Rigged Hilbert Space Approach to the Schrödinger Equation

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Abstract

It is shown that the natural framework for the solutions of any Schrödinger equation whose spectrum has a continuous part is the Rigged Hilbert Space rather than just the Hilbert space. The difficulties of using only the Hilbert space to handle unbounded Schrödinger Hamiltonians whose spectrum has a continuous part are disclosed. Those difficulties are overcome by using an appropriate Rigged Hilbert Space (RHS). The RHS is able to associate an eigenket to each energy in the spectrum of the Hamiltonian, regardless of whether the energy belongs to the discrete or to the continuous part of the spectrum. The collection of eigenkets corresponding to both discrete and continuous spectra forms a basis system that can be used to expand any physical wave function. Thus the RHS treats discrete energies (discrete spectrum) and scattering energies (continuous spectrum) on the same footing.

1. INTRODUCTION

Several authors have realized that the Hilbert space is not sufficient for the purposes of Quantum Mechanics, and that an extension of the Hilbert space to the Rigged Hilbert Space (RHS) is needed. The RHS was introduced in physics for the first time in the 1960s independently by J. P. Antoine [1], A. Bohm [2], and J. E. Roberts [3]. These authors realized that the RHS provides a rigorous mathematical rephrasing of Dirac's formalism. In essence, the Nuclear Spectral Theorem [4] (also known as Gelfand-Maurin Theorem) restates Dirac basis vector expansion along with the Dirac bras and kets within a mathematical theory. Later on, other authors such as A. Galindo and P. Pascual [5], and O. Melsheimer [6] came to the same conclusion.

Earlier attempts to go beyond the Hilbert space framework are reported in Refs. [7,8]. If two operators of the algebra of observables satisfy Heisenberg's commutation relation, at least one of them cannot be continuous (bounded) with respect to the Hilbert space topology. In Refs. [7,8], it is shown that there are subdomains of the Hilbert space that can be endowed with topologies that make those operators continuous.

Since the early 1990s, the RHS has become a standard tool in many areas of theoretical physics, especially in those that deal with continuous and resonance spectra. For instance, the RHS has been used to treat the Lippmann-Schwinger equation [9,10], the Gamow vectors (cf. [9,11–14] and references therein), and certain generalized spectral decompositions of chaotic maps [15,16].

The dynamical equation of Quantum Mechanics is the Schrödinger equation. Thus any attempt to show that the RHS contains the mathematical methods needed by Quantum Mechanics should show that the natural framework for the solutions of the Schrödinger equation is the RHS. The objective of this paper is to show that the solutions of the Schrödinger equation fall in a RHS. To illustrate this, we shall use the example of the square well-barrier potential Hamiltonian. We recall that none of Refs. [10–16] took the Schrödinger equation as the dynamical equation.

A RHS is a triplet of spaces

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

where $\mathcal{H}$ is a Hilbert space, $\mathbf{\Phi}$ is a dense subspace of the Hilbert space, and $\mathbf{\Phi}^{\times}$ is the dual space of $\mathbf{\Phi}$, i.e., $\mathbf{\Phi}^{\times}$ is the set of antilinear functionals over the space $\mathbf{\Phi}$. The space $\mathbf{\Phi}$ has a topology that is finer than the topology inherited from $\mathcal{H}$. The domain $\mathcal{D}(H)$ of the Hamiltonian lies between $\mathbf{\Phi}$ and $\mathcal{H}$,

$$\mathbf{\Phi} \subset \mathcal{D}(H) \subset \mathcal{H} \, . \tag{1.2}$$

If a Schrödinger Hamiltonian is defined on the whole Hilbert space and has only discrete spectrum, then the Hilbert space is sufficient for the purposes of Quantum Mechanics. However, if the Hamiltonian is not defined on the whole Hilbert space (e.g., it is unbounded) and its spectrum has a continuous part, then the mathematical methods of the Hilbert space are not sufficient, and an extension of those methods is needed. The RHS arises as the natural extension when dealing with unbounded operators that have continuous spectrum.

The reason why the RHS is the extension of the Hilbert space that we need is twofold. On the one hand, one of the key assumptions of Quantum Mechanics is that the quantity

$$(\varphi, H\varphi) \tag{1.3}$$

accounts for the expectation value of the measurement of the observable H in the state φ, and that

$$\Delta_{\varphi} H = \sqrt{(\varphi, H^2\varphi) - (\varphi, H\varphi)^2} \tag{1.4}$$

accounts for the uncertainty of the measurement of the observable H in the state φ. The expectation value (1.3) cannot be computed for every element of the Hilbert space $\mathcal{H}$, but only for those $\varphi \in \mathcal{H}$ that also belong to $\mathcal{D}(H)$. Similarly, the uncertainty (1.4) cannot be computed for every element of $\mathcal{H}$ either. If we take as physical states those square integrable functions for which physical quantities such as the expectation value (1.3) and the uncertainty (1.4) can be computed, then not every square integrable function (i.e., every element of $\mathcal{H}$) can represent a physical state. As we shall see, the natural space of physical wave functions is the space $\mathbf{\Phi}$ in (1.1), because all physical quantities such as expectation values and uncertainties can be computed for its elements.

On the other hand, in Quantum Mechanics it is assumed that for each energy in the spectrum of the Hamiltonian H, there corresponds a ket that is an eigenvector of H. If we denote the ket corresponding to an energy E_n in the discrete spectrum by $|E_n)$ and denote the ket corresponding to an energy E in the continuous spectrum by $|E\rangle$, then we should have

$$H|E_n) = E_n|E_n) \, , \tag{1.5a}$$

$$H|E\rangle = E|E\rangle \, . \tag{1.5b}$$

These eigenkets are normalized according to the following rule:

$$(E_n|E_m) = \delta_{nm} \, , \quad \langle E|E'\rangle = \delta(E - E') \, , \quad \langle E|E_n) = 0 \, . \tag{1.6}$$

It is also assumed that those kets form a complete basis that can be used to expand any wave function φ,

$$\varphi = \sum_n |E_n)(E_n|\varphi) + \int dE \, |E\rangle\langle E|\varphi\rangle \, . \tag{1.7}$$

The solutions of Eq. (1.5a) are square normalizable, i.e., they lie in the Hilbert space. However, the solutions of Eq. (1.5b) are not square normalizable, i.e., they lie outside the Hilbert space. Therefore, the Hilbert space is not large enough to contain the non-normalizable eigenkets that are associated to the energies in the continuous spectrum—a larger space than the Hilbert space is needed. This larger space, which contains the eigenkets $|E\rangle$, is the space $\mathbf{\Phi}^{\times}$ in (1.1). The action of the Hamiltonian, which is in principle defined only on the elements of $\mathbf{\Phi}$ (or on the elements of $\mathcal{D}(H)$), can be extended to the elements $|F\rangle$ of $\mathbf{\Phi}^{\times}$ by defining the following conjugate operator $H^{\times}$:

$$\langle \varphi|H^{\times}|F\rangle := \langle H^{\dagger}\varphi|F\rangle \, , \quad \forall \varphi \in \mathbf{\Phi} \, , \ |F\rangle \in \mathbf{\Phi}^{\times} \, . \tag{1.8}$$

The operator $H^{\times}$ is a uniquely defined extension of H. Using definition (1.8), the RHS formalism restates Eq. (1.5b) as

$$\langle\varphi|H^{\times}|E\rangle = \langle H^{\dagger}\varphi|E\rangle = E\langle\varphi|E\rangle\,, \quad \forall\varphi\in\mathbf{\Phi}\,. \tag{1.9}$$

When the arbitrary $\varphi \in \mathbf{\Phi}$ is omitted in this equation, we recover the formal equation (1.5b).

In this way, the Gelfand triplet (1.1) arises in a natural way. The Hilbert space $\mathcal{H}$ appears because the wave functions must be square normalizable. The subspace $\mathbf{\Phi}$ is the set of physical wave functions, i.e., the set of square integrable functions for which any expectation value and any uncertainty can be computed. The dual space $\mathbf{\Phi}^{\times}$ contains the eigenkets associated to energies in the continuous part of the spectrum of H. These eigenkets are defined as functionals over the space $\mathbf{\Phi}$, and they can be used to expand any $\varphi \in \mathbf{\Phi}$ as in Eq. (1.7). The eigenequation (1.5b) holds within the RHS in the sense of Eq. (1.9). Thus the Rigged Hilbert Space is the extension of the Hilbert space that is needed when the solutions of the Schrödinger equation are not normalizable. These non-normalizable solutions are treated as distributions in the dual space $\mathbf{\Phi}^{\times}$.

Unlike the Hilbert space, the RHS treats the discrete and continuous spectra on the same footing: for each energy of the spectrum of the Hamiltonian (either in the discrete or in the continuous part), there is an eigenket of the Hamiltonian (given by Eq. (1.5a) in the discrete case, and by Eq. (1.5b) in the continuous case) that belongs to a basis that expands any physical wave function as in Eq. (1.7).

The main shortcoming of the RHS theory is that it does not provide a prescription to construct the space $\mathbf{\Phi}$ and the eigenvectors $|E\rangle$. The general statement of the Nuclear Spectral Theorem [4] just assures the existence of the generalized eigenvectors $|E\rangle$. In that theorem, the space $\mathbf{\Phi}$ is assumed to be given beforehand. In this paper, the RHS of the square well-barrier will be constructed explicitly along with the eigenkets $|E\rangle$ by applying the method proposed in Ref. [9]. This method has been successfully applied to a Hamiltonian with purely continuous spectrum: the square *barrier* Hamiltonian [17]. Here we apply it to a Hamiltonian with both discrete and continuous spectrum: the square *well-barrier* Hamiltonian.

The steps of our method can be summarized as follows:

(i) Construction of the self-adjoint Hamiltonian from the formal Schrödinger differential operator.

(ii) Construction of the Green function and therewith of the resolvent.

(iii) Computation of the spectrum of the Hamiltonian.

(iv) Construction of the direct integral decomposition.

(v) Construction of the Rigged Hilbert Space.

Steps (i)-(iv) will be addressed by using the Sturm-Liouville theory [18]. Step (v) will be handled by the methods proposed in Ref. [9].

In Section 2, we construct the self-adjoint Hamiltonian from the formal Schrödinger differential operator and from a domain of the Hilbert space. In Section 3, we construct the Green function and the resolvent of H. In Section 4, we compute the spectrum of the Hamiltonian. In Section 5, we construct the direct integral decomposition of the Hilbert space generated by the Hamiltonian. In Section 6, the RHS of the square well-barrier Hamiltonian is constructed.

2. FORMAL DIFFERENTIAL OPERATOR AND SELF-ADJOINT HAMILTONIAN

The first step toward the construction of a RHS associated to a Hamiltonian is to define that Hamiltonian. In non-relativistic quantum mechanics, the Hamiltonian is defined by the formal differential operator of the time-independent Schrödinger equation and by a Hilbert space domain on which the Hamiltonian acts.

