_{22} are just the Lebesgue measure, since

$$\varrho_{11}((E_1,E_2)) = \lim_{\delta\to 0}\lim_{\varepsilon\to 0+} \frac{1}{2\pi{\rm i}} \int_{E_1+\delta}^{E_2-\delta} \left[\theta_{11}^+(E-{\rm i}\varepsilon) - \theta_{11}^+(E+{\rm i}\varepsilon) \right] {\rm d}E$$
$$= \int_{E_1}^{E_2} {\rm d}E = E_2 - E_1 \, , \tag{4.18}$$

and

$$\varrho_{22}((E_1,E_2)) = \lim_{\delta\to 0}\lim_{\varepsilon\to 0+} \frac{1}{2\pi{\rm i}} \int_{E_1+\delta}^{E_2-\delta} \left[\theta_{22}^+(E-{\rm i}\varepsilon) - \theta_{22}^+(E+{\rm i}\varepsilon) \right] {\rm d}E$$
$$= \int_{E_1}^{E_2} {\rm d}E = E_2 - E_1 \, . \tag{4.19}$$

Clearly, the functions $\theta_{11}^+(E)$ and $\theta_{22}^+(E)$ both have a branch cut along $(0,\infty)$, and therefore $(0,\infty)$ is included in ${\rm Sp}(H)$. Since ${\rm Sp}(H)$ is a closed set, it must hold that

$${\rm Sp}(H) = [0,\infty) \, . \tag{4.20}$$

We note that, instead of the "initial" basis (4.9*a*)-(4.9*b*), we could use the "final" basis:

$$\sigma_1(x;E) = \chi_{\rm l}^-(x;E) \, , \tag{4.21a}$$
$$\sigma_2(x;E) = \chi_{\rm r}^-(x;E) \, . \tag{4.21b}$$

This basis produces the same spectrum (as it should be) and the same spectral measures (cf. Appendix B).

To finish this section, we recall that the spectra of the position and momentum observables coincide with the full real line:

$${\rm Sp}(Q) = {\rm Sp}(P) = (-\infty,\infty) \, . \tag{4.22}$$

The spectra of Q and P are simple, whereas the spectrum of H is doubly degenerate. Indeed, to each energy $E \in [0,\infty)$ there correspond two linearly independent eigenfunctions, $\chi_{\rm l}^+$ and $\chi_{\rm r}^+$ (or, equivalently, $\chi_{\rm l}^-$ and $\chi_{\rm r}^-$).

5. Diagonalization and eigenfunction expansion

Theorem 2 of Sec. 4 provides the means to construct two unitary operators $U_\pm$ that diagonalize H. The operator U_+ is associated with the basis $\{\chi_{\rm l}^+, \chi_{\rm r}^+\}$, whereas U_- is associated with $\{\chi_{\rm l}^-, \chi_{\rm r}^-\}$. These unitary operators transform from the position into the energy representation, and they induce two eigenfunction expansions and two direct integral decompositions of the Hilbert space.

For the sake of brevity, we shall present each calculation associated with U_+ together with the corresponding calculation associated with U_-.

By Theorem 2, the mappings $U_\pm$ are given by

$$\begin{array}{rcl} U_\pm : L^2(\mathbb{R}, \mathrm{d}x) & \longmapsto & L^2([0,\infty), \mathrm{d}E) \oplus L^2([0,\infty), \mathrm{d}E) \\ f(x) & \longmapsto & \widehat{f}^\pm(E) \equiv U_\pm f(E) \equiv [(U_\pm f)_{\mathrm{l}}(E), (U_\pm f)_{\mathrm{r}}(E)] \, , \end{array} \tag{5.1}$$

where

$$\widehat{f}_{\mathrm{l}}^\pm(E) \equiv (U_\pm f)_{\mathrm{l}}(E) = \int_{-\infty}^{\infty} \mathrm{d}x \, f(x) \overline{\chi_{\mathrm{l}}^\pm(x;E)} \, , \tag{5.2}$$

$$\widehat{f}_{\mathrm{r}}^\pm(E) \equiv (U_\pm f)_{\mathrm{r}}(E) = \int_{-\infty}^{\infty} \mathrm{d}x \, f(x) \overline{\chi_{\mathrm{r}}^\pm(x;E)} \, . \tag{5.3}$$

Note that $\widehat{f}^\pm(E) \equiv U_\pm f(E)$ are two-component vectors, because the spectrum of H is doubly degenerate.

The inverses of $U_\pm$ can be obtained from the following theorem (cf. Theorem XIII.5.14 of Ref. [23]):

Theorem 4. *(Weyl-Kodaira) Let H, Λ, $\{\varrho_{ij}\}$, etc., be as in Theorem 2. Let E_0 and E_1 be the end points of Λ. Then the inverse of the isometric isomorphism U of $\mathsf{E}(\Lambda) L^2(\mathbb{R}, \mathrm{d}x)$ onto $L^2(\Lambda, \{\varrho_{ij}\})$ is given by the formula*

$$(U^{-1}F)(x) = \lim_{\mu_0 \to E_0} \lim_{\mu_1 \to E_1} \int_{\mu_0}^{\mu_1} \left(\sum_{i,j=1}^{2} F_i(E) \sigma_j(x;E) \varrho_{ij}(\mathrm{d}E) \right) \tag{5.4}$$

where $F = [F_1, F_2] \in L^2(\Lambda, \{\varrho_{ij}\})$, the limit existing in the topology of $L^2(\mathbb{R}, \mathrm{d}x)$.

By Theorem 4, the inverses of $U_\pm$ are given by

$$f(x) = (U_\pm^{-1} \widehat{f})(x) = \int_0^\infty \mathrm{d}E \, \widehat{f}_{\mathrm{l}}^\pm(E) \chi_{\mathrm{l}}^\pm(x;E) + \int_0^\infty \mathrm{d}E \, \widehat{f}_{\mathrm{r}}^\pm(E) \chi_{\mathrm{r}}^\pm(x;E) \, , \tag{5.5}$$

where

$$\widehat{f}_{\mathrm{l}}^\pm(E), \; \widehat{f}_{\mathrm{r}}^\pm(E) \in L^2([0,\infty), \mathrm{d}E) \, . \tag{5.6}$$

The operators $U_\pm^{-1}$ transform from $L^2([0,\infty), \mathrm{d}E) \oplus L^2([0,\infty), \mathrm{d}E)$ onto $L^2(\mathbb{R}, \mathrm{d}x)$. Note that Eq. (5.5) can also be seen as the eigenfunction expansions of any element $f(x)$ of $L^2(\mathbb{R}, \mathrm{d}x)$ in terms of the basis $\{\chi_{\mathrm{l}}^\pm, \chi_{\mathrm{r}}^\pm\}$. Similarly, we can write the two-component vectors $U_\pm f$, Eq. (5.1), as

$$\widehat{f}^\pm(E) \equiv \int_{-\infty}^{\infty} \mathrm{d}x \, f(x) \overline{\chi_{\mathrm{l}}^\pm(x;E)} \dotplus \int_{-\infty}^{\infty} \mathrm{d}x \, f(x) \overline{\chi_{\mathrm{r}}^\pm(x;E)} \, , \tag{5.7}$$

which provide the eigenfunction expansions of any element $\widehat{f}^\pm(E)$ of $L^2([0,\infty), \mathrm{d}E) \oplus L^2([0,\infty), \mathrm{d}E)$ in terms of $\{\chi_{\mathrm{l}}^\pm, \chi_{\mathrm{r}}^\pm\}$. (The symbol $\dotplus$ in Eq. (5.7) intends to mean that, from a mathematical point of view, this equation should be seen as a two-component vector equality rather than as an actual sum.)

A straightforward calculation shows that

$$\widehat{H} \widehat{f}^\pm(E) = U_\pm H U_\pm^{-1} \widehat{f}^\pm(E) = E \widehat{f}^\pm(E) \equiv [E \widehat{f}_{\mathrm{l}}^\pm(E), E \widehat{f}_{\mathrm{r}}^\pm(E)] \, , \quad f \in \mathcal{D}(H) \, . \tag{5.8}$$

The direct integral decompositions of the Hilbert space induced by $U_\pm$ read as

$$\begin{array}{rcl} U_\pm : \mathcal{H} & \longmapsto & \widehat{\mathcal{H}} = \int_0^\infty \widehat{\mathcal{H}}_{\rm l}(E)\mathrm{d}E \oplus \int_0^\infty \widehat{\mathcal{H}}_{\rm r}(E)\mathrm{d}E \\ f & \longmapsto & U_\pm f := [(U_\pm f)_{\rm l}, (U_\pm f)_{\rm r}] \, , \end{array} \tag{5.9}$$

where $\mathcal{H}$ is realized by $L^2(\mathbb{R}, \mathrm{d}x)$, and $\widehat{\mathcal{H}}$ is realized by $L^2([0,\infty), \mathrm{d}E) \oplus L^2([0,\infty), \mathrm{d}E)$. The Hilbert spaces $\widehat{\mathcal{H}}_{\rm l}(E)$ and $\widehat{\mathcal{H}}_{\rm r}(E)$, which are associated to each energy E in the spectrum of H, are realized by $\mathbb{C}$. The scalar product on $\widehat{\mathcal{H}}$ can be written as

$$\left(\widehat{f}, \widehat{g}\right)_{\widehat{\mathcal{H}}} = \int_0^\infty \mathrm{d}E \, \overline{\widehat{f}_{\rm l}^{\pm}(E)} \, \widehat{g}_{\rm l}^{\pm}(E) + \int_0^\infty \mathrm{d}E \, \overline{\widehat{f}_{\rm r}^{\pm}(E)} \, \widehat{g}_{\rm r}^{\pm}(E) \, . \tag{5.10}$$

It is worthwhile noticing the similarities between $U_\pm$ and the Fourier transform $\mathcal{F}$, which is given by

$$\begin{array}{rcl} \mathcal{F} : L^2(\mathbb{R}, \mathrm{d}x) & \longmapsto & L^2(\mathbb{R}, \mathrm{d}p) \\ f(x) & \longmapsto & \mathcal{F}f(p) = \frac{1}{\sqrt{2\pi\hbar}} \int_{-\infty}^{\infty} \mathrm{d}x \, f(x) \mathrm{e}^{-\mathrm{i}px/\hbar} \, . \end{array} \tag{5.11}$$

The operators $U_\pm$ transform between the position and the energy representations, and $\mathcal{F}$ transforms between the position and the momentum representations. The kernels of $U_\pm$, $\chi_{\rm l,r}^{\pm}$, are eigenfunctions of the energy operator, and the kernel of $\mathcal{F}$, $\frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{-\mathrm{i}px/\hbar}$, is an eigenfunction of the momentum operator. Like $\mathcal{F}$, $U_\pm$ are unitary operators. Thus, $U_\pm$ are Fourier-like transforms.

