# Rigged Hilbert Space Treatment of Continuous Spectrum


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(March 16, 2002)


## Abstract


The ability of the Rigged Hilbert Space formalism to deal with continuous spectrum is demonstrated within the example of the square barrier potential. The non-square integrable solutions of the time-independent Schrödinger equation are used to define Dirac kets, which are (generalized) eigenvectors of the Hamiltonian. These Dirac kets are antilinear functionals over the space of physical wave functions. They are also basis vectors that expand any physical wave function in a Dirac basis vector expansion. It is shown that an acceptable physical wave function must fulfill stronger conditions than just square integrability—the space of physical wave functions is not the whole Hilbert space but rather a dense subspace of the Hilbert space. We construct the position and energy representations of the Rigged Hilbert Space generated by the square barrier potential Hamiltonian. We shall also construct the unitary operator that transforms from the position into the energy representation. We shall see that in the energy representation the Dirac kets act as the antilinear Schwartz delta functional. In constructing the Rigged Hilbert Space of the square barrier potential, we will find a systematic procedure to construct the Rigged Hilbert Space of a large class of spherically symmetric potentials. The example of the square barrier potential will also make apparent that the natural framework for the solutions of a Schrödinger operator with continuous spectrum is the Rigged Hilbert Space rather than just the Hilbert space.



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## 1. INTRODUCTION

In the late 1920s, Dirac introduced a new mathematical model of Quantum Mechanics based upon a uniquely smooth and elegant abstract algebra of linear operators defined on an infinite dimensional complex vector space equipped with an inner product norm [1]. Dirac's abstract algebraic model of *bras* and *kets* (from the bracket notation for inner product) proved to be of great heuristic value in the ensuing years, especially in dealing with Hamiltonians whose spectrum is continuous.

The Hilbert space (HS) was the first mathematical idealization proposed for Quantum Mechanics [2]. However, as von Neumann explains in the introduction to his book [2], the HS theory and Dirac's formalism are two different things. Although there were attempts to realize the Dirac formalism in Hilbert space, there were a number of serious problems resulting from the fact that the Hilbert space cannot allocate such things as bras, kets, the Dirac delta function or the Dirac basis vector expansion, all of which are essential in any physical formulation of Quantum Mechanics that deals with continuous spectrum. Indeed in his textual presentation [1] Dirac himself states that "the bra and ket vectors that we now use form a more general space than a Hilbert Space" (see [1], page 40).

In the late 1940s, L. Schwartz gave a precise meaning to the Dirac delta function as a functional over a space of test functions (cf. [3]). This led to the development of a new branch of functional analysis, the theory of distributions [3]. About the same time, von Neumann published the theory of direct integral decompositions of a Hilbert space induced by a self-adjoint operator [4] (also valid for more general cases). This spectral theory was closer to classical Fourier analysis and represented an improvement over the earlier von Neumann's spectral theory [2].

I. Gelfand always thought that von Neumann's spectral theory was not the whole story of the theory of linear operators defined on infinite dimensional vector spaces. Prompted by the theory of distributions, he and his school introduced the Rigged Hilbert Space (RHS). Starting out with this RHS and von Neumann's direct integral decomposition, they were able to prove the Nuclear Spectral theorem (also called Gelfand-Maurin theorem) [5]. This theorem justifies Dirac basis vector expansion.

One of the aspects of Dirac's formalism, the continuity of the elements of the algebra of observables, was discussed in the early 1960s in Refs. [6,7]. If two operators of the algebra of observables satisfy the canonical (Heisenberg) commutation relation, at least one of them cannot be continuous (bounded) with respect to the Hilbert space topology. In Refs. [6,7], it is shown that there are subdomains of the Hilbert space that can be endowed with (locally convex) topologies that make those operators continuous; the largest of those subdomains is the Schwartz space.

In the mid 1960s, some physicists [8–10] independently realized that the RHS provides a rigorous mathematical rephrasing of all the aspects of Dirac's formalism. In particular, the Nuclear Spectral theorem restates Dirac basis vector expansion along with the Dirac bras and kets within a mathematical theory. Later on, the RHS was used to accommodate resonance states (Gamow vectors) (cf. [11–17] and references therein). Applications of the RHS formalism to Quantum Mechanics can now be found in some textbooks [18,19].

Although there are some explicit examples of RHS in the literature (see for instance [20]), no example of the RHS generated by a Schrödinger Hamiltonian with continuous spectrum has been constructed yet. Here we try to fill in this gap [17].

The dynamical equation that governs the behavior of a quantum system at any time is the time-dependent Schrödinger equation,

$$i\hbar \frac{\partial}{\partial t}\varphi(t) = H\varphi(t)\,, \tag{1.1}$$

where $H$ denotes the Hamiltonian of the system and $\varphi(t)$ denotes the value of the wave function $\varphi$ at time $t$. In order to solve (1.1), we associate to each energy $E$ in the spectrum $\mathrm{Sp}(H)$ of the Hamiltonian a ket $|E\rangle$ which is an eigenvector of $H$,

$$H|E\rangle = E|E\rangle\,, \quad E \in \mathrm{Sp}(H)\,. \tag{1.2}$$

These eigenkets form a complete basis system that expands any wave function $\varphi$ as

$$\varphi = \int dE\, |E\rangle\langle E|\varphi\rangle \equiv \int dE\, \varphi(E)|E\rangle\,. \tag{1.3}$$

The time-dependent solution of Eq. (1.1) is obtained by Fourier-transforming the time-independent solution (1.3),

$$\varphi(t) = \int dE\, e^{-iEt/\hbar}\,\varphi(E)\,. \tag{1.4}$$

If the spectrum of the Hamiltonian has a continuous part, and if the energy $E$ belongs to this continuous part of the spectrum, then the corresponding eigenket $|E\rangle$ that solves Eq. (1.2) is not square integrable, i.e., $|E\rangle$ is not an element of the Hilbert space. Therefore, the eigenket $|E\rangle$ cannot represent an experimentally preparable physical state.