The time-independent Schrödinger equation reads in the position representation as

$$\left(\frac{-\hbar^2}{2m}\Delta + V(\vec{x})\right)\langle\vec{x}|E\rangle = E\langle\vec{x}|E\rangle\,, \tag{2.1}$$

where Δ is the three-dimensional Laplacian and

$$V(\vec{x}) \equiv V(r) = \begin{cases} -V_1 & 0<r<a \\ V_2 & a<r<b \\ 0 & b<r<\infty \end{cases} \tag{2.2}$$

is the well-square potential, V_1 and V_2 being two positive real numbers. The potential $V(\vec{x})$ is rotational invariant, and spherical coordinates $\vec{x} \equiv (r,\theta,\phi)$ can be used to write Eq. (2.1) as

$$\left(\frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right)\langle r,\theta,\phi|E,l,l_3\rangle = E\langle r,\theta,\phi|E,l,l_3\rangle\,. \tag{2.3}$$

By splitting radial and angular dependences,

$$\langle r,\theta,\phi|E,l,l_3\rangle \equiv \langle r|E\rangle_l\,\langle\theta,\phi|l,l_3\rangle \equiv \frac{1}{r}\chi_l(r;E)Y_{l,l_3}(\theta,\phi), \tag{2.4}$$

where $Y_{l,l_3}(\theta,\phi)$ are the spherical harmonics, we obtain for the radial part

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2} + V(r)\right)\chi_l(r;E) = E\chi_l(r;E)\,. \tag{2.5}$$

For simplicity we study only the case $l=0$. Writing $\chi_{l=0}(r;E) \equiv \chi(r;E)$,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r)\right)\chi(r;E) = E\chi(r;E)\,. \tag{2.6}$$

Therefore, the formal Schrödinger differential operator for the zero angular momentum case is

$$h \equiv -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r)\,. \tag{2.7}$$

In order to construct the domain $\mathcal{D}(H)$ of the Hamiltonian, we need first the Hilbert space that contains it. Clearly, the Hilbert space that fits the differential operator (2.7) is $L^2([0,\infty),dr)$. Now, each element f in the domain $\mathcal{D}(H)$ must be square integrable (see condition (2.9a) below), the action of h on f must be well-defined (see condition (2.9b) below), and the action of h on f must remain square integrable (see condition (2.9c) below). Furthermore, the Hamiltonian H induced by h and by $\mathcal{D}(H)$ must be self-adjoint. It is well-known that all the possible self-adjoint operators associated to the formal differential operator (2.7) are determined by the following condition (cf. [18], page 1306):

$$f(0) + \alpha f'(0) = 0\,, \quad -\infty < \alpha \leq \infty\,. \tag{2.8}$$

Among all the possibilities in Eq. (2.8), the one that is used in physics is $\alpha = 0$, i.e., $f(0) = 0$. All the above mentioned conditions, which determine the domain $\mathcal{D}(H)$, can be written as

$$f(r) \in L^2([0,\infty), dr)\,, \tag{2.9a}$$
$$f(r) \in AC^2[0,\infty)\,, \tag{2.9b}$$
$$(hf)(r) \in L^2([0,\infty), dr)\,, \tag{2.9c}$$
$$f(0) = 0\,, \tag{2.9d}$$

where $AC^2([0,\infty))$ denotes the space of all functions f which have a continuous derivative in $[0,\infty)$, and for which f' is not only continuous but also absolutely continuous over each compact subinterval of $[0,\infty)$. Thus the domain of our Hamiltonian is

$$\mathcal{D}(H) = \{f \in L^2([0,\infty), dr) \mid f \in AC^2[0,\infty), hf \in L^2([0,\infty), dr), f(0) = 0\}\,. \tag{2.10}$$

It follows that the Hamiltonian defined by

$$(Hf)(r) := (hf)(r)\,, \quad f \in \mathcal{D}(H) \tag{2.11}$$

is a well-defined self-adjoint linear operator.

3. RESOLVENT AND GREEN FUNCTION

The second step toward the construction of the RHS is to compute the resolvent and the Green function of the (self-adjoint) Hamiltonian. The resolvent operator of H is defined as the inverse of the operator $(E-H)$ for those complex energies E for which that inverse exists. If we write the resolvent operator as an integral operator, the kernel of that integral operator is precisely the Green function,

$$\left[(E-H)^{-1}f\right](r) = \int_0^\infty ds\, G(r,s;E) f(s)\,. \tag{3.1}$$

The Green function $G(r,s;E)$ can be computed using the prescription provided by the following theorem (cf. Theorem XIII.3.16 of Ref. [18] and also Ref. [19]):

Theorem 1 Let H be the self-adjoint operator (2.11) derived from the real formal differential operator (2.7) by the imposition of the boundary condition (2.9d). Let $\mathrm{Im}(E) \neq 0$. Then there is exactly one solution $\chi(r;E)$ of $(h-E)\sigma = 0$ square-integrable at 0 and satisfying the boundary condition (2.9d), and exactly one solution $\Theta(r;E)$ of $(h-E)\sigma = 0$ square-integrable at infinity. The resolvent $(E-H)^{-1}$ is an integral operator whose kernel $G(r,s;E)$ is given by

$$G(r,s;E)=\left\{\begin{array}{ll} \frac{2m}{\hbar^2}\,\frac{\chi(r;E)\,\Theta(s;E)}{W(\chi,\Theta)} & r<s \\ \frac{2m}{\hbar^2}\,\frac{\chi(s;E)\,\Theta(r;E)}{W(\chi,\Theta)} & r>s\,, \end{array}\right. \tag{3.2}$$

where $W(\chi,\Theta)$ is the Wronskian of χ and Θ,

$$W(\chi,\Theta)=\chi\Theta'-\chi'\Theta\,. \tag{3.3}$$

In order to compute $G(r,s;E)$, we shall divide the complex energy plane in three different regions and obtain $G(r,s;E)$ for each region separately. In our calculations, we shall use the following branch of the square root function:

$$\sqrt{\cdot}:\{E\in\mathbb{C}\,|\ -\pi<\arg(E)\leq\pi\}\longmapsto\{E\in\mathbb{C}\,|\ -\pi/2<\arg(E)\leq\pi/2\}\,. \tag{3.4}$$

3.1. Region $\mathrm{Re}(E)<0$, $\mathrm{Im}(E)\neq 0$

We first apply Theorem 1 to the region of the complex energy plane where $\mathrm{Re}(E)<0$ and $\mathrm{Im}(E)\neq 0$. According to that theorem, the Green function reads

$$G(r,s;E)=\left\{\begin{array}{ll} -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\,\frac{\widetilde{\chi}(r;E)\,\widetilde{\Theta}(s;E)}{2\widetilde{\mathcal{J}}_3(E)} & r<s \\ -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\,\frac{\widetilde{\chi}(s;E)\,\widetilde{\Theta}(r;E)}{2\widetilde{\mathcal{J}}_3(E)} & r>s \end{array}\right. \qquad \mathrm{Re}(E)<0\,,\ \mathrm{Im}(E)\neq 0\,. \tag{3.5}$$

In this equation, the eigenfunction $\widetilde{\chi}(r;E)$ satisfies the time-independent Schrödinger equation (2.6) subject to the following boundary conditions:

$$\widetilde{\chi}(0;E)=0\,, \tag{3.6a}$$
$$\widetilde{\chi}(r;E)\in AC^2([0,\infty))\,, \tag{3.6b}$$
$$\widetilde{\chi}(r;E)\ \text{is square integrable at}\ 0\,, \tag{3.6c}$$

which yield

$$\widetilde{\chi}(r;E)=\left\{\begin{array}{ll} \frac{i}{2}\left(e^{\sqrt{-\frac{2m}{\hbar^2}(E+V_1)}\,r}-e^{-\sqrt{-\frac{2m}{\hbar^2}(E+V_1)}\,r}\right) & 0<r<a \\ \widetilde{\mathcal{J}}_1(E)e^{\sqrt{-\frac{2m}{\hbar^2}(E-V_2)}\,r}+\widetilde{\mathcal{J}}_2(E)e^{-\sqrt{-\frac{2m}{\hbar^2}(E-V_2)}\,r} & a<r<b \\ \widetilde{\mathcal{J}}_3(E)e^{\sqrt{-\frac{2m}{\hbar^2}E}\,r}+\widetilde{\mathcal{J}}_4(E)e^{-\sqrt{-\frac{2m}{\hbar^2}E}\,r} & b<r<\infty\,. \end{array}\right. \tag{3.7}$$

The expressions of the functions $\widetilde{\mathcal{J}}_1(E)$-$\widetilde{\mathcal{J}}_4(E)$ can be found in Appendix A.

The eigenfunction $\widetilde{\Theta}(r;E)$ of Eq. (3.5) satisfies the time-independent Schrödinger equation (2.6) subject to the following boundary conditions:

$$\widetilde{\Theta}(r;E)\in AC^2([0,\infty))\,, \tag{3.8a}$$
$$\widetilde{\Theta}(r;E)\ \text{is square integrable at}\ \infty\,, \tag{3.8b}$$

which yield

$$\widetilde{\Theta}(r;E)=\begin{cases}\widetilde{\mathcal{A}}_1(E)e^{\sqrt{-\frac{2m}{\hbar^2}(E+V_1)}\,r}+\widetilde{\mathcal{A}}_2(E)e^{-\sqrt{-\frac{2m}{\hbar^2}(E+V_1)}\,r} & 0<r<a\\ \widetilde{\mathcal{A}}_3(E)e^{\sqrt{-\frac{2m}{\hbar^2}(E-V_2)}\,r}+\widetilde{\mathcal{A}}_4(E)e^{-\sqrt{-\frac{2m}{\hbar^2}(E-V_2)}\,r} & a<r<b\\ e^{-\sqrt{-\frac{2m}{\hbar^2}E}\,r} & b<r<\infty\,.\end{cases} \tag{3.9}$$

The expressions of the functions $\widetilde{\mathcal{A}}_1(E)$-$\widetilde{\mathcal{A}}_4(E)$ can be found in Appendix A.

3.2. Region $\mathrm{Re}(E)>0$, $\mathrm{Im}(E)>0$

In this region of the complex plane, Theorem 1 leads to the following Green function:

$$G(r,s;E)=\begin{cases}\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(r;E)\,\Theta_+(s;E)}{2i\mathcal{J}_4(E)} & r<s\\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(s;E)\,\Theta_+(r;E)}{2i\mathcal{J}_4(E)} & r>s\end{cases}\qquad \mathrm{Re}(E)>0\,,\ \mathrm{Im}(E)>0\,. \tag{3.10}$$

In this equation, the eigenfunction $\chi(r;E)$ satisfies the differential equation (2.6) subject to the boundary conditions (3.6),

$$\chi(r;E)=\begin{cases}\sin(\sqrt{\frac{2m}{\hbar^2}(E+V_1)}\,r) & 0<r<a\\ \mathcal{J}_1(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_2)}\,r}+\mathcal{J}_2(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_2)}\,r} & a<r<b\\ \mathcal{J}_3(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}\,r}+\mathcal{J}_4(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}\,r} & b<r<\infty\,.\end{cases} \tag{3.11}$$

The functions $\mathcal{J}_1(E)$-$\mathcal{J}_4(E)$ are determined by the boundary conditions (3.6), and their expressions are listed in Appendix A.

The eigenfunction $\Theta_+(r;E)$ satisfies the differential equation (2.6) subject to the boundary conditions (3.8),

$$\Theta_+(r;E)=\begin{cases}\mathcal{A}_1^+(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E+V_1)}\,r}+\mathcal{A}_2^+(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E+V_1)}\,r} & 0<r<a\\ \mathcal{A}_3^+(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_2)}\,r}+\mathcal{A}_4^+(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_2)}\,r} & a<r<b\\ e^{i\sqrt{\frac{2m}{\hbar^2}E}\,r} & b<r<\infty\,.\end{cases} \tag{3.12}$$

The functions $\mathcal{A}_1^+(E)$-$\mathcal{A}_4^+(E)$ are determined by the boundary conditions (3.8), and their expressions are listed in Appendix A.

3.3. Region $\mathrm{Re}(E)>0$, $\mathrm{Im}(E)<0$

If $\mathrm{Re}(E)>0$, $\mathrm{Im}(E)<0$ and we use the branch of the square root function (3.4), then the Green function has the form

$$G(r,s;E)=\begin{cases}-\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(r;E)\,\Theta_-(s;E)}{2i\mathcal{J}_3(E)} & r<s\\ -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(s;E)\,\Theta_-(r;E)}{2i\mathcal{J}_3(E)} & r>s\end{cases}\qquad \mathrm{Re}(E)>0\,,\ \mathrm{Im}(E)<0\,. \tag{3.13}$$

The eigenfunction $\chi(r;E)$ satisfies the time-independent Schrödinger equation (2.6) subject to the boundary conditions (3.6). Thus $\chi(r;E)$ is given by Eq. (3.11)—hence the same symbol as in the previous subsection—although now E lies in the fourth quadrant of the complex energy plane.