6. The rigged Hilbert space and Dirac's formalism

In the previous sections, we have exhausted the Sturm-Liouville theory (i.e., the Hilbert space mathematics) when applied to the rectangular barrier. In this section, we equip the Sturm-Liouville theory with distribution theory, thereby constructing the equipped (i.e., rigged) Hilbert space of the rectangular barrier.

6.1. Construction of the rigged Hilbert space

As explained in the Introduction, we need a subdomain of the Hilbert space on which algebraic operations (sums, multiplications and commutation relations) involving P, Q and H are well defined and on which expectation values are finite. Essentially, that subdomain should remain stable under the action of any algebraic operation involving P, Q and H. The largest of such subdomains is the maximal invariant subspace of the algebra $\mathcal{A}$ [15, 16], which we shall denote by $\mathcal{D}$. Clearly, the elements of $\mathcal{D}$ 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 [16],
- the action of any power of the multiplication operator, of the differentiation operator and of h is square integrable.

Hence,

$$\mathcal{D} = \{\varphi \in L^2(\mathbb{R}, \mathrm{d}x) \ : \ \varphi \in C^\infty(\mathbb{R}), \ \varphi^{(n)}(a) = \varphi^{(n)}(b) = 0 \, , \ n = 0,1,\dots \, , \\ \frac{\mathrm{d}^n}{\mathrm{d}x^n} x^m h^l \varphi(x) \in L^2(\mathbb{R}, \mathrm{d}x) \, , \ n,m,l = 0,1,\dots\} \, . \quad (6.1)$$

The algebra of observables induces a natural topology on $\mathcal{D}$, whose definition of convergence is as follows:

$$\varphi_\alpha \xrightarrow[\alpha\to\infty]{\tau_{\mathbf{\Phi}}} \varphi \quad \text{iff} \quad \|\varphi_\alpha - \varphi\|_{n,m,l} \xrightarrow[\alpha\to\infty]{} 0 \, , \quad n,m,l = 0,1,\dots \, , \qquad (6.2)$$

where the norms $\| \cdot \|_{n,m,l}$ are defined as

$$\|\varphi\|_{n,m,l} := \sqrt{\int_{-\infty}^{\infty} \mathrm{d}x \ |P^n Q^m H^l \varphi(x)|^2} \, , \quad n,m,l = 0,1,\dots \, . \qquad (6.3)$$

When the space $\mathcal{D}$ is topologized by these norms, we obtain the locally convex space of test functions $\mathbf{\Phi}$. On $\mathbf{\Phi}$, the expectation values

$$(\varphi, A^n \varphi) \, , \quad \varphi \in \mathbf{\Phi} \, , \ A = P, Q, H \qquad (6.4)$$

are finite, and the commutation relations (1.5)-(1.7) are well defined. (Note that, when acting on $\varphi \in \mathbf{\Phi}$, the commutation relation (1.7) becomes $[H,P] = 0$, due to the vanishing of the derivatives of φ at the discontinuities of the potential.) Moreover, the restrictions of P, Q and H to $\mathbf{\Phi}$ are essentially self-adjoint, $\tau_{\mathbf{\Phi}}$-continuous operators. Equations (6.1) and (6.3) show that $\mathbf{\Phi}$ is very similar to the Schwartz space, the major differences being that the derivatives of the elements of $\mathbf{\Phi}$ vanish at $x = a, b$ and that $\mathbf{\Phi}$ is invariant not only under P and Q but also under H. This is why we shall write

$$\mathbf{\Phi} \equiv \mathcal{S}(\mathbb{R}\text{-}\{a,b\}) \, . \qquad (6.5)$$

Once we have constructed the space $\mathbf{\Phi}$, we can construct its topological antidual $\mathbf{\Phi}^\times$ as the space of $\tau_{\mathbf{\Phi}}$-continuous *antilinear* functionals on $\mathbf{\Phi}$, and therewith the RHS corresponding to the algebra of the 1D rectangular barrier potential,

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times \, , \qquad (6.6)$$

which in the position representation is realized by

$$\mathcal{S}(\mathbb{R}\text{-}\{a,b\}) \subset L^2(\mathbb{R}, \mathrm{d}x) \subset \mathcal{S}^\times(\mathbb{R}\text{-}\{a,b\}) \, . \qquad (6.7)$$

The space $\mathbf{\Phi}^\times$ is meant to contain the eigenkets $|p\rangle$, $|x\rangle$ and $|E^\pm\rangle_{\mathrm{l,r}}$ of P, Q and H. The definition of these eigenkets is borrowed from the theory of distributions. The eigenket $|p\rangle$ is defined as an integral operator whose kernel is the eigenfunction of the differential operator $-\mathrm{i}\hbar \mathrm{d}/\mathrm{d}x$ with eigenvalue p:

$$\begin{array}{rcl} |p\rangle : \mathbf{\Phi} & \longmapsto & \mathbb{C} \\ \varphi & \longmapsto & \langle\varphi|p\rangle := \int_{-\infty}^{\infty} \mathrm{d}x \, \overline{\varphi(x)} \frac{1}{\sqrt{2\pi\hbar}} \mathrm{e}^{\mathrm{i}px/\hbar} = \overline{(\mathcal{F}\varphi)(p)} \, . \end{array} \qquad (6.8)$$

Note that, although the eigenfunctions $\frac{1}{\sqrt{2\pi\hbar}}\mathrm{e}^{\mathrm{i}px/\hbar}$ are in principle well defined for any complex p, the momentum in Eq. (6.8) runs only over $\mathrm{Sp}(P) = (-\infty, \infty)$, because we are interested in assigning kets $|p\rangle$ only to the momenta in the spectrum of P, which are the only momenta that participate in the Dirac basis expansion associated to P. The eigenfunctions corresponding to the multiplication operator are just the delta function $\delta(x-x')$, and therefore the ket corresponding to each $x \in \mathrm{Sp}(Q)$ is defined as

$$\begin{array}{rcl} |x\rangle : \mathbf{\Phi} & \longmapsto & \mathbb{C} \\ \varphi & \longmapsto & \langle \varphi | x\rangle := \int_{-\infty}^{\infty} \mathrm{d}x' \, \overline{\varphi(x')} \delta(x-x') = \overline{\varphi(x)} \, . \end{array} \tag{6.9}$$

Similarly, we define the eigenkets corresponding to the Hamiltonian:

$$\begin{array}{rcl} |E^{\pm}\rangle_{\mathrm{l,r}} : \mathbf{\Phi} & \longmapsto & \mathbb{C} \\ \varphi & \longmapsto & \langle \varphi | E^{\pm}\rangle_{\mathrm{l,r}} := \int_{-\infty}^{\infty} \mathrm{d}x \, \overline{\varphi(x)} \chi_{\mathrm{l,r}}^{\pm}(x;E) = \overline{(U_{\pm}\varphi)_{\mathrm{l,r}}(E)} \, . \end{array} \tag{6.10}$$

Note that in Eq. (6.10) we have defined four different kets. Note also that, although the eigenfunctions $\chi_{\mathrm{l,r}}^{\pm}(x;E)$ are in principle well defined for any complex E, the energy in Eq. (6.10) runs only over $\mathrm{Sp}(H) = [0,\infty)$, because we are interested in assigning kets $|E^{\pm}\rangle_{\mathrm{l,r}}$ only to the energies in the spectrum of H, which are the only energies that participate in the Dirac basis expansion associated to H.

The following proposition, whose proof can be found in Appendix C, summarizes the results of this subsection:

Proposition 1. *The triplet of spaces (6.7) is a rigged Hilbert space, and it satisfies all the requirements demanded in the Introduction. More specifically,*

(i) *The quantities (6.3) fulfill the conditions to be a norm.*

(ii) *The space $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ is stable under the action of P, Q and H. The restrictions of P, Q and H to $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ are essentially self-adjoint, $\tau_{\mathbf{\Phi}}$-continuous operators. The space $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ is dense in $L^2(\mathbb{R},\mathrm{d}x)$.*

(iii) *The kets $|p\rangle$, $|x\rangle$ and $|E^{\pm}\rangle_{\mathrm{l,r}}$ are well-defined antilinear functionals on $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, i.e., they belong to $\mathcal{S}^{\times}(\mathbb{R}\text{-}\{a,b\})$.*

(iv) *The kets $|p\rangle$ are generalized eigenvectors of P,*

$$P|p\rangle = p|p\rangle \, , \quad p \in \mathbb{R} \, ; \tag{6.11}$$

the kets $|x\rangle$ are generalized eigenvectors of Q,

$$Q|x\rangle = x|x\rangle \, , \quad x \in \mathbb{R} \, ; \tag{6.12}$$

the kets $|E^{\pm}\rangle_{\mathrm{l,r}}$ are generalized eigenvectors of H,

$$H|E^{\pm}\rangle_{\mathrm{l,r}} = E|E^{\pm}\rangle_{\mathrm{l,r}} \, , \quad E \in [0,\infty) \, . \tag{6.13}$$

(Note that $|p\rangle$ and $|x\rangle$ are in particular tempered distributions, whereas $|E^{\pm}\rangle_{\mathrm{l,r}}$ are not.)

6.2. The Dirac bras

We have constructed the kets $|p\rangle$, $|x\rangle$ and $|E^{\pm}\rangle_{\mathrm{l,r}}$, and we have shown that they belong to the space of *antilinear* functionals over $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, which we denoted by $\mathcal{S}^{\times}(\mathbb{R}\text{-}\{a,b\})$.