We will show that the expansion (1.3) is only valid for those $\varphi$ that belong to a space of test functions $\mathbf{\Phi} \subset \mathcal{H}$. We will also show that the kets $|E\rangle$ can be understood mathematically as continuous antilinear functionals over the space of test functions $\mathbf{\Phi}$, i.e., $|E\rangle \in \mathbf{\Phi}^\times$. According to the RHS mathematics, equation (1.2) means that

$$\langle H\varphi|E\rangle = E\langle\varphi|E\rangle\,, \quad \text{for every } \varphi \in \mathbf{\Phi}\,, \tag{1.5}$$

where $H$ is (the restriction to $\mathbf{\Phi}$ of) the self-adjoint Hamiltonian operator, which is a continuous operator on the linear topological space $\mathbf{\Phi}$. For every such an operator, one defines the conjugate operator $H^\times$ on $\mathbf{\Phi}^\times$ by

$$\langle H\varphi|F\rangle = \langle\varphi|H^\times F\rangle\,, \quad \text{for all } \varphi \in \mathbf{\Phi}\,,\ F \in \mathbf{\Phi}^\times\,. \tag{1.6}$$

The operator $H^\times$ is a uniquely defined extension of the Hilbert space adjoint operator $H^\dagger$ (which for the case of a essentially self-adjoint operator coincides with the closure of $H$). Using the definition (1.6), we write (1.5) formally as

$$H^\times|E\rangle = E|E\rangle\,, \quad |E\rangle \in \mathbf{\Phi}^\times\,, \tag{1.7}$$

which is understood as a functional equation over the space $\mathbf{\Phi}$. The quantities $E$ and $|E\rangle$ are called generalized eigenvalues and generalized eigenvectors, respectively.

The general statement of the Nuclear Spectral theorem just assures the existence of the generalized eigenvectors $|E\rangle$, but it does not provide a prescription to construct them. In this paper, we construct the generalized eigenvectors $|E\rangle$ of the square barrier Hamiltonian along with the RHS. We shall use the Sturm-Liouville theory (Weyl theory) [21] to find the RHS of the square barrier potential.

By applying the Sturm-Liouville theory to the Schrödinger equation of the square barrier potential, we will obtain a domain $\mathcal{D}(H)$ on which the Hamiltonian is self-adjoint. The Green functions, the spectrum, and the unitary transformation that diagonalizes our Hamiltonian will be also computed. The diagonalization of the Hamiltonian will allow us to obtain the energy (spectral) representation and the direct integral decomposition of the Hilbert space induced by our Hamiltonian. We will see why this direct integral decomposition is not enough for the purposes of Quantum Mechanics and why the RHS is necessary. Next, we will construct the space $\mathbf{\Phi}$ and therewith the RHS of the square barrier potential,

$$\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^{\times} \, . \tag{1.8}$$

Dirac kets will be accommodated as elements of $\mathbf{\Phi}^{\times}$, and the Schwartz delta function will appear in the energy (spectral) representation of the triplet (1.8). The Nuclear Spectral theorem will be proved, and it will be shown that this theorem is just a restatement of the heuristic Dirac basis vector expansion.

## 2. STURM-LIOUVILLE THEORY APPLIED TO THE SQUARE BARRIER POTENTIAL

### 2.1. Schrödinger Equation in the Position Representation

In order to calculate the set of real generalized eigenvalues of the square barrier Hamiltonian (the physical spectrum) and their corresponding generalized eigenvectors, we solve equation (1.7) in the position representation,

$$\langle \vec{x}|H^{\times}|E\rangle = E\langle \vec{x}|E\rangle \, . \tag{2.1}$$

The expression of the Hamiltonian in the position representation is

$$\langle \vec{x}|H^{\times}|E\rangle = \left( \frac{-\hbar^2}{2m}\Delta + V(\vec{x}) \right) \langle \vec{x}|E\rangle \, , \tag{2.2}$$

where $\Delta$ is the three-dimensional Laplacian and

$$V(\vec{x}) = V(r) = \begin{cases} 0 & 0 < r < a \\ V_0 & a < r < b \\ 0 & b < r < \infty \end{cases} \tag{2.3}$$

is the square barrier potential. Writing Eqs. (2.1) and (2.2) in spherical coordinates and restricting ourselves to the case of zero angular momentum, we obtain the radial time-independent Schrödinger equation,

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)\right)\chi(r;E)=E\chi(r;E)\,. \tag{2.4}$$

Thus our Hamiltonian in the radial representation is given by the differential operator

$$h\equiv-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)\,. \tag{2.5}$$

Throughout this paper, the symbol $h$ will be used to denote the formal differential operator (2.5). The formal differential operator (2.5) is of the Sturm-Liouville type (cf. [21]), and therefore we are allowed to apply the Sturm-Liouville theory to our problem.

Mathematically, all the information about the differential operator $h$ that is provided by the Sturm-Liouville theory (resolvent, spectrum, spectral representation,...) is obtained from the generalized eigenvalue equation

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

subject to different boundary conditions. From a physical point of view, Eq. (2.6) is the time-independent Schrödinger equation. As mentioned in the introduction, the monoenergetic eigensolutions of (2.6) are not in general square integrable, i.e., they are not in the Hilbert space. Those monoenergetic eigensolutions will be associated to antilinear functionals $F_E\in\mathbf{\Phi}^\times$ by

$$F_E(\varphi)\equiv\int_0^\infty dr\,\overline{\varphi(r)}\chi(r;E)\,. \tag{2.7}$$

These functionals are generalized eigenvectors of the Hamiltonian $H$,

$$H^\times F_E=EF_E\,, \tag{2.8}$$

or more precisely,

$$\langle\varphi|H^\times|F_E\rangle=\langle H\varphi|F_E\rangle=E\langle\varphi|F_E\rangle\,,\quad\forall\varphi\in\mathbf{\Phi}\,. \tag{2.9}$$

### 2.2. Self-Adjoint Extension

Our first objective will be to define a linear operator on a Hilbert space corresponding to the formal differential operator $h$ and investigate its self-adjoint extensions. Among all the possibilities, we shall choose the self-adjoint extension that fits spherically symmetric potentials. Later sections will deal with the spectral properties of this self-adjoint extension and with the RHS induced by it.