The eigenfunction $\Theta_-(r;E)$ satisfies the differential equation (2.6) subject to the boundary conditions (3.8),

$$\Theta_-(r;E) = \begin{cases} \mathcal{A}_1^-(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E+V_1)}\,r} + \mathcal{A}_2^-(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E+V_1)}\,r} & 0<r<a \\ \mathcal{A}_3^-(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_2)}\,r} + \mathcal{A}_4^-(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_2)}\,r} & a<r<b \\ e^{-i\sqrt{\frac{2m}{\hbar^2}E}\,r} & b<r<\infty\,. \end{cases} \tag{3.14}$$

The functions $\mathcal{A}_1^-(E)$-$\mathcal{A}_4^-(E)$ are determined by the boundary conditions (3.8), and their expressions are listed in Appendix A.

4. SPECTRUM OF THE HAMILTONIAN

The third step toward the construction of the RHS is to obtain the (Hilbert space) spectrum Sp(H) of the self-adjoint Hamiltonian H. Since H is self-adjoint, the spectrum must be real. In order to elucidate which real numbers are in Sp(H) we make use of Theorem 3 below. Before stating Theorem 3, we need to state another theorem, which provides the unitary operator U that will be used to diagonalize H (cf. Theorem XIII.5.13 of Ref. [18]):

Theorem 2 (Weyl-Kodaira) Let h be the formally self-adjoint differential operator (2.7) defined on the interval $[0,\infty)$. Let H be the self-adjoint operator (2.11). Let Λ be an open interval of the real axis, and suppose that there is given a set $\{\sigma_1(r;E),\, \sigma_2(r;E)\}$ of functions, defined and continuous on $(0,\infty)\times\Lambda$, such that for each fixed E in Λ, $\{\sigma_1(r;E),\, \sigma_2(r;E)\}$ forms a basis for the space of solutions of $h\sigma = E\sigma$. Then there exists a positive 2×2 matrix measure $\{\rho_{ij}\}$ defined on Λ, such that the limit

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

exists in the topology of $L^2(\Lambda,\{\rho_{ij}\})$ for each f in $L^2([0,\infty),dr)$ and defines an isometric isomorphism U of $\mathsf{E}(\Lambda)L^2([0,\infty),dr)$ onto $L^2(\Lambda,\{\rho_{ij}\})$, $\mathsf{E}(\Lambda)$ being the spectral projection associated to Λ.

The spectral measures $\{\rho_{ij}\}$ are provided by the following theorem (cf. Theorem XIII.5.18 of Ref. [18]):

Theorem 3 (Titchmarsh-Kodaira) Let Λ be an open interval of the real axis, O be an open set in the complex plane containing Λ, and Re(H) := $\mathbb{C}$ − Sp(H). Let $\{\sigma_1(r;E),\, \sigma_2(r;E)\}$ 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 $(0,\infty)\times O$ and analytically dependent on E for E in O. Suppose that the kernel $G(r,s;E)$ for the resolvent $(E-H)^{-1}$ has a representation

$$G(r,s;E)=\begin{cases}\sum_{i,j=1}^{2}\theta_{ij}^{-}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})} & r<s\\ \sum_{i,j=1}^{2}\theta_{ij}^{+}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})} & r>s\,,\end{cases}\tag{4.2}$$

for all E in $\mathrm{Re}(H)\cap O$, and that $\{\rho_{ij}\}$ 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 $1\leq i,j\leq 2$,

$$\begin{aligned}\rho_{ij}((E_1,E_2)) &= \lim_{\delta\to 0}\lim_{\epsilon\to 0+}\tfrac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}[\theta_{ij}^{-}(E-i\epsilon)-\theta_{ij}^{-}(E+i\epsilon)]dE\\ &= \lim_{\delta\to 0}\lim_{\epsilon\to 0+}\tfrac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}[\theta_{ij}^{+}(E-i\epsilon)-\theta_{ij}^{+}(E+i\epsilon)]dE\,.\end{aligned}\tag{4.3}$$

Using these spectral measures we can compute the spectrum of H. This spectrum is the subset of the real line on which the Green function fails to be analytic. This non-analyticity of $G(r,s;E)$ will be built into the functions $\theta_{ij}^{\pm}(E)$ that appear in Theorem 3. From the expression of the Green function computed in Section 3, it is clear that the subsets $(-\infty,0)$ and $(0,\infty)$ should be studied separately. We will denote either of these subsets by Λ.

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

We first take Λ from Theorem 3 to be $(-\infty,0)$. We choose a basis for the space of solutions of the equation $h\sigma=E\sigma$ that is continuous on $(0,\infty)\times\Lambda$ and analytically dependent on E as

$$\sigma_1(r;E)=\begin{cases}\widetilde{\mathcal{B}}_1(E)e^{\sqrt{-\frac{2m}{\hbar^2}(E+V_1)}r}+\widetilde{\mathcal{B}}_2(E)e^{-\sqrt{-\frac{2m}{\hbar^2}(E+V_1)}r} & 0<r<a\\ \widetilde{\mathcal{B}}_3(E)e^{\sqrt{-\frac{2m}{\hbar^2}(E-V_2)}r}+\widetilde{\mathcal{B}}_4(E)e^{-\sqrt{-\frac{2m}{\hbar^2}(E-V_2)}r} & a<r<b\\ e^{\sqrt{-\frac{2m}{\hbar^2}E}r} & b<r<\infty\,,\end{cases}\tag{4.4a}$$

$$\sigma_2(r;E)=\widetilde{\Theta}(r;E)\,.\tag{4.4b}$$

The functions $\widetilde{\mathcal{B}}_1$-$\widetilde{\mathcal{B}}_4$ are such that $\sigma_1(r;E)$ and its derivative are continuous at $r=a$ and at $r=b$. Their expressions are listed in Eq. (A8) of Appendix A. The function $\widetilde{\Theta}(r;E)$ is given by Eq. (3.9). Obviously,

$$\widetilde{\chi}(r;E)=\widetilde{\mathcal{J}}_3(E)\sigma_1(r;E)+\widetilde{\mathcal{J}}_4(E)\sigma_2(r;E)\,,\tag{4.5}$$

which along with Eq. (3.5) leads to

$$G(r,s;E)=-\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\,\frac{1}{2}\left[\sigma_1(r;E)+\frac{\widetilde{\mathcal{J}}_4(E)}{\widetilde{\mathcal{J}}_3(E)}\sigma_2(r;E)\right]\sigma_2(s;E)\,,$$
$$r<s\,,\ \mathrm{Re}(E)<0\,,\mathrm{Im}(E)\neq 0\,.\tag{4.6}$$

Since

$$\overline{\sigma_2(s;\overline{E})} = \sigma_2(s;E)\,, \tag{4.7}$$

we can write Eq. (4.6) as

$$G(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\,\frac{1}{2}\left[\sigma_1(r;E)\overline{\sigma_2(s;\overline{E})} + \frac{\widetilde{\mathcal{J}}_4(E)}{\widetilde{\mathcal{J}}_3(E)}\,\sigma_2(r;E)\overline{\sigma_2(s;\overline{E})}\right],$$
$$r<s\,,\ \mathrm{Re}(E)<0\,,\mathrm{Im}(E)\neq 0\,. \tag{4.8}$$

By comparing Eqs. (4.2) and (4.8) we see that

$$\theta_{ij}^{-}(E) = \begin{pmatrix} 0 & -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\frac{1}{2} \\ 0 & -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\frac{1}{2}\frac{\widetilde{\mathcal{J}}_4(E)}{\widetilde{\mathcal{J}}_3(E)} \end{pmatrix}\,, \quad \mathrm{Re}(E)<0\,,\ \mathrm{Im}(E)\neq 0\,. \tag{4.9}$$

The functions $\theta_{ij}^{-}(E)$ are analytic in a neighborhood of $\Lambda = (-\infty, 0)$ except at the energies for which $\widetilde{\mathcal{J}}_3(E)$ vanishes. In this case, the function $\theta_{22}^{-}(E)$ has a pole. Since

$$\widetilde{\mathcal{J}}_3(\tilde{k}) = \widetilde{\mathcal{J}}_3(-ik) = \mathcal{J}_4(k) = \frac{i}{2}\,\mathcal{J}_+(k)\,, \tag{4.10}$$

where $\mathcal{J}_+(k)$ is the Jost function [20], the poles of $\theta_{22}^{-}(E)$ correspond to the zeros of the Jost function on the negative real axis of the energy plane, or on the positive imaginary k-axis. Those bound states have been calculated by Hogreve [20] for different values of V_1, V_2 in Eq. (2.2). In general, there is a finite number of bound states whose energies $E_1,\ldots,E_N$ are in the interval $(-V_1, 0)$. The corresponding normalized wave functions read [18]

$$\phi_n(r) = N_n\,\widetilde{\Theta}(r;E_n)\,, \quad n=1,\ldots,N\,, \tag{4.11}$$

where the square of N_n is given by the residue of the spectral function $\theta_{22}^{-}(E)$ at the bound state energy E_n,

$$N_n^2 = \mathrm{res}\left[\theta_{22}^{-}(E)\right]_{E=E_n} = \mathrm{res}\left[-\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\frac{1}{2}\frac{\widetilde{\mathcal{J}}_4(E)}{\widetilde{\mathcal{J}}_3(E)}\right]_{E=E_n}\,. \tag{4.12}$$

Therefore $E_1,\ldots,E_N$ are the only negative energies that belong to the spectrum of our Hamiltonian.

It is worthwhile noting that the normalization (4.12) provided by the residue of the spectral measure $\theta_{22}^{-}(E)$ is the same (as it should!) as the normalization obtained in Refs. [21–23]. To see this, we denote the momentum of those bound states by $k_n = i|k_n| = i\widetilde{k}_n$, $n=1,\ldots,N$. Then we have that

$$\widetilde{\Theta}(r;\widetilde{k}_n) = \widetilde{\Theta}(r;-ik_n) = \Theta_+(r;k_n)\,, \tag{4.13}$$

and that

$$\mathrm{res}\left[-\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\frac{1}{2}\frac{\widetilde{\mathcal{J}}_4(E)}{\widetilde{\mathcal{J}}_3(E)}\right]_{E=E_n} = \mathrm{res}\left[i\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{2}\frac{\mathcal{J}_-(E)}{\mathcal{J}_+(E)}\right]_{E=E_n} = i\,\mathrm{res}\left[S(k)\right]_{k=k_n}\,, \tag{4.14}$$

where $S(k)$ is the S-matrix in the k-momentum representation and

$$\mathcal{J}_-(E) = 2i\mathcal{J}_3(E)\,. \tag{4.15}$$

Since the eigenfunction $\phi_n(r)$ of Eq. (4.11) is normalized to one, from Eqs. (4.12)-(4.14) it follows that

$$\int_0^\infty dr\ [\Theta_+(r;k_n)]^2 = \frac{-i}{\mathrm{res}\,[S(k)]_{k=k_n}}\,, \tag{4.16}$$

which is the normalization that appears in Refs. [21–23]. (The normalization rule of Eq. (4.16) has been generalized to Gamow vectors in Refs. [24–26].)

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

Now we study the case $\Lambda = (0,\infty)$. In order to be able to apply Theorem 3, we choose the following basis for the space of solutions of $h\sigma = E\sigma$ that is continuous on $(0,\infty)\times\Lambda$ and analytically dependent on E:

$$\sigma_1(r;E) = \chi(r;E)\,, \tag{4.17a}$$

$$\sigma_2(r;E) = \begin{cases} \cos(\sqrt{\frac{2m}{\hbar^2}(E+V_1)}r) & 0<r<a \\ \mathcal{C}_1(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_2)}r} + \mathcal{C}_2(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_2)}r} & a<r<b \\ \mathcal{C}_3(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r} + \mathcal{C}_4(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & b<r<\infty\,. \end{cases} \tag{4.17b}$$

The functions $\mathcal{C}_1$-$\mathcal{C}_4$, whose expressions are given by Eq. (A9) of Appendix A, are such that σ_2 and its derivative are continuous at $r=a$ and at $r=b$. The eigenfunction $\chi(r;E)$ is given by Eq. (3.11).