In this subsection, we construct the corresponding bras $\langle x|$, $\langle p|$ and ${}_{\rm l,r}\langle^{\pm}E|$, and we show that they belong to the space of *linear* functionals over $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, which we shall denote by $\mathcal{S}'(\mathbb{R}\text{-}\{a,b\})$. The triplet of spaces

$$\mathcal{S}(\mathbb{R}\text{-}\{a,b\}) \subset L^2(\mathbb{R},\mathrm{d}x) \subset \mathcal{S}'(\mathbb{R}\text{-}\{a,b\}) \tag{6.14}$$

or, equivalently,

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}' \tag{6.15}$$

is also a rigged Hilbert space, although now suitable to contain the eigenbras of the observables.

The definition of the bra $\langle p|$ is as follows:

$$\begin{array}{rcl} \langle p| : \mathbf{\Phi} & \longmapsto & \mathbb{C} \\ \varphi & \longmapsto & \langle p|\varphi\rangle := \int_{-\infty}^{\infty} \mathrm{d}x\, \varphi(x) \frac{1}{\sqrt{2\pi\hbar}} \mathrm{e}^{-\mathrm{i}px/\hbar} = (\mathcal{F}\varphi)(p)\,. \end{array} \tag{6.16}$$

Comparison with Eq. (6.8) shows that the action of $\langle p|$ is the complex conjugate of the action of $|p\rangle$:

$$\langle p|\varphi\rangle = \overline{\langle \varphi|p\rangle}\,. \tag{6.17}$$

The bra $\langle x|$ is defined as

$$\begin{array}{rcl} \langle x| : \mathbf{\Phi} & \longmapsto & \mathbb{C} \\ \varphi & \longmapsto & \langle x|\varphi\rangle := \int_{-\infty}^{\infty} \mathrm{d}x'\, \varphi(x')\delta(x-x') = \varphi(x)\,. \end{array} \tag{6.18}$$

Comparison with Eq. (6.9) shows that the action of $\langle x|$ is complex conjugated to the action of $|x\rangle$:

$$\langle x|\varphi\rangle = \overline{\langle \varphi|x\rangle}\,. \tag{6.19}$$

Analogously, the eigenbras of the Hamiltonian are defined as

$$\begin{array}{rcl} {}_{\rm l,r}\langle^{\pm}E| : \mathbf{\Phi} & \longmapsto & \mathbb{C} \\ \varphi & \longmapsto & {}_{\rm l,r}\langle^{\pm}E|\varphi\rangle := \int_{-\infty}^{\infty} \mathrm{d}x\, \varphi(x)\overline{\chi_{\rm l,r}^{\pm}(x;E)} = (U_{\pm}\varphi)_{\rm l,r}(E)\,. \end{array} \tag{6.20}$$

(Note that in Eq. (6.20) we have defined four different bras.) Comparison with Eq. (6.10) shows that the actions of the bras ${}_{\rm l,r}\langle^{\pm}E|$ are the complex conjugates of the actions of the kets $|E^{\pm}\rangle_{\rm l,r}$:

$$ {}_{\rm l,r}\langle^{\pm}E|\varphi\rangle = \overline{\langle\varphi|E^{\pm}\rangle_{\rm l,r}}\,. \tag{6.21}$$

The bras $\langle p|$, $\langle x|$ and ${}_{\rm l,r}\langle^{\pm}E|$ are eigenvectors of P, Q and H, respectively, as the following proposition shows:

Proposition 2. *Within the rigged Hilbert space (6.14), it holds that*

(i) The bras $\langle p|$, $\langle x|$ and ${}_{\rm l,r}\langle^{\pm}E|$ are well-defined linear functionals over $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, i.e., they belong to $\mathcal{S}'(\mathbb{R}\text{-}\{a,b\})$.

(ii) The bras $\langle p|$ are generalized left-eigenvectors of P,

$$\langle p|P = p\langle p| \, , \quad p \in \mathbb{R} \, ; \tag{6.22}$$

the bras $\langle x|$ are generalized left-eigenvectors of Q,

$$\langle x|Q = x\langle x| \, , \quad x \in \mathbb{R} \, ; \tag{6.23}$$

the bras ${}_{\mathrm{l,r}}\langle^{\pm}E|$ are generalized left-eigenvectors of H,

$$ {}_{\mathrm{l,r}}\langle^{\pm}E|H = E \, {}_{\mathrm{l,r}}\langle^{\pm}E| \, , \quad E \in [0,\infty) \, . \tag{6.24}$$

The proof of Proposition 2 is included in Appendix C.

Note that, in particular, and in accordance with Dirac's prescription, there is a one-to-one correspondence between bras and kets: Given an observable A, to each element a in the spectrum of A, there corresponds 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 $\mathbf{\Phi}^{\times}$.

6.3. The Dirac basis vector expansions

Another important aspect of Dirac's formalism is that the bras and kets form a complete basis system such that [see also Eq. (1.11)]

$$\sum_{\alpha} \int_{\mathrm{Sp}(A)} \mathrm{d}a \, |a\rangle_{\alpha} \, {}_{\alpha}\langle a| = I \, . \tag{6.25}$$

In the present subsection, we derive various Dirac basis vector expansions for the algebra of the 1D rectangular barrier potential.

We start by writing

$$\langle x|E^{\pm}\rangle_{\mathrm{l,r}} := \chi^{\pm}_{\mathrm{l,r}}(x;E) \, , \tag{6.26}$$

and

$$ {}_{\mathrm{l,r}}\langle^{\pm}E|x\rangle := \overline{\chi^{\pm}_{\mathrm{l,r}}(x;E)} \, . \tag{6.27}$$

Then, the restriction of (5.5) to $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ yields the following basis expansions:

$$\langle x|\varphi\rangle = \int_0^{\infty} \mathrm{d}E \, \langle x|E^{\pm}\rangle_{\mathrm{l}} \, {}_{\mathrm{l}}\langle^{\pm}E|\varphi\rangle + \int_0^{\infty} \mathrm{d}E \, \langle x|E^{\pm}\rangle_{\mathrm{r}} \, {}_{\mathrm{r}}\langle^{\pm}E|\varphi\rangle \, . \tag{6.28}$$

The restriction of Eqs. (5.2) and (5.3) to $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ yields four other basis expansions:

$$ {}_{\mathrm{l,r}}\langle^{\pm}E|\varphi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x \, {}_{\mathrm{l,r}}\langle^{\pm}E|x\rangle\langle x|\varphi\rangle \, . \tag{6.29}$$

The basis vector expansions (6.28)-(6.29) are very similar to those given by the restriction of the Fourier transform to $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$. If we define

$$\langle x|p\rangle := \frac{1}{\sqrt{2\pi\hbar}} \mathrm{e}^{\mathrm{i}px/\hbar} \, , \tag{6.30}$$

$$\langle p|x\rangle := \frac{1}{\sqrt{2\pi\hbar}} \mathrm{e}^{-\mathrm{i}px/\hbar} \, , \tag{6.31}$$

then the restriction of (5.11) to $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ yields

$$\langle p|\varphi\rangle = \int_{-\infty}^{\infty} \mathrm{d}x \ \langle p|x\rangle\langle x|\varphi\rangle \, , \tag{6.32}$$

whereas the restriction of the inverse of (5.11) to $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ yields

$$\langle x|\varphi\rangle = \int_{-\infty}^{\infty} \mathrm{d}p \ \langle x|p\rangle\langle p|\varphi\rangle \, . \tag{6.33}$$

The similarity between the Dirac basis vector expansions (6.28)-(6.29) and the Fourier expansions (6.32)-(6.33) is another facet of the parallel between Dirac's formalism and Fourier methods.

For the sake of completeness, we include the 1D rectangular potential version of the Nuclear Spectral Theorem [24] (see Appendix C for its proof):

Proposition 3. *(Nuclear Spectral Theorem) Let*

$$\mathcal{S}(\mathbb{R}\text{-}\{a,b\}) \subset L^2(\mathbb{R},\mathrm{d}x) \subset \mathcal{S}^\times(\mathbb{R}\text{-}\{a,b\}) \tag{6.34}$$

be the RHS of the 1D rectangular barrier algebra such that $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ remains invariant under the action of the algebra $\mathcal{A}$, and such that the operators of $\mathcal{A}$ are $\tau_{\mathbf{\Phi}}$-continuous, essentially self-adjoint operators over $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$. Then, for each element in the spectrum of P, Q or H, there is a generalized eigenvector such that

$$P|p\rangle = p|p\rangle \, , \qquad p \in \mathbb{R} \, , \tag{6.35}$$

$$Q|x\rangle = x|x\rangle \, , \qquad x \in \mathbb{R} \, , \tag{6.36}$$

$$H|E^{\pm}\rangle_{\mathrm{l,r}} = E|E^{\pm}\rangle_{\mathrm{l,r}} \, , \quad E \in [0,\infty) \, , \tag{6.37}$$

and such that for all $\varphi, \psi \in \mathcal{S}(\mathbb{R}\text{-}\{a,b\})$

$$(\varphi,\psi) = \int_0^{\infty} \mathrm{d}E \, \langle\varphi|E^{\pm}\rangle_{\mathrm{l\,l}}\langle^{\pm}E|\psi\rangle + \int_0^{\infty} \mathrm{d}E \, \langle\varphi|E^{\pm}\rangle_{\mathrm{r\,r}}\langle^{\pm}E|\psi\rangle \tag{6.38}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}p \, \langle\varphi|p\rangle\langle p|\psi\rangle \tag{6.39}$$

$$= \int_{-\infty}^{\infty} \mathrm{d}x \, \langle\varphi|x\rangle\langle x|\psi\rangle \, , \tag{6.40}$$

and for all $\varphi, \psi \in \mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, $n = 1, 2, \dots$

$$(\varphi, H^n\psi) = \int_0^{\infty} \mathrm{d}E \, E^n \langle\varphi|E^{\pm}\rangle_{\mathrm{l\,l}}\langle^{\pm}E|\psi\rangle + \int_0^{\infty} \mathrm{d}E \, E^n \langle\varphi|E^{\pm}\rangle_{\mathrm{r\,r}}\langle^{\pm}E|\psi\rangle \, , \tag{6.41}$$

$$(\varphi, P^n\psi) = \int_{-\infty}^{\infty} \mathrm{d}p \, p^n \langle\varphi|p\rangle\langle p|\psi\rangle \, , \tag{6.42}$$

$$(\varphi, Q^n\psi) = \int_{-\infty}^{\infty} \mathrm{d}x \, x^n \langle\varphi|x\rangle\langle x|\psi\rangle \, . \tag{6.43}$$

If we "sandwich" Eq. (6.25) in between two elements φ and ψ of $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, then we obtain the expansions (6.38)-(6.43), when $A = H^n, P^n, Q^n$, $n = 0,1,2,\ldots$. If we "sandwich" Eq. (6.25) in between an element φ of $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ and a bra $\langle x|$, ${}_{\rm l,r}\langle^{\pm}E|$ or $\langle p|$, then we obtain the expansions (6.28)-(6.29) and (6.32)-(6.33). This "sandwiching," however, is not valid when φ or ψ lies outside $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, because then the action of the bras and kets is not well defined. Thus, the RHS, rather than just the Hilbert space, fully justifies Dirac's formalism.