The Hilbert space that is in the RHS of the square barrier potential is realized by the space $L^2([0,\infty),dr)$ of square integrable functions $f(r)$ defined on the interval $[0,\infty)$. In this section, we find a subdomain $\mathcal{D}(H)$ of this Hilbert space on which the differential operator $h$ is self-adjoint. This domain must be a proper dense linear subspace of $L^2([0,\infty),dr)$. The action of $h$ must be well-defined on $\mathcal{D}(H)$, and this action must remain in $L^2([0,\infty),dr)$. We need also a boundary condition that assures the self-adjointness of the Hamiltonian. Among all the possible boundary conditions that provide a self-adjoint extension (see Appendix A), we choose $f(0) = 0$. These requirements can be written as

$$f(r) \in L^2([0,\infty), dr)\,, \tag{2.10a}$$
$$hf(r) \in L^2([0,\infty), dr)\,, \tag{2.10b}$$
$$f(r) \in AC^2[0,\infty)\,, \tag{2.10c}$$
$$f(0) = 0\,, \tag{2.10d}$$

where $AC^2[0,\infty)$ denotes the space of functions whose derivative is absolutely continuous (see Appendix A). Condition (2.10a) just means that the wave functions are square normalizable. Condition (2.10b) assures that the action of $h$ on any $f(r) \in \mathcal{D}(H)$ is square integrable. Condition (2.10c) is the weakest condition sufficient for the second derivative of $f(r)$ to be well-defined. In our example, this condition implies that $f(r)$ and $f'(r)$ are continuous at $r = a$ and at $r = b$. Condition (2.10d) selects the self-adjoint extension needed in physics.

The reason why we choose (2.10d) is the following: in physics [1,22–24], the set of boundary conditions imposed on the Schrödinger equation (2.6) always includes

$$\chi(0; E) = 0\,, \tag{2.11a}$$
$$\chi(r; E),\ \text{and}\ \chi'(r; E)\ \text{are continuous at}\ r = a\ \text{and at}\ r = b\,. \tag{2.11b}$$

Condition (2.11b) is implied by (2.10c), so we just need to recover (2.11a). This is why we impose (2.10d).

The set of conditions (2.10) leads to the domain

$$\mathcal{D}(H) = \{ f(r) \mid f(r), hf(r) \in L^2([0,\infty), dr),\ f(r) \in AC^2[0,\infty),\ f(0) = 0 \}\,. \tag{2.12}$$

In choosing (2.12) as the domain of our formal differential operator $h$, we define a linear operator $H$ by

$$Hf(r) := hf(r) = \left( -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + V(r) \right) f(r)\,, \quad f(r) \in \mathcal{D}(H)\,. \tag{2.13}$$

### 2.3. Resolvent and Green Functions

The Green function is the kernel of integration needed to write the resolvent of $H$ as an integral operator,

$$(E - H)^{-1} f(r) = \int_0^\infty G(r, s; E) f(s)\, ds\,. \tag{2.14}$$

The procedure to compute the Green function of our operator (2.13) is explained in [21] (see also [25]). For the sake of completeness, we include in Appendix B the theorem that is used to calculate $G(r, s; E)$.

The expression of the Green function will be given in terms of eigenfunctions of the differential operator $h$ subject to different boundary conditions (see Theorem 1 of Appendix B). We shall consider three regions of the complex plane and compute the Green function for each region separately. In all our calculations, we will use the following branch of the square root function:

$$\sqrt{\cdot} : \{E \in \mathbb{C} \mid \; -\pi < \arg(E) \leq \pi\} \longmapsto \{E \in \mathbb{C} \mid \; -\pi/2 < \arg(E) \leq \pi/2\} \, . \tag{2.15}$$

**Region $\Re(E) < 0$, $\Im(E) \neq 0$**

For $\Re(E) < 0$, $\Im(E) \neq 0$, the Green function (see Theorem 1 of Appendix B) is given by

$$G(r,s;E) = \left\{ \begin{array}{ll} -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}} \frac{\widetilde{\chi}(r;E)\,\widetilde{\Theta}(s;E)}{2\widetilde{\mathcal{J}}_3(E)} & r<s \\ -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}} \frac{\widetilde{\chi}(s;E)\,\widetilde{\Theta}(r;E)}{2\widetilde{\mathcal{J}}_3(E)} & r>s \end{array} \right. \quad \Re(E)<0\,, \; \Im(E) \neq 0 \, . \tag{2.16}$$

The eigenfunction $\widetilde{\chi}(r;E)$ satisfies the Schrödinger equation (2.6) and the boundary conditions

$$\widetilde{\chi}(0;E) = 0 \, , \tag{2.17a}$$
$$\widetilde{\chi}(r;E) \in AC^2([0,\infty)) \, , \tag{2.17b}$$
$$\widetilde{\chi}(r;E) \text{ is square integrable at } 0 \, . \tag{2.17c}$$

The boundary conditions (2.17) can be written as

$$\widetilde{\chi}(0;E) = 0 \, , \tag{2.18a}$$
$$\widetilde{\chi}(a-0;E) = \widetilde{\chi}(a+0;E) \, , \tag{2.18b}$$
$$\widetilde{\chi}'(a-0;E) = \widetilde{\chi}'(a+0;E) \, , \tag{2.18c}$$
$$\widetilde{\chi}(b-0;E) = \widetilde{\chi}(b+0;E) \, , \tag{2.18d}$$
$$\widetilde{\chi}'(b-0;E) = \widetilde{\chi}'(b+0;E) \, , \tag{2.18e}$$
$$\widetilde{\chi}(r;E) \;\text{ is square integrable at } 0 \, , \tag{2.18f}$$

and lead to

$$\widetilde{\chi}(r;E) = \left\{ \begin{array}{ll} e^{\sqrt{-\frac{2m}{\hbar^2}E}r} - e^{-\sqrt{-\frac{2m}{\hbar^2}E}r} & 0<r<a \\ \widetilde{\mathcal{J}}_1(E) e^{\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r} + \widetilde{\mathcal{J}}_2(E) e^{-\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b \\ \widetilde{\mathcal{J}}_3(E) e^{\sqrt{-\frac{2m}{\hbar^2}E}r} + \widetilde{\mathcal{J}}_4(E) e^{-\sqrt{-\frac{2m}{\hbar^2}E}r} & b<r<\infty \, . \end{array} \right. \tag{2.19}$$