Eqs. (3.12), (3.14) and (4.17) lead to

$$\Theta_+(r;E) = -\frac{\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E) + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E)\,, \tag{4.18a}$$

$$\Theta_-(r;E) = \frac{\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E) - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\,, \tag{4.18b}$$

where

$$W(E) = \mathcal{J}_4(E)\mathcal{C}_3(E) - \mathcal{J}_3(E)\mathcal{C}_4(E)\,. \tag{4.19}$$

By substituting Eq. (4.18a) into Eq. (3.10) we get to

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{2i\mathcal{J}_4(E)}\left[-\frac{\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E) + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E)\right]\sigma_1(s;E)\,,$$
$$\mathrm{Re}(E)>0, \mathrm{Im}(E)>0\,,\ r>s\,. \tag{4.20}$$

By substituting Eq. (4.18b) into Eq. (3.13) we get to

$$G(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \frac{1}{2i\mathcal{J}_3(E)} \left[\frac{\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E) - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E) \right] \sigma_1(s;E)\,,$$
$$\mathrm{Re}(E)>0, \mathrm{Im}(E)<0\,,\ r>s\,. \tag{4.21}$$

Since

$$\overline{\sigma_1(s;\overline{E})} = \sigma_1(s;E)\,, \tag{4.22}$$

Eq. (4.20) can be written as

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \frac{1}{2i\mathcal{J}_4(E)} \left[-\frac{\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})} + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})} \right]$$
$$\mathrm{Re}(E)>0, \mathrm{Im}(E)>0\,,\ r>s\,, \tag{4.23}$$

whereas Eq. (4.21) can be written as

$$G(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \frac{1}{2i\mathcal{J}_3(E)} \left[\frac{\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})} - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})} \right]$$
$$\mathrm{Re}(E)>0, \mathrm{Im}(E)<0\,,\ r>s\,. \tag{4.24}$$

By comparing (4.2) to (4.23) we get to

$$\theta_{ij}^{+}(E) = \begin{pmatrix} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \frac{1}{2i} \frac{-\mathcal{C}_4(E)}{\mathcal{J}_4(E)W(E)} & 0 \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \frac{1}{2i} \frac{1}{W(E)} & 0 \end{pmatrix}\,, \quad \mathrm{Re}(E)>0\,,\ \mathrm{Im}(E)>0\,. \tag{4.25}$$

By comparing (4.2) to (4.24) we get to

$$\theta_{ij}^{+}(E) = \begin{pmatrix} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \frac{1}{2i} \frac{\mathcal{C}_3(E)}{\mathcal{J}_3(E)W(E)} & 0 \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \frac{1}{2i} \frac{1}{W(E)} & 0 \end{pmatrix}\,, \quad \mathrm{Re}(E)>0\,,\ \mathrm{Im}(E)<0\,. \tag{4.26}$$

From Eqs. (4.25) and (4.26) we can see that the measures ρ_{12}, ρ_{21} and ρ_{22} in Theorem 3 are zero and that the measure ρ_{11} is given by

$$\begin{aligned} \rho_{11}((E_1,E_2)) &= \lim_{\delta\to 0}\lim_{\epsilon\to 0+} \frac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta} \left[\theta_{11}^{+}(E-i\epsilon) - \theta_{11}^{+}(E+i\epsilon)\right] dE \\ &= \int_{E_1}^{E_2} \frac{1}{4\pi} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \frac{1}{\mathcal{J}_3(E)\mathcal{J}_4(E)}\, dE\,, \end{aligned} \tag{4.27}$$

which leads to

$$\rho(E) \equiv \rho_{11}(E) = \frac{1}{4\pi} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \frac{1}{|\mathcal{J}_4(E)|^2}\,, \quad E\in(0,\infty)\,. \tag{4.28}$$

The function $\theta_{11}^{+}(E)$ has a branch cut along $(0,\infty)$, and therefore $(0,\infty)$ is included in $\mathrm{Sp}(H)$. Since $\mathrm{Sp}(H)$ is a closed set, we have that

$$\mathrm{Sp}(H) = \{E_1,\ldots,E_N\} \cup [0,\infty)\,. \tag{4.29}$$

Therefore, the spectrum of H has a discrete part $\Lambda_{\mathrm{b}} = \{E_1,\ldots,E_N\}$ and a continuous part $\Lambda_{\mathrm{c}} = [0,\infty)$.

5. DIRECT INTEGRAL DECOMPOSITION

The fourth step toward the construction of the RHS is to compute the unitary operator that diagonalizes the Hamiltonian and the direct integral decomposition induced by that unitary operator. In order to compute them, we apply Theorem 2 of Section 4 to the discrete and continuous spectrum separately, since they can be treated independently. In the end, the independence of the discrete and continuous spectra will lead to the splitting of the Hilbert space into a direct sum of a Hilbert space associated to the discrete spectrum and another Hilbert space associated to the continuous spectrum.

We first apply Theorem 2 to the discrete part of the spectrum. By that theorem, there is a unitary operator $U_{\rm b}$ from $\mathcal{H}_{\rm b} := \mathsf{E}(\Lambda_{\rm b})L^2([0,\infty),dr)$ onto $\widehat{\mathcal{H}}_{\rm b} := \mathbb{C}^N$ defined by

$$\begin{aligned} U_{\rm b} : \mathcal{H}_{\rm b} &\longmapsto \widehat{\mathcal{H}}_{\rm b} \\ f_{\rm b}(r) &\longmapsto U_{\rm b}f_{\rm b} = \{(\phi_1, f_{\rm b}), \ldots, (\phi_N, f_{\rm b})\} \, . \end{aligned} \tag{5.1}$$

In this equation, $\mathcal{H}_{\rm b}$ is the Hilbert space spanned by the bound states $\phi_1, \ldots, \phi_N$, $\widehat{\mathcal{H}}_{\rm b}$ is the space of N-tuples of the form $\{(\phi_n, f_{\rm b})\}_{n=1}^N$ (hence $\widehat{\mathcal{H}}_{\rm b}$ is isomorphic to $\mathbb{C}^N$), $f_{\rm b} = \mathsf{E}(\Lambda_{\rm b})f$, i.e., $f_{\rm b}$ is the component of f along the space $\mathcal{H}_{\rm b}$,

$$f_{\rm b}(r) = \sum_{n=1}^{N} (\phi_n, f)\, \phi_n(r) \, , \tag{5.2}$$

and $(\phi_n, f_{\rm b})$ is the scalar product of the n-th bound state $\phi_n(r)$ of Eq. (4.11) with $f_{\rm b}$,

$$(\phi_n, f_{\rm b}) = \int_0^\infty dr\, \overline{\phi_n(r)} f_{\rm b}(r) \, , \quad n = 1, \ldots, N \, . \tag{5.3}$$

On the space $\widehat{\mathcal{H}}_{\rm b}$, the Hamiltonian acts as the following $N \times N$ diagonal matrix:

$$\widehat{H}_{\rm b} := U_{\rm b} H_{\rm b} U_{\rm b}^{-1} = \begin{pmatrix} E_1 & 0 & .. & 0 \\ 0 & E_2 & .. & 0 \\ .. & .. & .. & .. \\ 0 & 0 & .. & E_N \end{pmatrix} , \tag{5.4}$$

where $H_{\rm b}$ is the restriction of H to $\mathcal{H}_{\rm b}$.

Next, we apply Theorem 2 to the continuous part of the spectrum. By that theorem, there is a unitary map $\widetilde{U}_{\rm c}$ from $\mathcal{H}_{\rm c} := \mathsf{E}(\Lambda_{\rm c})L^2([0,\infty),dr)$ onto $L^2((0,\infty),\rho(E)dE)$ defined by

$$\begin{aligned} \widetilde{U}_{\rm c} : \mathcal{H}_{\rm c} &\longmapsto L^2((0,\infty),\rho(E)dE) \\ f_{\rm c}(r) &\longmapsto \widetilde{f}_{\rm c}(E) = (\widetilde{U}_{\rm c} f_{\rm c})(E) = \int_0^\infty dr f_{\rm c}(r) \overline{\chi(r;E)} \, , \end{aligned} \tag{5.5}$$

where $f_{\rm c} = \mathsf{E}(\Lambda_{\rm c})f$, i.e., $f_{\rm c}$ is the component of f along the Hilbert space $\mathcal{H}_{\rm c}$. The space $\mathcal{H}_{\rm c}$ is the Hilbert space that corresponds to the continuous part of the spectrum—hence the subscript c.

If we write

$$\mathcal{D}(H) = \mathcal{H}_{\rm b} \oplus \mathcal{D}(\mathcal{H}_{\rm c}) \tag{5.6}$$

and denote the restriction of H to $\mathcal{D}(H_{\rm c})$ by $H_{\rm c}$, then the operator $\widetilde{U}_{\rm c}$ of Eq. (5.5) provides a ρ-diagonalization of $H_{\rm c}$. If we seek a δ-normalization [9], we just have to define the following eigenfunction:

$$\phi(r;E) := \sqrt{\rho(E)}\, \chi(r;E)\,, \tag{5.7}$$

which is the eigensolution of the differential operator h that is δ-normalized, and the following unitary operator:

$$\begin{aligned} U_{\rm c} : \mathcal{H}_{\rm c} &\longmapsto \widehat{\mathcal{H}}_{\rm c} \\ f_{\rm c} &\longmapsto \widehat{f}_{\rm c}(E) = (U_{\rm c} f_{\rm c})(E) = \int_0^\infty dr\, f_{\rm c}(r)\overline{\phi(r;E)}\,, \end{aligned} \tag{5.8}$$

where $\widehat{\mathcal{H}}_{\rm c} = L^2([0,\infty), dE)$. We note that the normalization of the bound states (4.11) is different to the δ-normalization of (5.7).

The inverses of the operators $U_{\rm b}$ and $U_{\rm c}$ are provided by the following theorem (cf. Theorem XIII.5.14 of Ref. [18]):

Theorem 4 (Weyl-Kodaira) Let H, Λ, $\{\rho_{ij}\}$, 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 $\mathsf{E}(\Lambda)L^2([0,\infty), dr)$ onto $L^2(\Lambda, \{\rho_{ij}\})$ is given by the formula

$$(U^{-1}F)(r) = \lim_{\mu_0 \to E_0} \lim_{\mu_1 \to E_1} \int_{\mu_0}^{\mu_1} \left(\sum_{i,j=1}^{2} F_i(E)\sigma_j(r;E)\rho_{ij}(dE) \right)\,, \tag{5.9}$$

where $F = [F_1, F_2] \in L^2(\Lambda, \{\rho_{ij}\})$, the limit existing in the topology of $L^2([0,\infty), dr)$.

According to Theorem 4, the inverse of $U_{\rm b}$ is given by

$$(U_{\rm b}^{-1}\widehat{f}_{\rm b})(r) = \sum_{n=1}^{N} (\phi_n, f_{\rm b})\phi_n(r)\,, \tag{5.10}$$

where $\widehat{f}_{\rm b} = \{(\phi_1, f_{\rm b}), \ldots, (\phi_N, f_{\rm b})\}$ is an N-tuple of complex numbers. The operator $U_{\rm b}^{-1}$ transforms from $\widehat{\mathcal{H}}_{\rm b}$ onto $\mathcal{H}_{\rm b}$.