6.4. Energy, momentum and wave-number representations of the rigged Hilbert space

In subsection 6.1, we constructed the position representation of the rigged Hilbert space of the 1D rectangular barrier algebra [see Eq. (6.7)]. In this subsection, we construct three spectral representations of (6.7): the energy, the momentum and the wave-number representations.

We start with the energy representation. The unitary operators $U_{\pm}$ of Eq. (5.9) afford two energy representations of the RHS (6.7). The energy representations of $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ will be denoted as

$$\widehat{\mathcal{S}}_{\pm}(\mathbb{R}\text{-}\{a,b\}) \equiv U_{\pm}\mathcal{S}(\mathbb{R}\text{-}\{a,b\})\,. \tag{6.44}$$

On $\widehat{\mathcal{S}}_{\pm}(\mathbb{R}\text{-}\{a,b\})$, the Hamiltonian acts as the multiplication operator, as Eq. (5.8) shows. The spaces $\widehat{\mathcal{S}}_{\pm}(\mathbb{R}\text{-}\{a,b\})$ are linear subspaces of $L^2([0,\infty),{\rm d}E)\oplus L^2([0,\infty),{\rm d}E)$. In order to endow $\widehat{\mathcal{S}}_{\pm}(\mathbb{R}\text{-}\{a,b\})$ with a topology, we carry the topology on $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ onto $\widehat{\mathcal{S}}_{\pm}(\mathbb{R}\text{-}\{a,b\})$,

$$\tau_{\widehat{\mathbf{\Phi}}_{\pm}} := U_{\pm}\tau_{\mathbf{\Phi}}\,. \tag{6.45}$$

Endowed with these topologies, $\widehat{\mathcal{S}}_{\pm}(\mathbb{R}\text{-}\{a,b\})$ are linear topological spaces. If we denote the antidual spaces of $\widehat{\mathcal{S}}_{\pm}(\mathbb{R}\text{-}\{a,b\})$ by $\widehat{\mathcal{S}}_{\pm}^{\times}(\mathbb{R}\text{-}\{a,b\})$, then we have

$$U_{\pm}^{\times}\mathcal{S}^{\times}(\mathbb{R}\text{-}\{a,b\}) = \left[U_{\pm}\mathcal{S}(\mathbb{R}\text{-}\{a,b\})\right]^{\times} = \widehat{\mathcal{S}}_{\pm}^{\times}(\mathbb{R}\text{-}\{a,b\})\,. \tag{6.46}$$

We can further split the energy representations of the RHS into left and right components, which are associated to left and right incidences. In order to do so, we need to recall the definition of the left and right components of the wave functions [see Eqs. (5.2) and (5.3)]:

$$\widehat{\varphi}_{\rm l,r}^{\pm}(E) = (U_{\pm}\varphi)_{\rm l,r}(E)\,. \tag{6.47}$$

Any element $\widehat{\varphi}^{\pm}$ of $\widehat{\mathcal{S}}_{\pm}(\mathbb{R}\text{-}\{a,b\})$ can therefore be written as a two-component vector,

$$\widehat{\varphi}^{\pm} \equiv \left[\widehat{\varphi}_{\rm l}^{\pm},\widehat{\varphi}_{\rm r}^{\pm}\right]\,, \tag{6.48}$$

which is equivalent to write the spaces (6.44) as sums of left and right components:

$$\widehat{\mathcal{S}}_{\pm}(\mathbb{R}\text{-}\{a,b\}) \equiv \widehat{\mathcal{S}}_{\pm;l}(\mathbb{R}\text{-}\{a,b\}) \oplus \widehat{\mathcal{S}}_{\pm;r}(\mathbb{R}\text{-}\{a,b\})\,. \tag{6.49}$$

Their antiduals can be split in a similar way,

$$\widehat{\mathcal{S}}_{\pm}^{\times}(\mathbb{R}\text{-}\{a,b\}) \equiv \widehat{\mathcal{S}}_{\pm;l}^{\times}(\mathbb{R}\text{-}\{a,b\}) \oplus \widehat{\mathcal{S}}_{\pm;r}^{\times}(\mathbb{R}\text{-}\{a,b\})\,. \tag{6.50}$$

The energy representation of the kets $|E^\pm\rangle_{\rm l,r}$ is given by a familiar distribution. If we denote the energy representation of these kets by $|\widehat{E}^\pm\rangle_{\rm l,r}$, then the following equalities

$$\begin{aligned}
\langle \widehat{\varphi}^\pm_{\rm l,r}|\widehat{E}^\pm\rangle_{\rm l,r} &= \langle \widehat{\varphi}^\pm_{\rm l,r}|U^\times_\pm|E^\pm\rangle_{\rm l,r} && (6.51)\\
&= \langle U^{-1}_\pm \widehat{\varphi}^\pm_{\rm l,r}|E^\pm\rangle_{\rm l,r} \\
&= \int_{-\infty}^{\infty} {\rm d}x\, \overline{\varphi(x)}\chi^\pm_{\rm l,r}(x;E) \\
&= \overline{\widehat{\varphi}^\pm_{\rm l,r}(E)} && (6.52)
\end{aligned}$$

show that $|\widehat{E}^\pm\rangle_{\rm l}$ and $|\widehat{E}^\pm\rangle_{\rm r}$ act as the *antilinear* Schwartz delta functional over the spaces $\widehat{\mathcal{S}}_{\pm;l}(\mathbb{R}\text{-}\{a,b\})$ and $\widehat{\mathcal{S}}_{\pm;r}(\mathbb{R}\text{-}\{a,b\})$, respectively.

The different realizations of the RHS are easily visualized through the following diagram:

$$\begin{array}{cccccccc}
H;\ \varphi & \mathcal{S}(\mathbb{R}\text{-}\{a,b\}) & \subset & L^2(\mathbb{R},{\rm d}x) & \subset & \mathcal{S}^\times(\mathbb{R}\text{-}\{a,b\}) & |E^\pm\rangle_{\rm l,r} \\
 & \downarrow U_\pm & & \downarrow U_\pm & & \downarrow U^\times_\pm & \\
\widehat{H};\ \widehat{\varphi}_\pm & \widehat{\mathcal{S}}_\pm(\mathbb{R}\text{-}\{a,b\}) & \subset & \oplus L^2([0,\infty),{\rm d}E) & \subset & \widehat{\mathcal{S}}^\times_\pm(\mathbb{R}\text{-}\{a,b\}) & |\widehat{E}^\pm\rangle_{\rm l,r}
\end{array} \qquad (6.53)$$

where $\oplus L^2([0,\infty),{\rm d}E)$ denotes $L^2([0,\infty),{\rm d}E) \oplus L^2([0,\infty),{\rm d}E)$. The top line of diagram (6.53) displays the Hamiltonian, the wave functions, the RHS and the Dirac kets in the position representation. The bottom line displays their energy representation counterparts.

We can also construct the energy representation of the eigenbras ${}_{\rm l,r}\langle ^\pm E|$. To this end, we first construct the energy representation of $\mathcal{S}'(\mathbb{R}\text{-}\{a,b\})$, which we shall denote by $\widehat{\mathcal{S}}'_\pm(\mathbb{R}\text{-}\{a,b\})$. These two spaces are related as follows:

$$U'_\pm \mathcal{S}'(\mathbb{R}\text{-}\{a,b\}) = \Big[U_\pm \mathcal{S}(\mathbb{R}\text{-}\{a,b\})\Big]' = \widehat{\mathcal{S}}'_\pm(\mathbb{R}\text{-}\{a,b\})\,. \qquad (6.54)$$

Similarly to Eqs. (6.49) and (6.50), the dual space can be split into left and right components,

$$\widehat{\mathcal{S}}'_\pm(\mathbb{R}\text{-}\{a,b\}) = \widehat{\mathcal{S}}'_{\pm;l}(\mathbb{R}\text{-}\{a,b\}) \oplus \widehat{\mathcal{S}}'_{\pm;r}(\mathbb{R}\text{-}\{a,b\})\,. \qquad (6.55)$$

Now, if we denote the energy representation of the energy eigenbras by ${}_{\rm l,r}\langle ^\pm \widehat{E}|$, then the following equalities

$$\begin{aligned}
{}_{\rm l,r}\langle ^\pm \widehat{E}|\widehat{\varphi}^\pm_{\rm l,r}\rangle &= {}_{\rm l,r}\langle ^\pm E|U'_\pm|\widehat{\varphi}^\pm_{\rm l,r}\rangle && (6.56)\\
&= {}_{\rm l,r}\langle ^\pm E|U^{-1}_\pm \widehat{\varphi}^\pm_{\rm l,r}\rangle \\
&= \int_{-\infty}^{\infty} {\rm d}x\, \varphi(x)\overline{\chi^\pm_{\rm l,r}(x;E)} \\
&= \widehat{\varphi}^\pm_{\rm l,r}(E) && (6.57)
\end{aligned}$$

show that ${}_{\rm l}\langle ^\pm \widehat{E}|$ and ${}_{\rm r}\langle ^\pm \widehat{E}|$ are the *linear* Schwartz delta functional over the spaces $\widehat{\mathcal{S}}_{\pm;l}(\mathbb{R}\text{-}\{a,b\})$ and $\widehat{\mathcal{S}}_{\pm;r}(\mathbb{R}\text{-}\{a,b\})$, respectively.