The functions $\widetilde{\mathcal{J}}_1 - \widetilde{\mathcal{J}}_4$ are such that $\widetilde{\chi}(r;E)$ satisfies the boundary conditions (2.18), and their expressions are given by Eq. (B4) of Appendix B.

The eigenfunction $\widetilde{\Theta}(r;E)$ satisfies the Schrödinger equation (2.6) and the boundary conditions

$$\widetilde{\Theta}(r;E) \in AC^2([0,\infty)) \, , \tag{2.20a}$$
$$\widetilde{\Theta}(r;E) \text{ is square integrable at } \infty \, . \tag{2.20b}$$

The boundary conditions (2.20) can be written as

$$\widetilde{\Theta}(a-0;E)=\widetilde{\Theta}(a+0;E)\,, \tag{2.21a}$$
$$\widetilde{\Theta}'(a-0;E)=\widetilde{\Theta}'(a+0;E)\,, \tag{2.21b}$$
$$\widetilde{\Theta}(b-0;E)=\widetilde{\Theta}(b+0;E)\,, \tag{2.21c}$$
$$\widetilde{\Theta}'(b-0;E)=\widetilde{\Theta}'(b+0;E)\,, \tag{2.21d}$$
$$\widetilde{\Theta}(r;E)\ \text{ is square integrable at } \infty\,, \tag{2.21e}$$

and lead to

$$\widetilde{\Theta}(r;E)=\begin{cases} \widetilde{\mathcal{A}}_1(E)e^{\sqrt{-\frac{2m}{\hbar^2}E}r}+\widetilde{\mathcal{A}}_2(E)e^{-\sqrt{-\frac{2m}{\hbar^2}E}r} & 0<r<a \\ \widetilde{\mathcal{A}}_3(E)e^{\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r}+\widetilde{\mathcal{A}}_4(E)e^{-\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b \\ e^{-\sqrt{-\frac{2m}{\hbar^2}E}r} & b<r<\infty\,. \end{cases} \tag{2.22}$$

The functions $\widetilde{\mathcal{A}}_1-\widetilde{\mathcal{A}}_4$ are such that $\widetilde{\Theta}(r;E)$ satisfies the boundary conditions (2.21), and their expressions are given by Eq. (B5) of Appendix B.

**Region $\Re(E)>0$, $\Im(E)>0$**

When $\Re(E)>0$, $\Im(E)>0$, the expression of the Green function is

$$G(r,s;E)=\begin{cases} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(r;E)\,\Theta_+(s;E)}{2i\mathcal{J}_4(E)} & r<s \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(s;E)\,\Theta_+(r;E)}{2i\mathcal{J}_4(E)} & r>s \end{cases} \qquad \Re(E)>0,\ \Im(E)>0\,. \tag{2.23}$$

The eigenfunction $\chi(r;E)$ satisfies the Schrödinger equation (2.6) and the boundary conditions (2.17),

$$\chi(r;E)=\begin{cases} \sin(\sqrt{\frac{2m}{\hbar^2}E}r) & 0<r<a \\ \mathcal{J}_1(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r}+\mathcal{J}_2(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b \\ \mathcal{J}_3(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r}+\mathcal{J}_4(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & b<r<\infty\,. \end{cases} \tag{2.24}$$

The functions $\mathcal{J}_1-\mathcal{J}_4$ are determined by the boundary conditions (2.18), and their expressions are listed in Eq. (B8) of Appendix B.

The eigenfunction $\Theta_+(r;E)$ satisfies the Schrödinger equation (2.6) and the boundary conditions (2.20),

$$\Theta_+(r;E)=\begin{cases} \mathcal{A}_1^+(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r}+\mathcal{A}_2^+(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & 0<r<a \\ \mathcal{A}_3^+(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r}+\mathcal{A}_4^+(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b \\ e^{i\sqrt{\frac{2m}{\hbar^2}E}r} & b<r<\infty\,. \end{cases} \tag{2.25}$$

The functions $\mathcal{A}_1^+-\mathcal{A}_4^+$ are determined by the boundary conditions (2.21), and their expressions are listed in Eq. (B9) of Appendix B.

**Region $\Re(E)>0$, $\Im(E)<0$**

In the region $\Re(E)>0$, $\Im(E)<0$ the Green function reads

$$G(r,s;E)=\begin{cases} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(r;E)\,\Theta_-(s;E)}{2i\mathcal{J}_3(E)} & r<s \\ -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{\chi(s;E)\,\Theta_-(r;E)}{2i\mathcal{J}_3(E)} & r>s \end{cases}\qquad \Re(E)>0,\ \Im(E)<0\,. \tag{2.26}$$

The eigenfunction $\chi(r;E)$ is given by (2.24). The eigenfunction $\Theta_-(r;E)$ satisfies the Schrödinger equation (2.6) and the boundary conditions (2.20),

$$\Theta_-(r;E)=\begin{cases} \mathcal{A}_1^-(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r}+\mathcal{A}_2^-(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & 0<r<a \\ \mathcal{A}_3^-(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r}+\mathcal{A}_4^-(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b \\ e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & b<r<\infty\,. \end{cases} \tag{2.27}$$

The functions $\mathcal{A}_1^- - \mathcal{A}_4^-$ are such that $\Theta_-(r;E)$ and its derivative are continuous at $r=a$ and at $r=b$. Their expressions are listed in Eq. (B11) of Appendix B.