According to Theorem 4, the inverse of $U_{\rm c}$ is given by

$$f_{\rm c}(r) = (U_{\rm c}^{-1}\widehat{f}_{\rm c})(r) = \int_0^\infty dE\, \widehat{f}_{\rm c}(E)\phi(r;E)\,, \quad \widehat{f}_{\rm c}(E) \in L^2([0,\infty), dE)\,. \tag{5.11}$$

The operator $U_{\rm c}^{-1}$ transforms from $\widehat{\mathcal{H}}_{\rm c}$ onto $\mathcal{H}_{\rm c}$.

Using the operators $U_{\rm b}$ and $U_{\rm c}$ we can construct an operator U defined as

$$\begin{aligned} U : \mathcal{H} &\longmapsto \widehat{\mathcal{H}} = \oplus_{n=1}^{N} \widehat{\mathcal{H}}(E_n) \oplus \int_0^\infty \widehat{\mathcal{H}}(E) dE \\ f &\longmapsto Uf := [U_{\rm b} f, U_{\rm c} f] = \left[\widehat{f}_{\rm b}, \{\widehat{f}_{\rm c}(E)\} \right]\,, \end{aligned} \tag{5.12}$$

where $\mathcal{H}$ is realized by $\mathcal{H}_{\rm b} \oplus \mathcal{H}_{\rm c}$, and $\widehat{\mathcal{H}}$ is realized by $\widehat{\mathcal{H}}_{\rm b} \oplus \widehat{\mathcal{H}}_{\rm c}$. The Hilbert space $\widehat{\mathcal{H}}(E_n)$, which is associated to each energy E_n in the discrete spectrum, and the Hilbert space $\widehat{\mathcal{H}}(E)$, which is associated to each energy E in the continuous spectrum, are realized by the Hilbert space of complex numbers $\mathbb{C}$. On $\widehat{\mathcal{H}}$, the operator H acts as the multiplication operator,

$$Hf \longmapsto UHf \equiv \sum_{n=1}^{N} E_n(\phi_n, f_{\rm b}) + \{E\widehat{f}_{\rm c}(E)\}\,, \quad f \in \mathcal{D}(H)\,. \tag{5.13}$$

The scalar product on $\widehat{\mathcal{H}}$ can be written as

$$\left(\widehat{f}, \widehat{g}\right)_{\widehat{\mathcal{H}}} = \sum_{n=1}^{N}(f_{\rm b}, \phi_n)(\phi_n, g_{\rm b}) + \int_0^\infty dE\, \overline{\widehat{f}_{\rm c}(E)}\, \widehat{g}_{\rm c}(E)\,, \tag{5.14}$$

where $\widehat{f}_{\rm b} = \{(\phi_1, f_{\rm b}), \ldots, (\phi_N, f_{\rm b})\}$ and $\widehat{g}_{\rm b} = \{(\phi_1, g_{\rm b}), \ldots, (\phi_N, g_{\rm b})\}$.

Therefore, U induces a direct integral decomposition of the Hilbert space associated to the Hamiltonian H (see [27,4]). In particular, we can write the eigenfunction expansions of any element of the Hilbert spaces $L^2([0,\infty), dr)$ and $L^2([0,\infty), dE)$ in terms of the eigensolutions $\phi_n(r)$ and $\phi(r;E)$ of h,

$$f(r) = f_{\rm b}(r) + f_{\rm c}(r) = \sum_{n=1}^{N}(\phi_n, f)\phi_n(r) + \int_0^\infty dE\, \widehat{f}(E)\phi(r;E)\,, \tag{5.15}$$

$$\widehat{f} \equiv \widehat{f}_{\rm b} + \widehat{f}_{\rm c}(E) = \{(\phi_n, f)\}_{n=1}^N + \int_0^\infty dr\, f(r)\overline{\phi(r;E)}\,. \tag{5.16}$$

6. RIGGED HILBERT SPACE

As explained in the Introduction, the Hilbert space framework (in particular, the direct integral decomposition) is not sufficient for the purposes of Quantum Mechanics: an extension of the Hilbert space to the RHS is needed. To construct the RHS, we shall consider the discrete and the continuous spectra separately.

6.1. Construction of the Rigged Hilbert Space

First, we construct the RHS associated to the discrete spectrum. In this case, the Hilbert space $\mathcal{H}_{\rm b}$ is finite dimensional. Therefore, all the difficulties exposed in the Introduction do not arise. The "Gelfand triplet" that corresponds to the discrete spectrum consists of three copies of the Hilbert space $\mathcal{H}_{\rm b}$,

$$\mathbf{\Phi}_{\rm b} = \mathcal{H}_{\rm b} = \mathbf{\Phi}_{\rm b}^\times\,. \tag{6.1}$$

The eigenket $|E_n)$ associated to any energy E_n in the discrete spectrum is defined by

$$
\begin{aligned}
|E_n) : \mathbf{\Phi}_{\rm b} &\longmapsto \mathbb{C} \\
\varphi_{\rm b} &\longmapsto (\varphi_{\rm b}|E_n) := (\varphi_{\rm b}, \phi_n) = \int_0^\infty dr\, \overline{\varphi_{\rm b}(r)}\phi_n(r)\,.
\end{aligned} \tag{6.2}
$$

Clearly, the function $|E_n)$ is an antilinear functional over $\mathbf{\Phi}_{\rm b}$, i.e., $|E_n) \in \mathbf{\Phi}_{\rm b}^\times$. Besides being an eigenvector of the Hamiltonian in the usual sense, $|E_n)$ is also an eigenvector of $H_{\rm b}$ in the RHS sense of Eq. (1.8),

$$
(\varphi_{\rm b}|H_{\rm b}^\times|E_n) = E_n(\varphi_{\rm b}|E_n)\,, \quad \forall \varphi_{\rm b} \in \mathbf{\Phi}_{\rm b}\,. \tag{6.3}
$$

Although it is not necessary to use the RHS formalism when dealing with the discrete spectrum, we have constructed the "RHS" (6.1) and the eigenket (6.2) in order to make a parallel to the continuous case.

Now, we construct the RHS associated to the continuous spectrum. The first step is to make all the powers of the Hamiltonian well-defined. In order to do so, we construct the maximal invariant subspace $\mathcal{D}_{\rm c}$ of the operator $H_{\rm c}$,

$$
\mathcal{D}_{\rm c} := \bigcap_{n=0}^{\infty} \mathcal{D}(H_{\rm c}^n)\,. \tag{6.4}
$$

The space $\mathcal{D}_{\rm c}$ is the largest subspace of $\mathcal{D}(H_{\rm c})$ that remains stable under the action of the Hamiltonian $H_{\rm c}$ and of its powers. Recalling that h denotes the formal differential operator (2.7), it is easy to check that

$$
\begin{aligned}
\mathcal{D}_{\rm c} = \{\varphi_{\rm c} \in \mathcal{H}_{\rm c} \mid h^n\varphi_{\rm c}(r) \in \mathcal{H}_{\rm c},\ h^n\varphi_{\rm c}(0) = 0,\ \varphi_{\rm c}^{(n)}(a) = \varphi_{\rm c}^{(n)}(b) = 0,\ n = 0,1,2,\ldots; \\
\varphi_{\rm c}(r) \in C^\infty([0,\infty))\}\,.
\end{aligned} \tag{6.5}
$$

The second step is to find the subspace $\mathbf{\Phi}_{\rm c} \subset \mathcal{D}_{\rm c}$ on which the eigenkets $|E\rangle$ of Eq. (1.5b) act as antilinear functionals. Those eigenkets are to be defined as integral operators whose kernel is the eigenfunction $\phi(r;E)$,

$$
\begin{aligned}
|E\rangle : \mathbf{\Phi}_{\rm c} &\longmapsto \mathbb{C} \\
\varphi_{\rm c} &\longmapsto \langle\varphi_{\rm c}|E\rangle := \int_0^\infty dr\, \overline{\varphi_{\rm c}(r)}\phi(r;E) = \overline{(U_{\rm c}\varphi_{\rm c})(E)}\,.
\end{aligned} \tag{6.6}
$$

A necessary condition for $|E\rangle$ to be well-defined is that $\mathbf{\Phi}_{\rm c}$ be included in $\mathcal{D}_{\rm c}$. This condition, however, is not sufficient to obtain a continuous functional. In order to make the eigenfunctional $|E\rangle$ continuous, we have to impose further restrictions on the behavior at infinity of the elements of $\mathcal{D}_{\rm c}$,

$$
\int_0^\infty dr\ |(r+1)^n(h+1)^m\varphi_{\rm c}(r)|^2 < \infty\,, \quad n,m = 0,1,2,\ldots \tag{6.7}
$$

The imposition of (6.7) upon the space $\mathcal{D}_{\rm c}$ yields

$$
\mathbf{\Phi}_{\rm c} = \{\varphi_{\rm c} \in \mathcal{D}_{\rm c} \mid \int_0^\infty dr\ |(r+1)^n(h+1)^m\varphi_{\rm c}(r)|^2 < \infty, \quad n,m = 0,1,2,\ldots\}\,. \tag{6.8}
$$

On $\mathbf{\Phi}_{\rm c}$, we define the family of norms

$$\|\varphi_{\rm c}\|_{n,m} := \sqrt{\int_0^\infty dr\ |(r+1)^n (h+1)^m \varphi_{\rm c}(r)|^2}\, , \quad n,m = 0,1,2,\ldots \tag{6.9}$$

These norms can be used to define a countably normed topology $\tau_{\mathbf{\Phi}_{\rm c}}$ on $\mathbf{\Phi}_{\rm c}$ (see [4]),

$$\varphi_{{\rm c},\alpha} \xrightarrow[\alpha\to\infty]{\tau_{\mathbf{\Phi}_{\rm c}}} \varphi_{\rm c} \quad \text{iff} \quad \|\varphi_{{\rm c},\alpha} - \varphi_{\rm c}\|_{n,m} \xrightarrow[\alpha\to\infty]{} 0\, , \quad n,m = 0,1,2,\ldots \tag{6.10}$$

Once we have constructed the space $\mathbf{\Phi}_{\rm c}$, we can construct its topological dual $\mathbf{\Phi}_{\rm c}^\times$ as the space of $\tau_{\mathbf{\Phi}_{\rm c}}$-continuous antilinear functionals on $\mathbf{\Phi}_{\rm c}$ (see [4]) and therewith the RHS corresponding to the continuous part of the spectrum,

$$\mathbf{\Phi}_{\rm c} \subset \mathcal{H}_{\rm c} \subset \mathbf{\Phi}_{\rm c}^\times\, . \tag{6.11}$$

In order to show that the RHS (6.11) is what we are looking for, we need to prove the following proposition (the proof can be found in Appendix B):

Proposition 1 The triplet of spaces (6.11) is a Rigged Hilbert Space, and it satisfies all the requirements demanded in the Introduction. More specifically,

(i) The quantities (6.9) fulfill the conditions to be a norm.

(ii) The space $\mathbf{\Phi}_{\rm c}$ is stable under the action of $H_{\rm c}$, and $H_{\rm c}$ is $\tau_{\mathbf{\Phi}_{\rm c}}$-continuous.

(iii) The ket $|E\rangle$ of Eq. (6.6) is a well-defined antilinear functional on $\mathbf{\Phi}_{\rm c}$, i.e., $|E\rangle$ belongs to $\mathbf{\Phi}_{\rm c}^\times$.

(iv) The ket $|E\rangle$ is a generalized eigenvector of $H_{\rm c}$,

$$H_{\rm c}^\times |E\rangle = E|E\rangle\, , \tag{6.12}$$

i.e.,

$$\langle\varphi_{\rm c}|H_{\rm c}^\times|E\rangle = \langle H_{\rm c}^\dagger\varphi_{\rm c}|E\rangle = E\langle\varphi_{\rm c}|E\rangle\, , \quad \forall\varphi_{\rm c}\in\mathbf{\Phi}_{\rm c}\, . \tag{6.13}$$

(This proposition is a generalization to infinite dimensional spaces of the results that hold in finite dimensional spaces.)