The diagram corresponding to the bras is as follows:

$$\begin{array}{llllll} H;\ \varphi & \mathcal{S}(\mathbb{R}\text{-}\{a,b\}) & \subset & L^2(\mathbb{R},\mathrm{d}x) & \subset & \mathcal{S}'(\mathbb{R}\text{-}\{a,b\}) & {}_{\mathrm{l,r}}\langle^{\pm}E| \\ & \downarrow U_{\pm} & & \downarrow U_{\pm} & & \downarrow U_{\pm}' & \\ \widehat{H};\ \widehat{\varphi}_{\pm} & \widehat{\mathcal{S}}_{\pm}(\mathbb{R}\text{-}\{a,b\}) & \subset & \oplus L^2([0,\infty),\mathrm{d}E) & \subset & \widehat{\mathcal{S}}_{\pm}'(\mathbb{R}\text{-}\{a,b\}) & {}_{\mathrm{l,r}}\langle^{\pm}\widehat{E}| \end{array} \tag{6.58}$$

The energy representations of P and Q have not been included, since they are fairly complicated.

The momentum representation of the RHS (6.7) can be constructed in a similar fashion, by way of the Fourier transform $\mathcal{F}$. We shall not reproduce the calculations here but only provide the resulting diagrams. The diagram corresponding to the position and momentum kets reads as

$$\begin{array}{llllll} P,Q;\ \varphi & \mathcal{S}(\mathbb{R}\text{-}\{a,b\}) & \subset & L^2(\mathbb{R},\mathrm{d}x) & \subset & \mathcal{S}^{\times}(\mathbb{R}\text{-}\{a,b\}) & |p\rangle,\, |x\rangle \\ & \downarrow \mathcal{F} & & \downarrow \mathcal{F} & & \downarrow \mathcal{F}^{\times} & \\ \widehat{P},\widehat{Q};\ \widehat{\varphi} & \widehat{\mathcal{S}}(\mathbb{R}\text{-}\{a,b\}) & \subset & L^2(\mathbb{R},\mathrm{d}p) & \subset & \widehat{\mathcal{S}}^{\times}(\mathbb{R}\text{-}\{a,b\}) & |\widehat{p}\rangle,\, |\widehat{x}\rangle \end{array} \tag{6.59}$$

where $\widehat{P}$ acts as the multiplication operator by p, $\widehat{Q}$ acts as the differential operator $\mathrm{i}\hbar\mathrm{d}/\mathrm{d}p$, $|\widehat{p}\rangle$ is the *antilinear* Schwartz delta functional, and $|\widehat{x}\rangle$ is the *antilinear* functional whose kernel is $(2\pi\hbar)^{-1/2}\exp(-\mathrm{i}px/\hbar)$. The momentum diagram for the position and momentum bras is

$$\begin{array}{llllll} P,Q;\ \varphi & \mathcal{S}(\mathbb{R}\text{-}\{a,b\}) & \subset & L^2(\mathbb{R},\mathrm{d}x) & \subset & \mathcal{S}'(\mathbb{R}\text{-}\{a,b\}) & \langle p|,\, \langle x| \\ & \downarrow \mathcal{F} & & \downarrow \mathcal{F} & & \downarrow \mathcal{F}' & \\ \widehat{P},\widehat{Q};\ \widehat{\varphi} & \widehat{\mathcal{S}}(\mathbb{R}\text{-}\{a,b\}) & \subset & L^2(\mathbb{R},\mathrm{d}p) & \subset & \widehat{\mathcal{S}}'(\mathbb{R}\text{-}\{a,b\}) & \langle\widehat{p}|,\, \langle\widehat{x}| \end{array} \tag{6.60}$$

where $\langle\widehat{p}|$ is the *linear* Schwartz delta functional, and $\langle\widehat{x}|$ is the *linear* functional with kernel $(2\pi\hbar)^{-1/2}\exp(\mathrm{i}px/\hbar)$. The momentum representation of H has not been included, since in the momentum representation H has a complicated expression.

The momentum representation should not be confused with the wave number representation, which we construct in the remainder of this subsection.

The eigenfunctions of the Schrödinger differential operator, the Green function and the transmission and reflection coefficients depend on the square root of the energy rather than on the energy itself. Thus, the wave number, which is defined as

$$k := \sqrt{\frac{2m}{\hbar^2}\,E}\,, \tag{6.61}$$

is a more convenient variable. In terms of k, the δ-normalized eigensolutions of the differential operator (2.1) read as

$$\langle x|k^{\pm}\rangle_{\mathrm{l,r}} \equiv \sqrt{\frac{\hbar^2 k}{m}}\ \chi^{\pm}_{\mathrm{l,r}}(x;E)\,. \tag{6.62}$$

These eigensolutions can be used to obtain the unitary operators $V_{\pm}$ that transform between the position and the wave-number representations,

$$\widehat{\widehat{f}}_{\pm}(k) = (V_{\pm}f)(k) = \int_{-\infty}^{\infty}\mathrm{d}x\, f(x)\overline{\langle x|k^{\pm}\rangle}_{\mathrm{l}} + \int_{-\infty}^{\infty}\mathrm{d}x\, f(x)\overline{\langle x|k^{\pm}\rangle}_{\mathrm{r}}\,,\ f\in\mathcal{H}\,, \tag{6.63}$$

where "$\widehat{\ }$" denotes the k-representation. On this representation, the Hamiltonian acts as multiplication by $\frac{\hbar^2}{2m}k^2$. To each $k \in [0,\infty)$, there correspond four eigenkets $|k^{\pm}\rangle_{\mathrm{l,r}}$ that act on $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ as the following integral operators:

$$\langle\varphi|k^{\pm}\rangle_{\mathrm{l,r}} := \int_{-\infty}^{\infty} \mathrm{d}x\, \langle\varphi|x\rangle\langle x|k^{\pm}\rangle_{\mathrm{l,r}} = \overline{(V_{\pm}\varphi)_{\mathrm{l,r}}(k)}\,, \quad \varphi \in \mathcal{S}(\mathbb{R}\text{-}\{a,b\})\,. \tag{6.64}$$

These eigenkets are generalized eigenvectors of the Hamiltonian with eigenvalue $\frac{\hbar^2}{2m}k^2$. The following diagram provides the k-representation counterpart of (6.53):

$$\begin{array}{cccccccc} H;\ \varphi & \mathcal{S}(\mathbb{R}\text{-}\{a,b\}) & \subset & L^2(\mathbb{R},\mathrm{d}x) & \subset & \mathcal{S}^{\times}(\mathbb{R}\text{-}\{a,b\}) & |k^{\pm}\rangle_{\mathrm{l,r}} \\ & \downarrow V_{\pm} & & \downarrow V_{\pm} & & \downarrow V_{\pm}^{\times} & \\ \widehat{\widehat{H}};\ \widehat{\widehat{\varphi}}_{\pm} & \widehat{\widehat{\mathcal{S}}}_{\pm}(\mathbb{R}\text{-}\{a,b\}) & \subset & \oplus L^2([0,\infty),\mathrm{d}k) & \subset & \widehat{\widehat{\mathcal{S}}}{}^{\times}_{\pm}(\mathbb{R}\text{-}\{a,b\}) & |\widehat{\widehat{k}}{}^{\pm}\rangle_{\mathrm{l,r}} \end{array} \tag{6.65}$$

where $\oplus L^2([0,\infty),\mathrm{d}k)$ denotes $L^2([0,\infty),\mathrm{d}k) \oplus L^2([0,\infty),\mathrm{d}k)$, and $|\widehat{\widehat{k}}{}^{\pm}\rangle_{\mathrm{l,r}}$ act as the *antilinear* Schwartz delta functional. The k-representation counterpart of (6.58) is given by the following diagram:

$$\begin{array}{cccccccc} H;\ \varphi & \mathcal{S}(\mathbb{R}\text{-}\{a,b\}) & \subset & L^2(\mathbb{R},\mathrm{d}x) & \subset & \mathcal{S}'(\mathbb{R}\text{-}\{a,b\}) & {}_{\mathrm{l,r}}\langle^{\pm}k| \\ & \downarrow V_{\pm} & & \downarrow V_{\pm} & & \downarrow V_{\pm}' & \\ \widehat{\widehat{H}};\ \widehat{\widehat{\varphi}}_{\pm} & \widehat{\widehat{\mathcal{S}}}_{\pm}(\mathbb{R}\text{-}\{a,b\}) & \subset & \oplus L^2([0,\infty),\mathrm{d}k) & \subset & \widehat{\widehat{\mathcal{S}}}{}'_{\pm}(\mathbb{R}\text{-}\{a,b\}) & {}_{\mathrm{l,r}}\langle^{\pm}\widehat{\widehat{k}}| \end{array} \tag{6.66}$$

where ${}_{\mathrm{l,r}}\langle^{\pm}\widehat{\widehat{k}}|$ act as the *linear* Schwartz delta functional.

The wave number is particularly useful in writing the Green function in a simple, compact form, as we are going to see now. Expressions (A.8) for $T(k)$ and (A.15) for $T^*(k)$ yield

$$T(-k) = T^*(k)\,, \quad k > 0\,. \tag{6.67}$$

From Eqs. (3.13) and (3.18) it results that

$$\chi_{\mathrm{r}}^{+}(x;-k) = \mathrm{i}\chi_{\mathrm{r}}^{-}(x;k)\,, \quad k > 0\,, \tag{6.68}$$

and from Eqs. (3.15) and (3.19) it results that

$$\chi_{\mathrm{l}}^{+}(x;-k) = \mathrm{i}\chi_{\mathrm{l}}^{-}(x;k)\,, \quad k > 0\,. \tag{6.69}$$

We can use the last three equations to write the Green function for all values of k (and therefore for all values of E):

$$G(x,x';k) = \frac{2\pi}{\mathrm{i}}\,\frac{\chi_{\mathrm{r}}^{+}(x_<;k)\chi_{\mathrm{l}}^{+}(x_>;k)}{T(k)}\,, \quad k \in \mathbb{C}\,, \tag{6.70}$$

where $x_<, x_>$ refer to the smaller and to the bigger of x and x', respectively.