### 2.4. Diagonalization of $H$ and Eigenfunction Expansion

In the present section, we diagonalize the Hamiltonian and construct the eigenfunction expansion generated by the eigenfunctions of the differential operator $h$. In order to do so, we compute the spectrum of $H$ and then construct a unitary operator $U$ that transforms from the position representation into the energy representation. We will see that the spectrum of $H$ is the positive real line $[0,\infty)$. In the energy representation, $H$ will act as the multiplication operator, the Hilbert space will be realized by $L^2([0,\infty),dE)$ and the domain of the Hamiltonian will be realized by the maximal domain on which the multiplication operator is well-defined. On our way, we shall take advantage of some theorems of the Sturm-Liouville theory that are proved in Ref. [21]. For the sake of completeness, we include those theorems in Appendix C.

#### *2.4.1.* Spectrum of $H$

We first compute the spectrum Sp$(H)$ of the operator $H$ by applying Theorem 4 of Appendix C (see also [21]). Since $H$ is self-adjoint, its spectrum is real. The 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 4 of Appendix C.

From the expression of the Green function computed above, it is clear that the subsets $(-\infty,0)$ and $(0,\infty)$ should be studied separately. We will denote either of these subsets by $\Lambda$.

**Subset $\Lambda=(-\infty,0)$**

We first take $\Lambda$ from Theorem 4 of Appendix C 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

$$\sigma_1(r;E) = \begin{cases} \widetilde{\mathcal{B}}_1(E) e^{\sqrt{-\frac{2m}{\hbar^2}E}r} + \widetilde{\mathcal{B}}_2(E) e^{-\sqrt{-\frac{2m}{\hbar^2}E}r} & 0 < r < a \\ \widetilde{\mathcal{B}}_3(E) e^{\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r} + \widetilde{\mathcal{B}}_4(E) e^{-\sqrt{-\frac{2m}{\hbar^2}(E-V_0)}r} & a < r < b \\ e^{\sqrt{-\frac{2m}{\hbar^2}E}r} & b < r < \infty \,, \end{cases} \tag{2.28a}$$

$$\sigma_2(r;E) = \widetilde{\Theta}(r;E) \, . \tag{2.28b}$$

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. (C9) of Appendix C. The function $\widetilde{\Theta}(r;E)$ is given by Eq. (2.22).

Obviously,

$$\widetilde{\chi}(r;E) = \widetilde{\mathcal{J}}_3(E)\sigma_1(r;E) + \widetilde{\mathcal{J}}_4(E)\sigma_2(r;E) \, , \tag{2.29}$$

which along with Eq. (2.16) leads to

$$G(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}} \frac{1}{2} \left[ \sigma_1(r;E) + \frac{\widetilde{\mathcal{J}}_4(E)}{\widetilde{\mathcal{J}}_3(E)} \sigma_2(r;E) \right] \sigma_2(s;E) \, , \qquad r < s \, , \ \Re(E) < 0 \, , \Im(E) \neq 0 \, . \tag{2.30}$$

Since

$$\overline{\sigma_2(s;\overline{E})} = \sigma_2(s;E) \, , \tag{2.31}$$

we can write Eq. (2.30) as

$$G(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}} \frac{1}{2} \left[ \sigma_1(r;E)\overline{\sigma_2(s;\overline{E})} + \frac{\widetilde{\mathcal{J}}_4(E)}{\widetilde{\mathcal{J}}_3(E)} \sigma_2(r;E)\overline{\sigma_2(s;\overline{E})} \right] , \qquad r < s \, , \ \Re(E) < 0 \, , \Im(E) \neq 0 \, . \tag{2.32}$$

On the other hand, by Theorem 4 in Appendix C we have

$$G(r,s;E) = \sum_{i,j=1}^{2} \theta_{ij}^{-}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})} \, , \qquad r < s \, . \tag{2.33}$$

By comparing Eqs. (2.32) and (2.33) we see that

$$\theta_{ij}^{-}(E) = \begin{pmatrix} 0 & -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}} \frac{1}{2} \\ 0 & -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}} \frac{1}{2} \frac{\widetilde{\mathcal{J}}_4(E)}{\widetilde{\mathcal{J}}_3(E)} \end{pmatrix} , \quad \Re(E) < 0 \, , \ \Im(E) \neq 0 \, . \tag{2.34}$$

The functions $\theta_{ij}^{-}(E)$ are analytic in a neighborhood of $\Lambda = (-\infty, 0)$. Therefore, the interval $(-\infty, 0)$ is in the resolvent set $\mathrm{Re}(H)$ of the operator $H$.

**Subset** $\Lambda = (0, \infty)$

Now we study the case $\Lambda = (0,\infty)$. In order to be able to apply Theorem 4 of Appendix C, 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 $E$:

$$\sigma_1(r;E) = \chi(r;E)\,, \tag{2.35a}$$

$$\sigma_2(r;E) = \begin{cases} \cos(\sqrt{\frac{2m}{\hbar^2}E}r) & 0<r<a \\ \mathcal{C}_1(E)e^{i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} + \mathcal{C}_2(E)e^{-i\sqrt{\frac{2m}{\hbar^2}(E-V_0)}r} & a<r<b \\ \mathcal{C}_3(E)e^{i\sqrt{\frac{2m}{\hbar^2}E}r} + \mathcal{C}_4(E)e^{-i\sqrt{\frac{2m}{\hbar^2}E}r} & b<r<\infty\,. \end{cases} \tag{2.35b}$$

The functions $\mathcal{C}_1 - \mathcal{C}_4$, whose expressions are given by Eq. (C10) of Appendix C, are such that $\sigma_2$ and its derivative are continuous at $r=a$ and at $r=b$. The eigenfunction $\chi(r;E)$ is given by Eq. (2.24).