We now combine the RHSs (6.1) and (6.11) corresponding to the discrete and continuous spectrum into the RHS of the square well-barrier potential,

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^\times\, , \tag{6.14}$$

where

$$\mathbf{\Phi} := \mathbf{\Phi}_{\rm b} \oplus \mathbf{\Phi}_{\rm c}\, ; \qquad \mathcal{H} := \mathcal{H}_{\rm b} \oplus \mathcal{H}_{\rm c}\, ; \qquad \mathbf{\Phi}^\times := \mathbf{\Phi}_{\rm b}^\times \oplus \mathbf{\Phi}_{\rm c}^\times\, . \tag{6.15}$$

On the space $\mathbf{\Phi}$, all the expectation values of the Hamiltonian and all the algebraic operations involving H are well-defined, and the eigenvalue equations (1.5) hold. The kets $|E_n)$ and $|E\rangle$

satisfy the normalization (1.6). Since the spaces $\mathbf{\Phi}_{\rm b}$ and $\mathbf{\Phi}_{\rm c}$ are orthogonal to each other, we also have that

$$(\varphi|E_n) = (\varphi_{\rm b}|E_n) \, ; \quad \langle \varphi|E\rangle = \langle \varphi_{\rm c}|E\rangle \, . \tag{6.16}$$

As we shall see in the next section, the kets $|E_n)$ and $|E\rangle$ form a complete basis system.

Before finishing this section, we would like to remark that $\phi(r;E)$ is *not* the same object as the ket $|E\rangle$ of Eq. (6.6). The function $\phi(r;E)$ is an eigenfunction of the formal differential operator h, whereas the ket $|E\rangle$ is a generalized eigenvector of the Hamiltonian. The eigenket $|E\rangle$ is defined by the eigenfunction $\phi(r;E)$ *and* by the space of test functions $\mathbf{\Phi}_{\rm c}$ on which it acts as an antilinear functional.

6.2. Dirac Basis Vector Expansion

In the Introduction, we mentioned that in Quantum Mechanics it is assumed that the eigenkets of the Hamiltonian form a complete basis system that can be used to expand any physical wave function φ as in Eq. (1.7). This expansion is derived in the present section. That derivation consists of the restriction of the eigenfunction expansion (5.15) to the space $\mathbf{\Phi}$.

If we denote $\langle r|\varphi\rangle \equiv \varphi(r)$, $\langle r|E_n) \equiv \phi_n(r)$, and $\langle r|E\rangle \equiv \phi(r;E)$, and if we define the action of the bra $\langle E|$ on the wave function φ by $\langle E|\varphi\rangle := \overline{\langle \varphi|E\rangle}$, then Eq. (5.15) can be written as

$$\langle r|\varphi\rangle = \sum_{n=0}^{\infty} \langle r|E_n)(E_n|\varphi) + \int_0^\infty dE \, \langle r|E\rangle\langle E|\varphi\rangle \, , \quad \varphi \in \mathbf{\Phi} \, . \tag{6.17}$$

This is the Dirac basis vector expansion of the square well-barrier potential. Although the eigenfunction expansion (5.15) is valid for every element of the Hilbert space, Dirac basis vector expansion (6.17) is only valid for functions $\varphi \in \mathbf{\Phi}$, because only those functions fulfill both

$$\overline{\widehat{\varphi}_{\rm c}(E)} = \langle \varphi|E\rangle \tag{6.18}$$

and

$$\langle \varphi|H^\times|E\rangle = \langle H^\dagger\varphi|E\rangle = E\langle \varphi|E\rangle \, . \tag{6.19}$$

For the sake of completeness, we include the Nuclear Spectral Theorem [4], which is usually referred to as the mathematical justification of the heuristic Dirac basis vector expansion [1–6]. Instead of using the general proof of Ref. [4], we prove that theorem using the machinery of the Sturm-Liouville theory (our proof can be found in Appendix B).

Proposition 2 (Nuclear Spectral Theorem) Let

$$\mathbf{\Phi} \subset L^2([0,\infty),dr) \subset \mathbf{\Phi}^\times \tag{6.20}$$

be the RHS of the square well-barrier Hamiltonian H such that $\mathbf{\Phi}$ remains invariant under H and H is a $\tau_{\mathbf{\Phi}}$-continuous operator on $\mathbf{\Phi}$. Then, for each energy in the spectrum of H there is a generalized eigenvector such that

$$H|E_n) = E_n|E_n)\,, \quad E_n \in \{E_1, \ldots, E_N\}\,, \tag{6.21a}$$
$$H^\times|E\rangle = E|E\rangle\,, \quad E \in [0, \infty)\,, \tag{6.21b}$$

and such that

$$(\varphi, \psi) = \sum_{n=1}^{N} (\varphi|E_n)(E_n|\psi) + \int_0^\infty dE\, \langle\varphi|E\rangle\langle E|\psi\rangle\,, \quad \forall\varphi, \psi \in \mathbf{\Phi}\,, \tag{6.22}$$

and

$$(\varphi, H^m\psi) = \sum_{n=1}^{N} E_n^m (\varphi|E_n)(E_n|\psi) + \int_0^\infty dE\, E^m \langle\varphi|E\rangle\langle E|\psi\rangle\,, \quad \forall\varphi, \psi \in \mathbf{\Phi}\,, m = 1, 2, \ldots \tag{6.23}$$

Thus this theorem allows us to write the scalar product (6.22) of any two functions φ, ψ of $\mathbf{\Phi}$ and the matrix elements (6.23) in terms of the action of the kets $|E_n)$ and $|E\rangle$ on φ, ψ.

6.3. Energy and Momentum Representations of the Rigged Hilbert Space

In this section, we construct the energy representation of the RHS (6.14) by applying to it the unitary operator U of Eq. (5.12). As done throughout this paper, we study the discrete and the continuous case separately.

In the discrete case (6.1), we have already seen that the energy representation of $\mathcal{H}_{\rm b}$ is $\mathbb{C}^N$. Hence the energy representation of the RHS (6.1) consists of three copies of the space $\mathbb{C}^N$. The image of the eigenket $|E_n)$ under $U_{\rm b}^\times$ is the N-tuple that has zeros everywhere but at the n-th position, $\{\delta_{in}\}_{i=1}^N$. In the energy representation, the Hamiltonian $H_{\rm b}$ acts as the diagonal matrix (5.4).

In the continuous case (6.11), we have already shown that in the energy representation the Hamiltonian $H_{\rm c}$ acts as the multiplication operator. The energy representation of the space $\mathbf{\Phi}_{\rm c}$ is defined as

$$\widehat{\mathbf{\Phi}}_{\rm c} := U_{\rm c}\mathbf{\Phi}_{\rm c}\,. \tag{6.24}$$

The space $\widehat{\mathbf{\Phi}}_{\rm c}$ is a linear subspace of $L^2([0,\infty), dE)$. In order to endow $\widehat{\mathbf{\Phi}}_{\rm c}$ with a topology $\tau_{\widehat{\mathbf{\Phi}}_{\rm c}}$, we carry the topology on $\mathbf{\Phi}_{\rm c}$ into $\widehat{\mathbf{\Phi}}_{\rm c}$,

$$\tau_{\widehat{\mathbf{\Phi}}_{\rm c}} := U_{\rm c}\tau_{\mathbf{\Phi}_{\rm c}}\,. \tag{6.25}$$

With this topology, the space $\widehat{\mathbf{\Phi}}_{\rm c}$ is a linear topological space. If we denote the dual space of $\widehat{\mathbf{\Phi}}_{\rm c}$ by $\widehat{\mathbf{\Phi}}_{\rm c}^\times$, then we have

$$U_{\rm c}^\times \mathbf{\Phi}_{\rm c}^\times = (U_{\rm c}\mathbf{\Phi}_{\rm c})^\times = \widehat{\mathbf{\Phi}}_{\rm c}^\times\,. \tag{6.26}$$

From the following chain of equalities:

$$
\begin{aligned}
\langle\widehat{\varphi}_{\rm c}|U_{\rm c}^{\times}|E\rangle &= \langle U_{\rm c}^{-1}\widehat{\varphi}_{\rm c}|E\rangle \\
&= \int_0^\infty dr\, \overline{\varphi_{\rm c}(r)}\phi(r;E) \\
&= \overline{\widehat{\varphi}_{\rm c}(E)}\,,
\end{aligned}
\tag{6.27}
$$

it follows that the energy representation of the Dirac ket $|E\rangle$, that we denote by $|\widehat{E}\rangle$, is the antilinear Schwartz delta functional, i.e., $|\widehat{E}\rangle$ is the antilinear functional that associates to each function $\widehat{\varphi}_{\rm c}$ the complex conjugate of its value at the point E.

In order to summarize all these results, it is very helpful to show the different realizations of the RHS through the following diagram:

$$
\begin{array}{cccccccc}
H;\ \varphi & \mathbf{\Phi}_{\rm b}\oplus\mathbf{\Phi}_{\rm c} & \subset & \mathcal{H}_{\rm b}\oplus\mathcal{H}_{\rm c} & \subset & \mathbf{\Phi}_{\rm b}^{\times}\oplus\mathbf{\Phi}_{\rm c}^{\times} & & |E_n)\oplus|E\rangle \\
& U_{\rm b}\downarrow\oplus\downarrow U_{\rm c} & & U_{\rm b}\downarrow\oplus\downarrow U_{\rm c} & & U_{\rm b}^{\times}\downarrow\oplus\downarrow U_{\rm c}^{\times} & & \\
\widehat{H};\ \widehat{\varphi} & \widehat{\mathbf{\Phi}}_{\rm b}\oplus\widehat{\mathbf{\Phi}}_{\rm c} & \subset & \widehat{\mathcal{H}}_{\rm b}\oplus\widehat{\mathcal{H}}_{\rm c} & \subset & \widehat{\mathbf{\Phi}}_{\rm b}^{\times}\oplus\widehat{\mathbf{\Phi}}_{\rm c}^{\times} & & |\widehat{E}_n)\oplus|\widehat{E}\rangle
\end{array}
\tag{6.28}
$$

On the top line of the diagram (6.28), we have the RHS, the Hamiltonian, the wave functions and the Dirac kets in the position representation. On the bottom line, we have their energy representation counterparts.

Since every function we have computed (eigenfunctions of the Schrödinger differential operator, Green function, etc.) depends on the square root of the energy rather than on the energy itself, the momentum k is a more convenient variable, especially for the continuous case. The momentum k is defined by

$$
k := \sqrt{\frac{2m}{\hbar^2}\,E}\,. \tag{6.29}
$$

In terms of k, the δ-normalized eigensolution of the differential operator (2.7) reads

$$
\langle r|k\rangle = \left[2\pi\mathcal{J}_3(k)\mathcal{J}_4(k)\right]^{-1/2}\chi(r;k)\,. \tag{6.30}
$$

This eigensolution can be used to obtain the unitary operator $V_{\rm c}$ that transforms from the position into the momentum representation,

$$
\widehat{f}_{\rm c}(k) = (V_{\rm c}f_{\rm c})(k) = \int_0^\infty dr\, f_{\rm c}(r)\overline{\langle r|k\rangle}\,, \quad f_{\rm c}\in\mathcal{H}_{\rm c}\,. \tag{6.31}
$$

(The operator $V_{\rm b}$ corresponding to the discrete case is $U_{\rm b}$.) On the k-representation, the (continuous part of the) Hamiltonian acts as multiplication by k^2. To each $k\in[0,\infty)$, there corresponds an eigenket $|k\rangle$ that acts on $\mathbf{\Phi}_{\rm c}$ as the following integral operator:

$$
\langle\varphi_{\rm c}|k\rangle := \int_0^\infty dr\,\langle\varphi_{\rm c}|r\rangle\langle r|k\rangle = \overline{(V_{\rm c}\varphi_{\rm c})(k)}\,, \quad \varphi_{\rm c}\in\mathbf{\Phi}_{\rm c}\,. \tag{6.32}
$$

This eigenket is a generalized eigenvector of the Hamiltonian corresponding to the eigenvalue k^2. In this way, we can construct the k-representation of all the objects of the diagram (6.28).