7. Conclusions

We have explicitly constructed the RHSs of the algebra of the 1D rectangular potential. In the position representation, these RHSs are given by

$$\mathcal{S}(\mathbb{R}\text{-}\{a,b\}) \subset L^2(\mathbb{R},\mathrm{d}x) \subset \mathcal{S}^{\times}(\mathbb{R}\text{-}\{a,b\})\,, \tag{7.1}$$

$$\mathcal{S}(\mathbb{R}\text{-}\{a,b\}) \subset L^2(\mathbb{R},\mathrm{d}x) \subset \mathcal{S}'(\mathbb{R}\text{-}\{a,b\})\,. \tag{7.2}$$

On $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, the observables are essentially self-adjoint, continuous operators. Algebraic operations such as commutation relations are well defined on $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$.

We have also constructed the Dirac bras and kets of each observable of the algebra, as well as the basis expansions generated by the bras and kets. By doing so, we have shown (once again) that the RHS fully accounts for Dirac's formalism.

By comparing the results for the Fourier transform $\mathcal{F}$ with those for the unitary operators $U_{\pm}$, we have seen that Dirac's formalism can be viewed as an extension of Fourier methods: Monoenergetic eigenfunctions extend the notion of monochromatic plane waves, $U_{\pm}$ extend the notion of Fourier transform, and Dirac's basis expansions extend the notion of Fourier decomposition.

The results of this paper can be applied to many other algebras, at least when resonance eigenvalues are not considered. In general, the space of test functions $\mathbf{\Phi}$ is given by the maximal invariant subspace of the algebra, and the spaces of distributions $\mathbf{\Phi}^{\times}$ and $\mathbf{\Phi}'$ are given by the antidual and dual spaces of $\mathbf{\Phi}$.

As a corollary to the results of this paper, we can derive the RHSs of the algebra of the 1D free Hamiltonian. By making V_0 tend to zero, we can see that these RHSs are given by

$$\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R},\mathrm{d}x) \subset \mathcal{S}^{\times}(\mathbb{R})\,, \tag{7.3}$$

$$\mathcal{S}(\mathbb{R}) \subset L^2(\mathbb{R},\mathrm{d}x) \subset \mathcal{S}'(\mathbb{R})\,, \tag{7.4}$$

where $\mathcal{S}(\mathbb{R})$ is the Schwartz space.

Finally, of mathematical interest is the introduction of a new space of test functions, the Schwartz-like space $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, and new spaces of distributions, the spaces of tempered-like distributions $\mathcal{S}^{\times}(\mathbb{R}\text{-}\{a,b\})$ and $\mathcal{S}'(\mathbb{R}\text{-}\{a,b\})$.

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Appendix A. Auxiliary functions

For the sake of completeness, we provide the explicit expressions of the coefficients of the eigenfunctions:

$$\widetilde{T}(\widetilde{k}) = \mathrm{e}^{\widetilde{k}(b-a)} \frac{4\widetilde{Q}/\widetilde{k}}{(1+\widetilde{Q}/\widetilde{k})^2\mathrm{e}^{\widetilde{Q}(b-a)} - (1-\widetilde{Q}/\widetilde{k})^2\mathrm{e}^{-\widetilde{Q}(b-a)}} \tag{A.1}$$

$$\widetilde{A}_{\mathrm{r}}(\widetilde{k}) = \frac{-2\mathrm{e}^{\widetilde{k}b}\mathrm{e}^{\widetilde{Q}a}(1-\widetilde{Q}/\widetilde{k})}{(1+\widetilde{Q}/\widetilde{k})^2\mathrm{e}^{\widetilde{Q}(b-a)} - (1-\widetilde{Q}/\widetilde{k})^2\mathrm{e}^{-\widetilde{Q}(b-a)}} \tag{A.2}$$

$$\widetilde{B}_{\rm r}(\widetilde{k}) = \frac{2{\rm e}^{\widetilde{k}b}{\rm e}^{-\widetilde{Q}a}(1+\widetilde{Q}/\widetilde{k})}{(1+\widetilde{Q}/\widetilde{k})^2{\rm e}^{\widetilde{Q}(b-a)}-(1-\widetilde{Q}/\widetilde{k})^2{\rm e}^{-\widetilde{Q}(b-a)}} \tag{A.3}$$

$$\widetilde{R}_{\rm r}(\widetilde{k}) = {\rm e}^{2\widetilde{k}b}\frac{(1-(\widetilde{Q}/\widetilde{k})^2){\rm e}^{\widetilde{Q}(b-a)}-(1-(\widetilde{Q}/\widetilde{k})^2){\rm e}^{-\widetilde{Q}(b-a)}}{(1+\widetilde{Q}/\widetilde{k})^2{\rm e}^{\widetilde{Q}(b-a)}-(1-\widetilde{Q}/\widetilde{k})^2{\rm e}^{-\widetilde{Q}(b-a)}} \tag{A.4}$$

$$\widetilde{R}_{\rm l}(\widetilde{k}) = {\rm e}^{-2\widetilde{k}a}\frac{(1-(\widetilde{Q}/\widetilde{k})^2){\rm e}^{\widetilde{Q}(b-a)}-(1-(\widetilde{Q}/\widetilde{k})^2){\rm e}^{-\widetilde{Q}(b-a)}}{(1+\widetilde{Q}/\widetilde{k})^2{\rm e}^{\widetilde{Q}(b-a)}-(1-\widetilde{Q}/\widetilde{k})^2{\rm e}^{-\widetilde{Q}(b-a)}} \tag{A.5}$$

$$\widetilde{A}_{\rm l}(\widetilde{k}) = \frac{2{\rm e}^{-\widetilde{k}a}{\rm e}^{\widetilde{Q}b}(1+\widetilde{Q}/\widetilde{k})}{(1+\widetilde{Q}/\widetilde{k})^2{\rm e}^{\widetilde{Q}(b-a)}-(1-\widetilde{Q}/\widetilde{k})^2{\rm e}^{-\widetilde{Q}(b-a)}} \tag{A.6}$$

$$\widetilde{B}_{\rm l}(\widetilde{k}) = \frac{-2{\rm e}^{-\widetilde{k}a}{\rm e}^{-\widetilde{Q}b}(1-\widetilde{Q}/\widetilde{k})}{(1+\widetilde{Q}/\widetilde{k})^2{\rm e}^{\widetilde{Q}(b-a)}-(1-\widetilde{Q}/\widetilde{k})^2{\rm e}^{-\widetilde{Q}(b-a)}} \tag{A.7}$$

$$T(k) = {\rm e}^{-{\rm i}k(b-a)}\frac{-4Q/k}{(1-Q/k)^2{\rm e}^{{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}} \tag{A.8}$$

$$A_{\rm r}(k) = \frac{2{\rm e}^{-{\rm i}kb}{\rm e}^{-{\rm i}Qa}(1-Q/k)}{(1-Q/k)^2{\rm e}^{{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}} \tag{A.9}$$

$$B_{\rm r}(k) = \frac{-2{\rm e}^{-{\rm i}kb}{\rm e}^{{\rm i}Qa}(1+Q/k)}{(1-Q/k)^2{\rm e}^{{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}} \tag{A.10}$$

$$R_{\rm r}(k) = {\rm e}^{-2{\rm i}kb}\frac{(1-(Q/k)^2)\,{\rm e}^{{\rm i}Q(b-a)}-(1-(Q/k)^2)\,{\rm e}^{-{\rm i}Q(b-a)}}{(1-Q/k)^2{\rm e}^{{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}} \tag{A.11}$$

$$R_{\rm l}(k) = {\rm e}^{2{\rm i}ka}\frac{(1-(Q/k)^2)\,{\rm e}^{{\rm i}Q(b-a)}-(1-(Q/k)^2)\,{\rm e}^{-{\rm i}Q(b-a)}}{(1-Q/k)^2{\rm e}^{{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}} \tag{A.12}$$

$$A_{\rm l}(k) = \frac{-2{\rm e}^{{\rm i}ka}{\rm e}^{-{\rm i}Qb}(1+Q/k)}{(1-Q/k)^2{\rm e}^{{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}} \tag{A.13}$$

$$B_{\rm l}(k) = \frac{2{\rm e}^{{\rm i}ka}{\rm e}^{{\rm i}Qb}(1-Q/k)}{(1-Q/k)^2{\rm e}^{{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}} \tag{A.14}$$

$$T^*(k) = {\rm e}^{{\rm i}k(b-a)}\frac{-4Q/k}{(1-Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{{\rm i}Q(b-a)}} \tag{A.15}$$

$$A_{\rm r}^*(k) = \frac{2{\rm e}^{{\rm i}kb}{\rm e}^{{\rm i}Qa}(1-Q/k)}{(1-Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{{\rm i}Q(b-a)}} \tag{A.16}$$

$$B_{\rm r}^*(k) = \frac{-2{\rm e}^{{\rm i}kb}{\rm e}^{-{\rm i}Qa}(1+Q/k)}{(1-Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{{\rm i}Q(b-a)}} \tag{A.17}$$

$$R_{\rm r}^*(k) = {\rm e}^{2{\rm i}kb}\frac{(1-(Q/k)^2)\,{\rm e}^{-{\rm i}Q(b-a)}-(1-(Q/k)^2)\,{\rm e}^{{\rm i}Q(b-a)}}{(1-Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{{\rm i}Q(b-a)}} \tag{A.18}$$

$$R_{\rm l}^*(k) = {\rm e}^{-2{\rm i}ka}\frac{(1-(Q/k)^2)\,{\rm e}^{-{\rm i}Q(b-a)}-(1-(Q/k)^2)\,{\rm e}^{{\rm i}Q(b-a)}}{(1-Q/k)^2{\rm e}^{-{\rm i}Q(b-a)}-(1+Q/k)^2{\rm e}^{{\rm i}Q(b-a)}} \tag{A.19}$$

$$A_{\mathrm{l}}^{*}(k) = \frac{-2\mathrm{e}^{-\mathrm{i}ka}\mathrm{e}^{\mathrm{i}Qb}(1+Q/k)}{(1-Q/k)^2\mathrm{e}^{-\mathrm{i}Q(b-a)} - (1+Q/k)^2\mathrm{e}^{\mathrm{i}Q(b-a)}} \tag{A.20}$$

$$B_{\mathrm{l}}^{*}(k) = \frac{2\mathrm{e}^{-\mathrm{i}ka}\mathrm{e}^{-\mathrm{i}Qb}(1-Q/k)}{(1-Q/k)^2\mathrm{e}^{-\mathrm{i}Q(b-a)} - (1+Q/k)^2\mathrm{e}^{\mathrm{i}Q(b-a)}} \tag{A.21}$$