Eqs. (2.25), (2.27) and (2.35) lead to

$$\Theta_+(r;E) = -\frac{\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E) + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E) \tag{2.36}$$

and to

$$\Theta_-(r;E) = \frac{\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E) - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\,, \tag{2.37}$$

where

$$W(E) = \mathcal{J}_4(E)\mathcal{C}_3(E) - \mathcal{J}_3(E)\mathcal{C}_4(E)\,. \tag{2.38}$$

By substituting Eq. (2.36) into Eq. (2.23) we get to

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{2i\mathcal{J}_4(E)}\left[-\frac{\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E) + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E)\right]\sigma_1(s;E)\,,$$
$$\Re(E)>0, \Im(E)>0\,,\ r>s\,. \tag{2.39}$$

By substituting Eq. (2.37) into Eq. (2.26) we get to

$$G(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{2i\mathcal{J}_3(E)}\left[\frac{\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E) - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\right]\sigma_1(s;E)\,,$$
$$\Re(E)>0, \Im(E)<0\,,\ r>s\,, \tag{2.40}$$

Since

$$\overline{\sigma_1(s;\overline{E})} = \sigma_1(s;E)\,, \tag{2.41}$$

Eq. (2.39) leads to

$$G(r,s;E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{2i\mathcal{J}_4(E)}\left[-\frac{\mathcal{C}_4(E)}{W(E)}\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})} + \frac{\mathcal{J}_4(E)}{W(E)}\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right]$$
$$\Re(E)>0, \Im(E)>0\,,\ r>s\,, \tag{2.42}$$

and Eq. (2.40) leads to

$$G(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{2i\mathcal{J}_3(E)}\,\left[\frac{\mathcal{C}_3(E)}{W(E)}\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})} - \frac{\mathcal{J}_3(E)}{W(E)}\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right]$$
$$\Re(E)>0, \Im(E)<0\,,\ r>s\,, \qquad (2.43)$$

The expression of the resolvent in terms of the basis $\sigma_1, \sigma_2$ can be written as (see Theorem 4 in Appendix C)

$$G(r,s;E) = \sum_{i,j=1}^{2} \theta_{ij}^{+}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})}\,, \quad r>s\,. \qquad (2.44)$$

By comparing (2.44) to (2.42) we get to

$$\theta_{ij}^{+}(E) = \begin{pmatrix} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{2i}\frac{-\mathcal{C}_4(E)}{\mathcal{J}_4(E)W(E)} & 0 \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{2i}\frac{1}{W(E)} & 0 \end{pmatrix}\,, \quad \Re(E)>0\,,\ \Im(E)>0\,, \qquad (2.45)$$

By comparing (2.44) to (2.43) we get to

$$\theta_{ij}^{+}(E) = \begin{pmatrix} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{2i}\frac{\mathcal{C}_3(E)}{\mathcal{J}_3(E)W(E)} & 0 \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\frac{1}{2i}\frac{1}{W(E)} & 0 \end{pmatrix}\,, \quad \Re(E)>0\,,\ \Im(E)<0\,, \qquad (2.46)$$

From Eqs. (2.45) and (2.46) we can see that the measures $\rho_{12}$, $\rho_{21}$ and $\rho_{22}$ in Theorem 4 of Appendix C are zero and that the measure $\rho_{11}$ is given by

$$\begin{aligned}\rho_{11}((E_1,E_2)) &= \lim_{\delta\to 0}\lim_{\epsilon\to 0+}\frac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}\left[\theta_{11}^{+}(E-i\epsilon)-\theta_{11}^{+}(E+i\epsilon)\right]dE \\ &= \int_{E_1}^{E_2}\frac{1}{4\pi}\,\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{\mathcal{J}_3(E)\mathcal{J}_4(E)}\,dE\,,\end{aligned} \qquad (2.47)$$

which leads to

$$\rho(E)\equiv\rho_{11}(E) = \frac{1}{4\pi}\,\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,\frac{1}{|\mathcal{J}_4(E)|^2}\,, \quad E\in(0,\infty)\,. \qquad (2.48)$$

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, $\mathrm{Sp}(H) = [0,\infty)$. Thus the resolvent set of $H$ is $\mathrm{Re}(H) = \mathbb{C} - [0,\infty)$.

### *2.4.2.* **Diagonalization and Eigenfunction Expansion**

We are now in a position to diagonalize the Hamiltonian. By Theorem 2 of Appendix C, there is a unitary map $\widetilde{U}$ defined by

$$
\begin{aligned}
\widetilde{U} : L^2([0,\infty), dr) &\longmapsto L^2((0,\infty), \rho(E)dE) \\
f(r) &\longmapsto \widetilde{f}(E) = (\widetilde{U} f)(E) = \int_0^\infty dr f(r)\overline{\chi(r;E)}
\end{aligned}
\tag{2.49}
$$

that brings $\mathcal{D}(H)$ onto the space

$$
\mathcal{D}(\widetilde{E}) = \{\widetilde{f}(E) \in L^2((0,\infty), \rho(E)dE) \mid \int_0^\infty dE\, E^2 |\widetilde{f}(E)|^2 \rho(E) < \infty\} . \tag{2.50}
$$

Eqs. (2.49) and (2.50) provide a $\rho$-diagonalization of $H$. If we seek a $\delta$-diagonalization, i.e., if we seek eigenfunctions that are $\delta$-normalized, then the measure $\rho(E)$ must be absorbed by the eigenfunctions and by the wave functions.[1] This is why we define

$$
\sigma(r;E) := \sqrt{\rho(E)}\, \chi(r;E) , \tag{2.51}
$$

which is the eigensolution of the differential operator $h$ that is $\delta$-normalized, and

$$
\widehat{f}(E) := \sqrt{\rho(E)} \widetilde{f}(E) , \quad \widetilde{f}(E) \in L^2((0,\infty), \rho(E)dE) , \tag{2.52}
$$

and construct the unitary operator

$$
\begin{aligned}
\widehat{U} : L^2((0,\infty)), \rho(E)dE) &\longmapsto L^2((0,\infty), dE) \\
\widetilde{f} &\longmapsto \widehat{f}(E) = \widehat{U} \widetilde{f}(E) := \sqrt{\rho(E)} \widetilde{f}(E) .
\end{aligned}
\tag{2.53}
$$