If we express our functions in terms of k, there is no need to distinguish different regions in the E-plane, because in the k-plane the resolvent and the S-matrix do not have a cut. There is no need to work with a particular branch of the square root either, because Eq. (6.29) provides a Riemann surface in a natural way. For instance, we can define the Jost function

$$\mathcal{J}(k) := \mathcal{J}_+(k)\,, \quad k \in \mathbb{C}\,, \tag{6.33}$$

the eigensolution

$$f(r;k) := \Theta_+(r;k)\,, \quad k \in \mathbb{C}\,, \tag{6.34}$$

and the Green function

$$G(r,r';k) := -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}\frac{\chi(r_<;k)f(r_>;k)}{\mathcal{J}(k)}\,, \quad k \in \mathbb{C}\,, \tag{6.35}$$

where $r_<$, $r_>$ refer to the smaller and to the bigger of r and r', respectively. Then, as k approaches the real positive k axis, or as E approaches the right-hand cut from above, $\mathcal{J}(k)$, $f(r;k)$ and $G(r,r';k)$ become $\mathcal{J}_+(k)$, $\Theta_+(r;k)$ and $G^+(r,r';k)$, respectively; as k approaches the negative real axis (from above), or E the right-hand cut from below, $\mathcal{J}(k)$, $f(r;k)$ and $G(r,r';k)$ become $\mathcal{J}_-(k)$, $\Theta_-(r;k)$ and $G^-(r,r';k)$, respectively [21]. Also, the values that the functions of Eqs. (6.33)-(6.35) take on the second sheet of the Riemann surface are already specified (the Sturm-Liouville theory deals only with energies in the first sheet). This is particularly useful when studying resonance energies, which lie on the second sheet [24–26].

7. CONCLUSIONS

We have shown that the solutions of the Schrödinger equation corresponding to the square well-barrier potential fall in the Rigged Hilbert Space

$$\mathbf{\Phi}_{\rm b} \oplus \mathbf{\Phi}_{\rm c} \subset \mathcal{H}_{\rm b} \oplus \mathcal{H}_{\rm c} \subset \mathbf{\Phi}_{\rm b}^\times \oplus \mathbf{\Phi}_{\rm c}^\times\,. \tag{7.1}$$

The spectrum of the Hamiltonian has a discrete part $\{E_1, \ldots, E_N\}$ and a continuous part $[0,\infty)$. For each energy in the spectrum of H, we have constructed an eigenket that is an eigenvector of H. If the energy E_n belongs to the discrete spectrum, its corresponding eigenket $|E_n)$, which is given by Eq. (6.2), is an element of $\mathbf{\Phi}_{\rm b}^\times$. If the energy E belongs to the continuous spectrum, its corresponding eigenket $|E\rangle$, which is given by Eq (6.6), is an element of $\mathbf{\Phi}_{\rm c}^\times$. Thus the RHS treats the discrete and the continuous spectra independently and on the same footing. Each element φ of $\mathbf{\Phi}_{\rm b} \oplus \mathbf{\Phi}_{\rm c}$ can be expanded by the eigenkets of the Hamiltonian as in Eq. (6.17). The elements of $\mathbf{\Phi}_{\rm b} \oplus \mathbf{\Phi}_{\rm c}$ are the only square normalizable functions for which such an expansion is possible. The expectation values and the uncertainties of the Hamiltonian are well defined quantities in each element φ of $\mathbf{\Phi}_{\rm b} \oplus \mathbf{\Phi}_{\rm c}$.

Therefore, the RHS (7.1) contains all the physically meaningful solutions of the Schrödinger equation—the physical wave functions are included in $\mathbf{\Phi}_{\rm b} \oplus \mathbf{\Phi}_{\rm c}$, whereas the monoenergetic solutions of the time independent Schrödinger equation are included in $\mathbf{\Phi}_{\rm b}^\times \oplus \mathbf{\Phi}_{\rm c}^\times$.

Although illustrated within the example of the square well-barrier potential, these conclusions hold in general: the solutions of the Schrödinger equation fall in a RHS rather than just in a Hilbert space.

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APPENDIX A: LIST OF AUXILIARY FUNCTIONS

If we define

$$\widetilde{k} := \sqrt{-\frac{2m}{\hbar^2}\, E}\,; \quad \widetilde{Q}_1 := \sqrt{-\frac{2m}{\hbar^2}\,(E+V_1)}\,; \quad \widetilde{Q}_2 := \sqrt{-\frac{2m}{\hbar^2}\,(E-V_2)}\,. \tag{A1}$$

then the coefficients in Eq. (3.7) are given by

$$\widetilde{\mathcal{J}}_1(E) \equiv \widetilde{\mathcal{J}}_1(\widetilde{k}) = \frac{i}{4} e^{-\widetilde{Q}_2 a} \left[\left(1+\frac{\widetilde{Q}_1}{\widetilde{Q}_2}\right) e^{\widetilde{Q}_1 a} - \left(1-\frac{\widetilde{Q}_1}{\widetilde{Q}_2}\right) e^{-\widetilde{Q}_1 a} \right], \tag{A2a}$$

$$\widetilde{\mathcal{J}}_2(E) \equiv \widetilde{\mathcal{J}}_2(\widetilde{k}) = \frac{i}{4} e^{\widetilde{Q}_2 a} \left[\left(1-\frac{\widetilde{Q}_1}{\widetilde{Q}_2}\right) e^{\widetilde{Q}_1 a} - \left(1+\frac{\widetilde{Q}_1}{\widetilde{Q}_2}\right) e^{-\widetilde{Q}_1 a} \right], \tag{A2b}$$

$$\widetilde{\mathcal{J}}_3(E) \equiv \widetilde{\mathcal{J}}_3(\widetilde{k}) = \frac{1}{2} e^{-\widetilde{k} b} \left[\left(1+\frac{\widetilde{Q}_2}{\widetilde{k}}\right) e^{\widetilde{Q}_2 b} \widetilde{\mathcal{J}}_1(\widetilde{k}) + \left(1-\frac{\widetilde{Q}_2}{\widetilde{k}}\right) e^{-\widetilde{Q}_2 b} \widetilde{\mathcal{J}}_2(\widetilde{k}) \right], \tag{A2c}$$

$$\widetilde{\mathcal{J}}_4(E) \equiv \widetilde{\mathcal{J}}_4(\widetilde{k}) = \frac{1}{2} e^{\widetilde{k} b} \left[\left(1-\frac{\widetilde{Q}_2}{\widetilde{k}}\right) e^{\widetilde{Q}_2 b} \widetilde{\mathcal{J}}_1(\widetilde{k}) + \left(1+\frac{\widetilde{Q}_2}{\widetilde{k}}\right) e^{-\widetilde{Q}_2 b} \widetilde{\mathcal{J}}_2(\widetilde{k}) \right], \tag{A2d}$$

and the coefficients in Eq. (3.9) by

$$\widetilde{\mathcal{A}}_3(E) \equiv \widetilde{\mathcal{A}}_3(\widetilde{k}) = \frac{1}{2} e^{-\widetilde{Q}_2 b} \left(1-\frac{\widetilde{k}}{\widetilde{Q}_2}\right) e^{-\widetilde{k} b}, \tag{A3a}$$

$$\widetilde{\mathcal{A}}_4(E) \equiv \widetilde{\mathcal{A}}_4(\widetilde{k}) = \frac{1}{2} e^{\widetilde{Q}_2 b} \left(1+\frac{\widetilde{k}}{\widetilde{Q}_2}\right) e^{-\widetilde{k} b}, \tag{A3b}$$

$$\widetilde{\mathcal{A}}_1(E) \equiv \widetilde{\mathcal{A}}_1(\widetilde{k}) = \frac{1}{2} e^{-\widetilde{Q}_1 a} \left[\left(1+\frac{\widetilde{Q}_2}{\widetilde{Q}_1}\right) e^{\widetilde{Q}_2 a} \widetilde{\mathcal{A}}_3(\widetilde{k}) + \left(1-\frac{\widetilde{Q}_2}{\widetilde{Q}_1}\right) e^{-\widetilde{Q}_2 a} \widetilde{\mathcal{A}}_4(\widetilde{k}) \right], \tag{A3c}$$

$$\widetilde{\mathcal{A}}_2(E) \equiv \widetilde{\mathcal{A}}_2(\widetilde{k}) = \frac{1}{2} e^{\widetilde{Q}_1 a} \left[\left(1-\frac{\widetilde{Q}_2}{\widetilde{Q}_1}\right) e^{\widetilde{Q}_2 a} \widetilde{\mathcal{A}}_3(\widetilde{k}) + \left(1+\frac{\widetilde{Q}_2}{\widetilde{Q}_1}\right) e^{-\widetilde{Q}_2 a} \widetilde{\mathcal{A}}_4(\widetilde{k}) \right]. \tag{A3d}$$

If we define

$$k := \sqrt{\frac{2m}{\hbar^2}\, E}\,; \quad Q_1 := \sqrt{\frac{2m}{\hbar^2}\,(E+V_1)}\,; \quad Q_2 := \sqrt{\frac{2m}{\hbar^2}\,(E-V_2)}\,. \tag{A4}$$

then the functions $\mathcal{J}(E)$ of Eq. (3.11) are given by

$$\mathcal{J}_1(E) \equiv \mathcal{J}_1(k) = \frac{1}{2} e^{-iQ_2 a} \left(\sin(Q_1 a) + \frac{Q_1}{iQ_2} \cos(Q_1 a) \right), \tag{A5a}$$

$$\mathcal{J}_2(E) \equiv \mathcal{J}_2(k) = \frac{1}{2} e^{iQ_2 a} \left(\sin(Q_1 a) - \frac{Q_1}{iQ_2} \cos(Q_1 a) \right), \tag{A5b}$$

$$\mathcal{J}_3(E) \equiv \mathcal{J}_3(k) = \frac{1}{2} e^{-ikb} \left[\left(1 + \frac{Q_2}{k}\right) e^{iQ_2 b} \mathcal{J}_1(k) + \left(1 - \frac{Q_2}{k}\right) e^{-iQ_2 b} \mathcal{J}_2(k) \right], \tag{A5c}$$

$$\mathcal{J}_4(E) \equiv \mathcal{J}_4(k) = \frac{1}{2} e^{ikb} \left[\left(1 - \frac{Q_2}{k}\right) e^{iQ_2 b} \mathcal{J}_1(k) + \left(1 + \frac{Q_2}{k}\right) e^{-iQ_2 b} \mathcal{J}_2(k) \right], \tag{A5d}$$

and the functions $\mathcal{A}^+(E)$ of Eq. (3.12) by

$$\mathcal{A}_3^+(E) \equiv \mathcal{A}_3^+(k) = \frac{1}{2} e^{-iQ_2 b} \left(1 + \frac{k}{Q_2}\right) e^{ikb}, \tag{A6a}$$

$$\mathcal{A}_4^+(E) \equiv \mathcal{A}_4^+(k) = \frac{1}{2} e^{iQ_2 b} \left(1 - \frac{k}{Q_2}\right) e^{ikb}, \tag{A6b}$$

$$\mathcal{A}_1^+(E) \equiv \mathcal{A}_1^+(k) = \frac{1}{2} e^{-iQ_1 a} \left[\left(1 + \frac{Q_2}{Q_1}\right) e^{iQ_2 a} \mathcal{A}_3^+(k) + \left(1 - \frac{Q_2}{Q_1}\right) e^{-iQ_2 a} \mathcal{A}_4^+(k) \right], \tag{A6c}$$

$$\mathcal{A}_2^+(E) \equiv \mathcal{A}_2^+(k) = \frac{1}{2} e^{iQ_1 a} \left[\left(1 - \frac{Q_2}{Q_1}\right) e^{iQ_2 a} \mathcal{A}_3^+(k) + \left(1 + \frac{Q_2}{Q_1}\right) e^{-iQ_2 a} \mathcal{A}_4^+(k) \right]. \tag{A6d}$$