Appendix B. Spectral measures associated to $\{\chi_{\mathrm{l}}^{-}, \chi_{\mathrm{r}}^{-}\}$

The "final" basis $\{\chi_{\mathrm{l}}^{-}, \chi_{\mathrm{r}}^{-}\}$ can be used as well as the "initial" basis $\{\chi_{\mathrm{l}}^{+}, \chi_{\mathrm{r}}^{+}\}$ to calculate $\mathrm{Sp}(H)$. This calculation, which follows the procedure of Sec. 4, is provided in this appendix.

If we choose

$$\sigma_1(x;E) = \chi_{\mathrm{l}}^{-}(x;E) \tag{B.1}$$

$$\sigma_2(x;E) = \chi_{\mathrm{r}}^{-}(x;E) \tag{B.2}$$

as the basis of Theorem 3, then Eqs. (3.15), (3.18), (3.19), (4.10b), (B.1) and (B.2) lead to

$$\chi_{\mathrm{l}}^{+}(x;E) = -\frac{T(E)R_{\mathrm{r}}^{*}(E)}{T^{*}(E)}\sigma_1(x;E) + T(E)\sigma_2(x;E)\,, \tag{B.3}$$

$$\chi_{\mathrm{r}}^{-}(x';E) = T^{*}(E)\overline{\sigma_1(x';\overline{E})} - \frac{R_{\mathrm{l}}(E)T^{*}(E)}{T(E)}\overline{\sigma_2(x';\overline{E})}\,. \tag{B.4}$$

By substituting Eq. (B.3) into Eq. (3.17) and after some calculations, we get to

$$G(x,x';E) = \frac{2\pi}{\mathrm{i}}\left[-\frac{R_{\mathrm{r}}^{*}(E)}{T^{*}(E)}\sigma_1(x;E)\overline{\sigma_2(x';\overline{E})} + \sigma_2(x;E)\overline{\sigma_2(x';\overline{E})}\right]\,,$$
$$\mathrm{Re}(E)>0, \mathrm{Im}(E)>0\,,\ x>x'\,. \tag{B.5}$$

By substituting Eq. (B.4) into Eq. (3.21) and after some calculations, we get to

$$G(x,x';E) = \frac{2\pi}{\mathrm{i}}\left[-\sigma_1(x;E)\overline{\sigma_1(x';\overline{E})} + \frac{R_{\mathrm{l}}(E)}{T(E)}\sigma_1(x;E)\overline{\sigma_2(x';\overline{E})}\right]\,,$$
$$\mathrm{Re}(E)>0, \mathrm{Im}(E)<0\,,\ x>x'\,. \tag{B.6}$$

By comparing (4.2) to (B.5) we obtain

$$\theta_{ij}^{+}(E) = \begin{pmatrix} 0 & -\frac{2\pi}{\mathrm{i}}\frac{R_{\mathrm{r}}^{*}(E)}{T^{*}(E)} \\ 0 & \frac{2\pi}{\mathrm{i}} \end{pmatrix}\,, \quad \mathrm{Re}(E)>0\,,\ \mathrm{Im}(E)>0\,. \tag{B.7}$$

By comparing (4.2) to (B.6) we obtain

$$\theta_{ij}^{+}(E) = \begin{pmatrix} -\frac{2\pi}{\mathrm{i}} & \frac{2\pi}{\mathrm{i}}\frac{R_{\mathrm{l}}(E)}{T(E)} \\ 0 & 0 \end{pmatrix}\,, \quad \mathrm{Re}(E)>0\,,\ \mathrm{Im}(E)<0\,. \tag{B.8}$$

As expected, the functions $\theta_{11}^{+}(E)$ and $\theta_{22}^{+}(E)$ both have a branch cut along the spectrum of H.

The measures ϱ_{ij} of Theorem 3 can be readily obtained from Eqs. (B.7) and (B.8). The measure ϱ_{21} is clearly zero. So is the measure ϱ_{12}, since

$$\varrho_{12}((E_1,E_2)) = \int_{E_1}^{E_2} -\left(\frac{R_{\mathrm{l}}(E)}{T(E)} - \frac{R_{\mathrm{r}}^{*}(E)}{T^{*}(E)}\right)\mathrm{d}E = 0\,. \tag{B.9}$$

The measures ϱ_{11} and ϱ_{22} are simply the Lebesgue measure:

$$\varrho_{11}((E_1, E_2)) = \varrho_{22}((E_1, E_2)) = \int_{E_1}^{E_2} \mathrm{d}E = E_2 - E_1 \, . \tag{B.10}$$

Appendix C. Proofs of propositions

In this appendix, we provide the proofs of some propositions we stated in the main body of the paper. For the sake of clarity, in the proofs we shall denote the antidual and dual extensions of H by respectively $H^\times$ and H'.

Proof of Proposition 1. (*i*) This is immediate.

(*ii*) From the definition of $\mathcal{D}$, Eq. (6.1), and from the expressions of the differential operators associated to P, Q and H, it can be seen after straightforward (though tedious) calculations that $\mathcal{D}$ is stable under the algebra of observables. It is also easy to see that $\mathcal{D}$ is indeed the largest subdomain of $L^2(\mathbb{R}, \mathrm{d}x)$ that remains stable under the action of the algebra of observables, i.e., $\mathcal{D}$ is the maximal invariant subspace of $\mathcal{A}$.

That P, Q and H are essentially self-adjoint over $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ is obvious, since their only possible self-adjoint extensions are those with domains $\mathcal{D}(P)$, $\mathcal{D}(Q)$ and $\mathcal{D}(H)$.

In order to prove that H is $\tau_{\mathbf{\Phi}}$-continuous, we just have to realize that

$$\begin{aligned} \|H\varphi\|_{n,m,l} &= \|P^n Q^m H^l H\varphi\| \\ &= \|\varphi\|_{n,m,l+1} \, . \end{aligned} \tag{C.1}$$

In order to prove that P and Q are $\tau_{\mathbf{\Phi}}$-continuous, we need the following commutation relations:

$$[H^n, Q] = -\frac{1}{\mathrm{m}} n\mathrm{i}\hbar P H^{n-1} \, , \ n = 1, 2, \ldots \tag{C.2}$$

where m refers to the mass,

$$[Q^n, P] = n\mathrm{i}\hbar Q^{n-1} \, , \ n = 1, 2, \ldots \tag{C.3}$$

and

$$[H^n, P] = 0 \, , \ n = 1, 2, \ldots . \tag{C.4}$$

(Note that all these commutation relations are well defined on $\mathbf{\Phi}$.) Then, the $\tau_{\mathbf{\Phi}}$-continuity of P follows from

$$\begin{aligned} \|P\varphi\|_{n,m,l} &= \|P^n Q^m H^l P\varphi\| \\ &= \|P^n Q^m P H^l \varphi\| \qquad \text{from (C.4)} \\ &= \|P^n (P Q^m + m\mathrm{i}\hbar Q^{m-1}) H^l \varphi\| \qquad \text{from (C.3)} \\ &\leq \|P^{n+1} Q^m H^l \varphi\| + m\hbar \|P^n Q^{m-1} H^l \varphi\| \\ &= \|\varphi\|_{n+1,m,l} + m\hbar \|\varphi\|_{n,m-1,l} \, , \end{aligned} \tag{C.5}$$

and the $\tau_{\mathbf{\Phi}}$-continuity of Q follows from

$$
\begin{aligned}
\|Q\varphi\|_{n,m,l} &= \|P^nQ^mH^lQ\varphi\| \\
&= \|P^nQ^m(QH^l - \frac{1}{\mathrm{m}}li\hbar PH^{l-1})\varphi\| \qquad \text{from (C.2)} \\
&\leq \|P^nQ^{m+1}H^l\varphi\| + \frac{1}{\mathrm{m}}l\hbar\|P^nQ^mPH^{l-1}\varphi\| \\
&= \|\varphi\|_{n,m+1,l} + \frac{1}{\mathrm{m}}l\hbar\|P^n(PQ^m + mi\hbar Q^{m-1})H^{l-1}\varphi\| \qquad \text{from (C.3)} \\
&\leq \|\varphi\|_{n,m+1,l} + \frac{1}{\mathrm{m}}l\hbar\left(\|P^{n+1}Q^mH^{l-1}\varphi\| + m\hbar\|P^nQ^{m-1}H^{l-1}\varphi\|\right) \\
&= \|\varphi\|_{n,m+1,l} + \frac{1}{\mathrm{m}}l\hbar\|\varphi\|_{n+1,m,l-1} + \frac{1}{\mathrm{m}}l\hbar^2m\|\varphi\|_{n,m-1,l-1}\,. \qquad \text{(C.6)}
\end{aligned}
$$

In order to show that $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ is dense in $L^2(\mathbb{R},\mathrm{d}x)$, we need to define the space of infinitely differentiable functions with compact support that vanish at $x=a,b$ along with all their derivatives [16]:

$$
\begin{aligned}
C_0^\infty(\mathbb{R}\text{-}\{a,b\}) := \{f \in L^2(\mathbb{R},\mathrm{d}x) \ : \ & f \in C^\infty(\mathbb{R})\,, f^{(n)}(a) = f^{(n)}(b) = 0\,, \\
& f \text{ has compact support}\}\,. \qquad \text{(C.7)}
\end{aligned}
$$

Because

$$
C_0^\infty(\mathbb{R}\text{-}\{a,b\}) \subset \mathcal{S}(\mathbb{R}\text{-}\{a,b\})\,, \tag{C.8}
$$

and because $C_0^\infty(\mathbb{R}\text{-}\{a,b\})$ is dense in $L^2(\mathbb{R},\mathrm{d}x)$ [16], the space $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$ is dense in $L^2(\mathbb{R},\mathrm{d}x)$.