The operator that $\delta$-diagonalizes our Hamiltonian is $U := \widehat{U}\widetilde{U}$,

$$
\begin{aligned}
U : L^2([0,\infty)), dr) &\longmapsto L^2((0,\infty), dE) \\
f &\longmapsto Uf := \widehat{f} .
\end{aligned}
\tag{2.54}
$$

The action of $U$ can be written as an integral operator,

$$
\widehat{f}(E) = (Uf)(E) = \int_0^\infty dr f(r)\overline{\sigma(r;E)} , \quad f(r) \in L^2([0,\infty), dr) . \tag{2.55}
$$

The image of $\mathcal{D}(H)$ under the action of $U$ is

$$
\mathcal{D}(\widehat{E}) := U\mathcal{D}(H) = \{\widehat{f}(E) \in L^2((0,\infty), dE) \mid \int_0^\infty E^2 |\widehat{f}(E)|^2 dE < \infty\} . \tag{2.56}
$$

Therefore, we have constructed a unitary operator

$$
\begin{aligned}
U : \mathcal{D}(H) \subset L^2([0,\infty), dr) &\longmapsto \mathcal{D}(\widehat{E}) \subset L^2((0,\infty), dE) \\
f &\longmapsto \widehat{f} = Uf
\end{aligned}
\tag{2.57}
$$

that transforms from the position representation into the energy representation. The operator $U$ diagonalizes our Hamiltonian in the sense that $\widehat{E} \equiv UHU^{-1}$ is the multiplication operator,

[1]The meaning of the $\delta$-normalization of the eigenfunctions will be explained in Section 2.9.

$$\widehat{E} : \mathcal{D}(\widehat{E}) \subset L^2((0,\infty), dE) \longmapsto L^2((0,\infty), dE)$$
$$\widehat{f} \longmapsto (\widehat{E}\widehat{f})(E) := E\widehat{f}(E) \, . \tag{2.58}$$

The inverse operator of $U$ is given by (see Theorem 3 of Appendix C)

$$f(r) = (U^{-1}\widehat{f})(r) = \int_0^\infty dE \, \widehat{f}(E)\sigma(r,E) \, , \quad \widehat{f}(E) \in L^2((0,\infty), dE) \, . \tag{2.59}$$

The operator $U^{-1}$ transforms from the energy representation into the position representation.

The expressions (2.55) and (2.59) provide the eigenfunction expansion of any square integrable function in terms of the eigensolutions $\sigma(r;E)$ of $h$.

The unitary operator $U$ can be looked at as a sort of generalized Fourier transform: the Fourier transform connects the position and the momentum representations. $U$ connects the position and the energy representations. The role played by the plane waves $e^{-ipx}$ (which are generalized eigenfunctions of the operator $-id/dx$) is here played by the $\sigma(r;E)$ (which are generalized eigenfunctions of the differential operator $h$). Therefore $\sigma(r;E) \equiv \langle r|E\rangle$, which are the $\delta$-normalized eigensolutions of the Schrödinger equation, can be viewed as "transition elements" between the $r$- and the $E$-representations.

The label $f$ of the functions in the position representation is different to the label $\widehat{f}$ of the functions in the energy representation, because they have different functional dependences. Similar considerations apply to the Hamiltonian, the domain, the resolvent, etc. This is not the standard practice in the physics literature, where different representations are usually identified and labeled by the same symbol (see, for instance, [22–24,18]).

### 2.5. The Need of the Rigged Hilbert Space

The Sturm-Liouville theory only provides a domain $\mathcal{D}(H)$ on which the Hamiltonian $H$ is self-adjoint and a unitary operator $U$ that diagonalizes $H$. This unitary operator induces a direct integral decomposition of the Hilbert space (see [4,5]),

$$\mathcal{H} \longmapsto U\mathcal{H} \equiv \widehat{\mathcal{H}} = \oplus \int_{\mathrm{Sp}(H)} \mathcal{H}(E) dE$$
$$f \longmapsto Uf \equiv \{\widehat{f}(E)\}, \quad \widehat{f}(E) \in \mathcal{H}(E) \, , \tag{2.60}$$

where $\mathcal{H}$ is realized by $L^2([0,\infty), dr)$, and $\widehat{\mathcal{H}}$ is realized by $L^2([0,\infty), dE)$. The Hilbert space $\mathcal{H}(E)$ associated to each energy eigenvalue of $\mathrm{Sp}(H)$ is realized by the Hilbert space of complex numbers $\mathbb{C}$. On $\widehat{\mathcal{H}}$, the operator $H$ acts as the multiplication operator,

$$Hf \longmapsto UHf \equiv \{E\widehat{f}(E)\} \, , \quad f \in \mathcal{D}(H) \, . \tag{2.61}$$

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

$$\left(\widehat{f}, \widehat{g}\right)_{\widehat{\mathcal{H}}} = \int_{\mathrm{Sp}(H)} \left(\widehat{f}(E), \widehat{g}(E)\right)_E dE \, , \tag{2.62}$$

where the scalar product $(\,\cdot\,,\,\cdot\,)_E$ on $\mathcal{H}(E)$ is the usual scalar product on $\mathbb{C}$,

$$\left(\widehat{f}(E), \widehat{g}(E)\right)_E = \overline{\widehat{f}(E)}\, \widehat{g}(E)\,. \tag{2.63}$$

As we shall explain below, the direct integral decomposition does not accommodate some of the basic requirements needed in Quantum Mechanics. These requirements can be accommodated by the RHS.