The coefficients in Eq. (3.14) are given by

$$\mathcal{A}_3^-(E) \equiv \mathcal{A}_3^-(k) = \frac{1}{2} e^{-iQ_2 b} \left(1 - \frac{k}{Q_2}\right) e^{-ikb}, \tag{A7a}$$

$$\mathcal{A}_4^-(E) \equiv \mathcal{A}_4^-(k) = \frac{1}{2} e^{iQ_2 b} \left(1 + \frac{k}{Q_2}\right) e^{-ikb}, \tag{A7b}$$

$$\mathcal{A}_1^-(E) \equiv \mathcal{A}_1^-(k) = \frac{1}{2} e^{-iQ_1 a} \left[\left(1 + \frac{Q_2}{Q_1}\right) e^{iQ_2 a} \mathcal{A}_3^-(k) + \left(1 - \frac{Q_2}{Q_1}\right) e^{-iQ_2 a} \mathcal{A}_4^-(k) \right], \tag{A7c}$$

$$\mathcal{A}_2^-(E) \equiv \mathcal{A}_2^-(k) = \frac{1}{2} e^{iQ_1 a} \left[\left(1 - \frac{Q_2}{Q_1}\right) e^{iQ_2 a} \mathcal{A}_3^-(k) + \left(1 + \frac{Q_2}{Q_1}\right) e^{-iQ_2 a} \mathcal{A}_4^-(k) \right]. \tag{A7d}$$

The coefficients in Eq. (4.4a) are given by

$$\widetilde{\mathcal{B}}_3(E) \equiv \widetilde{\mathcal{B}}_3(\widetilde{k}) = \frac{1}{2} e^{-\widetilde{Q}_2 b} \left(1 + \frac{\widetilde{k}}{\widetilde{Q}_2}\right) e^{\widetilde{k} b}, \tag{A8a}$$

$$\widetilde{\mathcal{B}}_4(E) \equiv \widetilde{\mathcal{B}}_4(\widetilde{k}) = \frac{1}{2} e^{\widetilde{Q}_2 b} \left(1 - \frac{\widetilde{k}}{\widetilde{Q}_2}\right) e^{\widetilde{k} b}, \tag{A8b}$$

$$\widetilde{\mathcal{B}}_1(E) \equiv \widetilde{\mathcal{B}}_1(\widetilde{k}) = \frac{1}{2} e^{-\widetilde{Q}_1 a} \left[\left(1 + \frac{\widetilde{Q}_2}{\widetilde{Q}_1}\right) e^{\widetilde{Q}_2 a} \widetilde{\mathcal{B}}_3(\widetilde{k}) + \left(1 - \frac{\widetilde{Q}_2}{\widetilde{Q}_1}\right) e^{-\widetilde{Q}_2 a} \widetilde{\mathcal{B}}_4(\widetilde{k}) \right], \tag{A8c}$$

$$\widetilde{\mathcal{B}}_2(E) \equiv \widetilde{\mathcal{B}}_2(\widetilde{k}) = \frac{1}{2} e^{\widetilde{Q}_1 a} \left[\left(1 - \frac{\widetilde{Q}_2}{\widetilde{Q}_1}\right) e^{\widetilde{Q}_2 a} \widetilde{\mathcal{B}}_3(\widetilde{k}) + \left(1 + \frac{\widetilde{Q}_2}{\widetilde{Q}_1}\right) e^{-\widetilde{Q}_2 a} \widetilde{\mathcal{B}}_4(\widetilde{k}) \right]. \tag{A8d}$$

The functions $\mathcal{C}(E)$ of Eq. (4.17b) are given by

$$\mathcal{C}_1(E) \equiv \mathcal{C}_1(k) = \frac{1}{2} e^{-iQ_2 a} \left(\cos(Q_1 a) - \frac{Q_1}{iQ_2} \sin(Q_1 a) \right) , \tag{A9a}$$

$$\mathcal{C}_2(E) \equiv \mathcal{C}_2(k) = \frac{1}{2} e^{iQ_2 a} \left(\cos(Q_1 a) + \frac{Q_1}{iQ_2} \sin(Q_1 a) \right) , \tag{A9b}$$

$$\mathcal{C}_3(E) \equiv \mathcal{C}_3(k) = \frac{1}{2} e^{-ikb} \left[\left(1 + \frac{Q_2}{k}\right) e^{iQ_2 b} \mathcal{C}_1(k) + \left(1 - \frac{Q_2}{k}\right) e^{-iQ_2 b} \mathcal{C}_2(k) \right] , \tag{A9c}$$

$$\mathcal{C}_4(E) \equiv \mathcal{C}_4(k) = \frac{1}{2} e^{ikb} \left[\left(1 - \frac{Q_2}{k}\right) e^{iQb} \mathcal{C}_1(k) + \left(1 + \frac{Q_2}{k}\right) e^{-iQb} \mathcal{C}_2(k) \right] . \tag{A9d}$$

APPENDIX B: PROOFS OF PROPOSITIONS 1 AND 2

Proof of Proposition 1.

(i) It is very easy to show that the quantities (6.9) fulfill the conditions to be a norm,

$$\|\varphi_{\rm c} + \psi_{\rm c}\|_{n,m} \leq \|\varphi_{\rm c}\|_{n,m} + \|\psi_{\rm c}\|_{n,m} , \tag{B1a}$$

$$\|\alpha \varphi_{\rm c}\|_{n,m} = |\alpha| \, \|\varphi_{\rm c}\|_{n,m} , \tag{B1b}$$

$$\|\varphi_{\rm c}\|_{n,m} \geq 0 , \tag{B1c}$$

$$\text{If } \|\varphi_{\rm c}\|_{n,m} = 0, \text{ then } \varphi_{\rm c} = 0 . \tag{B1d}$$

The only condition that is somewhat difficult to prove is (B1d): if $\|\varphi_{\rm c}\|_{n,m} = 0$, then

$$(1+r)^n (h+1)^m \varphi_{\rm c}(r) = 0 , \tag{B2}$$

which yields

$$(h+1)^m \varphi_{\rm c}(r) = 0 . \tag{B3}$$

If $m = 0$, then Eq. (B3) implies $\varphi_{\rm c}(r) = 0$. If $m = 1$, then Eq. (B3) implies that -1 is an eigenvalue of $H_{\rm c}$ whose corresponding eigenvector is $\varphi_{\rm c}$. Since there is no discrete eigenvalue in the continuous part of the spectrum, $\varphi_{\rm c}$ must be the zero vector. The proof for $m > 1$ is similar.

(ii) In order to see that $H_{\rm c}$ is $\tau_{\mathbf{\Phi}_{\rm c}}$-continuous, we just have to realize that

$$\begin{aligned} \|H_{\rm c}\varphi_{\rm c}\|_{n,m} &= \|(H_{\rm c}+I)\varphi_{\rm c} - \varphi_{\rm c}\|_{n,m} \\ &\leq \|(H_{\rm c}+I)\varphi_{\rm c}\|_{n,m} + \|\varphi_{\rm c}\|_{n,m} \\ &= \|\varphi_{\rm c}\|_{n,m+1} + \|\varphi_{\rm c}\|_{n,m} . \end{aligned} \tag{B4}$$

The stability of $\mathbf{\Phi}_{\rm c}$ under the action of $H_{\rm c}$ also follows from Eq. (B4).

(iii) From the definition (6.6), it is pretty easy to see that $|E\rangle$ is an antilinear functional. In order to show that $|E\rangle$ is continuous, we define

$$\mathcal{M}(E) := \sup_{r \in [0,\infty)} |\phi(r;E)| . \tag{B5}$$

Since

$$
\begin{aligned}
|\langle \varphi_{\rm c}|E\rangle| &= \left| \int_0^\infty dr\, \overline{\varphi_{\rm c}(r)}\phi(r;E) \right| \\
&\leq \mathcal{M}(E) \int_0^\infty dr\, |\varphi_{\rm c}(r)| \\
&= \mathcal{M}(E) \int_0^\infty dr\, \frac{1}{1+r}(1+r)|\varphi_{\rm c}(r)| \\
&\leq \mathcal{M}(E) \left(\int_0^\infty dr\, \frac{1}{(1+r)^2} \right)^{1/2} \left(\int_0^\infty dr\, |(1+r)\varphi_{\rm c}(r)|^2 \right)^{1/2} \\
&= \mathcal{M}(E) \|\varphi_{\rm c}\|_{1,0} \, ,
\end{aligned} \tag{B6}
$$

the functional $|E\rangle$ is continuous when $\mathbf{\Phi}_{\rm c}$ is endowed with the $\tau_{\mathbf{\Phi}_{\rm c}}$ topology.

(iv) In order to prove that $|E\rangle$ is a generalized eigenvector of $H_{\rm c}$, we make use of the conditions (6.5) and (6.7) satisfied by the elements of $\mathbf{\Phi}_{\rm c}$,

$$
\begin{aligned}
\langle \varphi_{\rm c}|H_{\rm c}^{\times}|E\rangle &= \langle H_{\rm c}^{\dagger}\varphi_{\rm c}|E\rangle \\
&= \int_0^\infty dr \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) \right) \overline{\varphi_{\rm c}(r)}\phi(r;E) \\
&= -\frac{\hbar^2}{2m} \left[\frac{d\overline{\varphi_{\rm c}(r)}}{dr}\phi(r;E) \right]_0^\infty + \frac{\hbar^2}{2m} \left[\overline{\varphi_{\rm c}(r)}\frac{d\phi(r;E)}{dr} \right]_0^\infty \\
&\quad + \int_0^\infty dr\, \overline{\varphi_{\rm c}(r)} \left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) \right) \phi(r;E) \\
&= E\langle \varphi_{\rm c}|E\rangle \, .
\end{aligned} \tag{B7}
$$

Proof of Proposition 2.

Let φ and ψ be in $\mathbf{\Phi}$. Since U of Eq. (5.12) is unitary,

$$
(\varphi, \psi) = (U\varphi, U\psi) = (\widehat{\varphi}_{\rm b}, \widehat{\psi}_{\rm b})_{\mathcal{H}_{\rm b}} + (\widehat{\varphi}_{\rm c}, \widehat{\psi}_{\rm c})_{\mathcal{H}_{\rm c}} \, . \tag{B8}
$$

The scalar product of $\widehat{\varphi}_{\rm b}$ and $\widehat{\psi}_{\rm b}$ can be written as

$$
(\widehat{\varphi}_{\rm b}, \widehat{\psi}_{\rm b})_{\mathcal{H}_{\rm b}} = \sum_{n=1}^{N} (\varphi|E_n)(E_n|\psi) \, . \tag{B9}
$$

The wave functions $\widehat{\varphi}_{\rm c}$ and $\widehat{\psi}_{\rm c}$ are in particular elements of $L^2([0,\infty), dE)$. Hence their scalar product is well-defined,

$$
(\widehat{\varphi}_{\rm c}, \widehat{\psi}_{\rm c})_{\mathcal{H}_{\rm c}} = \int_0^\infty dE\, \overline{\widehat{\varphi}_{\rm c}(E)}\, \widehat{\psi}_{\rm c}(E) \, . \tag{B10}
$$

Since $\varphi_{\rm c}$ and $\psi_{\rm c}$ belong to $\mathbf{\Phi}_{\rm c}$, the action of each eigenket $|E\rangle$ on them is well-defined,

$$
\langle \varphi_{\rm c}|E\rangle = \overline{\widehat{\varphi}_{\rm c}(E)} \, , \tag{B11a}
$$

$$
\langle E|\psi_{\rm c}\rangle = \widehat{\psi}_{\rm c}(E) \, . \tag{B11b}
$$

By plugging Eq. (B11) into Eq. (B10) and Eqs. (B10) and (B9) into Eq. (B8), we get to Eq. (6.22). The proof of (6.23) follows the same pattern.

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