(*iii*) From definition (6.10), it is pretty easy to see that $|E^{\pm}\rangle_{\mathrm{l,r}}$ are antilinear functionals. In order to show that $|E^{\pm}\rangle_{\mathrm{l,r}}$ are continuous, we define

$$
\mathcal{M}_{\mathrm{l,r}}^{\pm}(E) := \sup_{x\in\mathbb{R}} \left|\chi_{\mathrm{l,r}}^{\pm}(x;E)\right| \tag{C.9}
$$

and

$$
C_{\mathrm{l,r}}^{\pm}(E) := \mathcal{M}_{\mathrm{l,r}}^{\pm}(E)\left(\int_{-\infty}^{\infty}\mathrm{d}x\,\frac{1}{(1+x^2)^2}\right)^{1/2}\,. \tag{C.10}
$$

Since

$$
\begin{aligned}
|\langle\varphi|E^{\pm}\rangle_{\mathrm{l,r}}| &= \left|\int_{-\infty}^{\infty}\mathrm{d}x\,\overline{\varphi(x)}\chi_{\mathrm{l,r}}^{\pm}(x;E)\right| \\
&\leq \mathcal{M}_{\mathrm{l,r}}^{\pm}(E)\int_{-\infty}^{\infty}\mathrm{d}x\,|\varphi(x)| \\
&= \mathcal{M}_{\mathrm{l,r}}^{\pm}(E)\int_{-\infty}^{\infty}\mathrm{d}x\,\frac{1}{1+x^2}(1+x^2)|\varphi(x)| \\
&\leq \mathcal{M}_{\mathrm{l,r}}^{\pm}(E)\left(\int_{-\infty}^{\infty}\mathrm{d}x\,\frac{1}{(1+x^2)^2}\right)^{1/2}\left(\int_{-\infty}^{\infty}\mathrm{d}x\,\left|(1+x^2)\varphi(x)\right|^2\right)^{1/2} \\
&= C_{\mathrm{l,r}}^{\pm}(E)\,\|(1+Q^2)\varphi\| \\
&\leq C_{\mathrm{l,r}}^{\pm}(E)\,(\|\varphi\| + \|Q^2\varphi\|)
\end{aligned}
$$

$$= C^{\pm}_{\mathrm{l,r}}(E)\,(\|\varphi\|_{0,0,0} + \|\varphi\|_{0,2,0})\,, \tag{C.11}$$

the functionals $|E^{\pm}\rangle_{\mathrm{l,r}}$ are continuous when $\mathbf{\Phi}$ is endowed with the topology $\tau_{\mathbf{\Phi}}$. The proof that $|p\rangle$ and $|x\rangle$ are also continuous antilinear functionals over $\mathbf{\Phi}$ is similar.

(*iv*) In order to prove that $|E^{\pm}\rangle_{\mathrm{l,r}}$ are generalized eigenvectors of H, we make use of the conditions (6.1) and (6.3) satisfied by the elements of $\mathbf{\Phi}$,

$$\begin{aligned}
\langle\varphi|H^{\times}|E^{\pm}\rangle_{\mathrm{l,r}} &= \langle H^{\dagger}\varphi|E^{\pm}\rangle_{\mathrm{l,r}} \\
&= \int_{-\infty}^{\infty} \mathrm{d}x \left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right)\overline{\varphi(x)}\chi^{\pm}_{\mathrm{l,r}}(x;E) \\
&= -\frac{\hbar^2}{2m}\left[\frac{\mathrm{d}\overline{\varphi(x)}}{\mathrm{d}x}\chi^{\pm}_{\mathrm{l,r}}(x;E)\right]_{-\infty}^{\infty} + \frac{\hbar^2}{2m}\left[\overline{\varphi(x)}\frac{\mathrm{d}\chi^{\pm}_{\mathrm{l,r}}(x;E)}{\mathrm{d}x}\right]_{-\infty}^{\infty} \\
&\quad + \int_{-\infty}^{\infty} \mathrm{d}x\, \overline{\varphi(x)}\left(-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\right)\chi^{\pm}_{\mathrm{l,r}}(x;E) \\
&= E\int_{-\infty}^{\infty} \mathrm{d}x\, \overline{\varphi(x)}\chi^{\pm}_{\mathrm{l,r}}(x;E) \\
&= E\langle\varphi|E^{\pm}\rangle_{\mathrm{l,r}}\,.
\end{aligned} \tag{C.12}$$

The proof that $|p\rangle$ and $|x\rangle$ are generalized eigenvectors of P and Q, respectively, is similar.

□

Proof of Proposition 2. (*i*) It is clear from definitions (6.16), (6.18) and (6.20) that $\langle p|$, $\langle x|$ and ${}_{\mathrm{l,r}}\langle^{\pm}E|$ are *linear* functionals over $\mathbf{\Phi}$. Because

$$\begin{aligned}
\left|{}_{\mathrm{l,r}}\langle^{\pm}E|\varphi\rangle\right| &= \left|\langle\varphi|E^{\pm}\rangle_{\mathrm{l,r}}\right| && \text{from (6.21)} \\
&\leq C^{\pm}_{\mathrm{l,r}}(E)\,(\|\varphi\|_{0,0,0} + \|\varphi\|_{0,2,0})\,, && \text{from (C.11)}
\end{aligned} \tag{C.13}$$

the bras ${}_{\mathrm{l,r}}\langle^{\pm}E|$ are continuous. That $|p\rangle$ and $|x\rangle$ are also continuous over $\mathbf{\Phi}$ can be proved in a similar way.

(*ii*) Because

$$\begin{aligned}
{}_{\mathrm{l,r}}\langle^{\pm}E|H'|\varphi\rangle &= {}_{\mathrm{l,r}}\langle^{\pm}E|H^{\dagger}\varphi\rangle \\
&= \overline{\langle H^{\dagger}\varphi|E^{\pm}\rangle}_{\mathrm{l,r}} && \text{from (6.21)} \\
&= E\,\overline{\langle\varphi|E^{\pm}\rangle}_{\mathrm{l,r}} && \text{from (C.12)} \\
&= E\;{}_{\mathrm{l,r}}\langle^{\pm}E|\varphi\rangle\,, && \text{from (6.21)}
\end{aligned} \tag{C.14}$$

the bras ${}_{\mathrm{l,r}}\langle^{\pm}E|$ are generalized left-eigenvectors of H.

Similarly, it can be proved that $\langle p|$ and $\langle x|$ are generalized left-eigenvectors of respectively P and Q. □

Proof of Proposition 3. We only need to prove Eqs. (6.38)-(6.43), since Eqs. (6.35)-(6.37) were proved in Proposition 1. Let us start with Eq. (6.38). Take φ and ψ in $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$. Because $U_{\pm}$ of Eq. (5.9) are unitary, we have that

$$(\varphi, \psi) = (U_{\pm}\varphi, U_{\pm}\psi) = (\widehat{\varphi}^{\pm}, \widehat{\psi}^{\pm}) \, . \tag{C.15}$$

Since $\widehat{\varphi}^{\pm}$ and $\widehat{\psi}^{\pm}$ are in particular elements of $L^2([0,\infty), \mathrm{d}E) \oplus L^2([0,\infty), \mathrm{d}E)$, their scalar product is given by

$$(\widehat{\varphi}^{\pm}, \widehat{\psi}^{\pm}) = \int_0^{\infty} \mathrm{d}E \, \overline{\widehat{\varphi}_{\mathrm{l}}^{\pm}(E)} \, \widehat{\psi}_{\mathrm{l}}^{\pm}(E) + \int_0^{\infty} \mathrm{d}E \, \overline{\widehat{\varphi}_{\mathrm{r}}^{\pm}(E)} \, \widehat{\psi}_{\mathrm{r}}^{\pm}(E) \, . \tag{C.16}$$

Since φ and ψ belong to $\mathcal{S}(\mathbb{R}\text{-}\{a,b\})$, the actions of the eigenkets and eigenbras of H are well defined on them:

$$\langle \varphi | E^{\pm} \rangle_{\mathrm{l,r}} = \overline{\widehat{\varphi}_{\mathrm{l,r}}^{\pm}(E)} \, , \tag{C.17}$$

$$_{\mathrm{l,r}}\langle {}^{\pm}E | \psi \rangle = \widehat{\psi}_{\mathrm{l,r}}^{\pm}(E) \, . \tag{C.18}$$

By plugging Eqs. (C.17) and (C.18) into Eq. (C.16), and Eq. (C.16) into Eq. (C.15), we get to Eq. (6.38).

It is clear that the trick to prove (6.38) was to go to the energy representation by way of $U_{\pm}$, in which representation H acts as the multiplication operator. The same trick can be used to prove Eq. (6.41). A similar trick applies to the proof of equations (6.39) and (6.42), although instead of $U_{\pm}$ we must use the Fourier transform to go to the momentum representation, where P acts as the multiplication operator. The calculations are straightforward and will not be reproduced here. Finally, Eqs. (6.40) and (6.43) are immediate. □

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[12] Note that, because we dealt with the radial part of a spherical shell potential for zero angular momentum, in Refs. [9, 11] we used the unfortunate term *square barrier potential*, although we should have used *spherical shell potential*. Analogously, in Ref. [10], we used the unfortunate term *square well-barrier potential*.

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