One of the most important principles of Quantum Mechanics is that the quantity $(\varphi, H\varphi)$ should fit the experimental expectation value of the observable $H$ in the state $\varphi$. However, $(\varphi, H\varphi)$ is not defined for every element in $\mathcal{H}$, but only for those square normalizable wave functions that are also in $\mathcal{D}(H)$. Therefore, not every square normalizable function can represent a "physical wave function", but only those that are (at least) in $\mathcal{D}(H)$. Another fundamental assumption of quantum physics is that the quantity

$$\mathrm{disp}_\varphi H = (\varphi, H^2\varphi) - (\varphi, H\varphi)^2 \tag{2.64}$$

represents the dispersion of the observable $H$ in the state $\varphi$, and that

$$\Delta_\varphi H \equiv \sqrt{\mathrm{disp}_\varphi H} \tag{2.65}$$

represents the uncertainty of the observable $H$ in the state $\varphi$. The quantities (2.64) and (2.65) are not defined for every element of the Hilbert space either. Therefore, we would like to find a subdomain $\mathbf{\Phi}$ included in $\mathcal{D}(H)$ on which the expectation values

$$(\varphi, H^n\varphi)\,, \quad n = 0, 1, 2, \ldots\,, \quad \varphi \in \mathbf{\Phi} \tag{2.66}$$

are well-defined.

Another important requirement of Quantum Mechanics is that algebraic operations such as the sum and multiplication of two operators are well-defined. In the HS formalism, these algebraic operations are not always well-defined because the domains on which these operators are self-adjoint do not remain stable under their actions in general. In fact, much of the trouble of the HS formalism comes from domain questions. In our case, the domain $\mathcal{D}(H)$ in (2.12) does not remain stable under $H$. We therefore would like to find a subdomain $\mathbf{\Phi}$ included in $\mathcal{D}(H)$ that remains stable under the action of $H$ and all of its powers,

$$H^n : \mathbf{\Phi} \longmapsto \mathbf{\Phi}\,, \quad n = 0, 1, 2, \ldots \tag{2.67}$$

One can see that if Eq. (2.67) holds, then the expectation values (2.66) are well-defined for each $\varphi$ in $\mathbf{\Phi}$, i.e., if the domain $\mathbf{\Phi}$ remains stable under the action of $H$, then the expectation values of $H$ in any state $\varphi \in \mathbf{\Phi}$ are well-defined.

In Quantum Mechanics, it is always assumed that for each $E \in \mathrm{Sp}(H)$ there is a Dirac ket $|E\rangle$ such that

$$H^\times|E\rangle = E|E\rangle \tag{2.68}$$

and such that the Dirac basis vector expansion (1.3) holds. Equation (2.68) has no solution in the Hilbert space when $E$ belongs to the continuous part of the spectrum of the Hamiltonian. In fact, Eq. (2.68) has to be related to the equation

$$\langle\vec{x}|H^\times|E\rangle = E\langle\vec{x}|E\rangle\,, \tag{2.69}$$

which in the radial representation reads

$$h\sigma(r;E) = E\sigma(r;E)\,, \tag{2.70}$$

where $h$ is the differential operator (2.5) and $\sigma(r;E)$ is the delta-normalized eigenfunction (2.51). Since $\sigma(r;E) \equiv \langle r|E\rangle$ lies outside $L^2([0,\infty), dr)$, i.e.,

$$\int_0^\infty dr\, |\sigma(r;E)|^2 = \infty\,, \tag{2.71}$$

the corresponding eigenket $|E\rangle$, which is defined by

$$\begin{aligned} |E\rangle : \mathbf{\Phi} &\longmapsto \mathbb{C} \\ \varphi &\longmapsto \langle\varphi|E\rangle := \int_0^\infty \overline{\varphi(r)}\sigma(r;E)dr\,, \end{aligned} \tag{2.72}$$

should also lie outside the Hilbert space. We shall show that $|E\rangle$ is an element of $\mathbf{\Phi}^\times$.

In summary, what our mathematical framework should provide us with is:

1. a dense invariant domain $\mathbf{\Phi}$ on which all the powers of $H$ and all the expectation values (2.66) are well-defined,
2. smooth enough wave functions so that Eq. (2.68) holds in the sense
$$\langle\varphi|H^\times|E\rangle = E\langle\varphi|E\rangle\,, \tag{2.73}$$
3. any wave function can be expanded by a Dirac basis vector expansion.

In the direct integral decomposition formalism, there is not enough room for either of these three requirements. This is why we introduce the RHS.

### 2.6. Construction of the Rigged Hilbert Space

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 $\mathcal{D}$ of the operator $H$,

$$\mathcal{D} := \bigcap_{n=0}^{\infty} \mathcal{D}(H^n)\,. \tag{2.74}$$

The space $\mathcal{D}$ is the largest subspace of $\mathcal{D}(H)$ that remains stable under the action of the Hamiltonian $H$ and all of its powers. It is easy to check that

$$\begin{aligned} \mathcal{D} = \{\varphi \in L^2([0,\infty), dr) \mid h^n\varphi(r) \in L^2([0,\infty), dr),\ h^n\varphi(0) = 0, \varphi^{(n)}(a) = \varphi^{(n)}(b) = 0, \\ n = 0,1,2,\ldots;\ \varphi(r) \in C^\infty([0,\infty))\}\,. \end{aligned} \tag{2.75}$$

The conditions $\varphi^{(n)}(a) = \varphi^{(n)}(b) = 0$ in (2.75) come from taking the discontinuities of the potential $V(r)$ at $r=a$ and at $r=b$ into consideration (cf. [9]).

The second step is to find a subspace $\mathbf{\Phi}$ on which the eigenkets $|E\rangle$ of $H$ are well-defined as antilinear functionals. For each $E \in \mathrm{Sp}(H)$, we associate a ket $|E\rangle$ to the generalized eigenfunction $\sigma(r;E)$ through

$$
\begin{aligned}
|E\rangle : \mathbf{\Phi} &\longmapsto \mathbb{C} \\
\varphi &\longmapsto \langle\varphi|E\rangle := \int_0^\infty \overline{\varphi(r)}\sigma(r;E)dr = \overline{(U\varphi)(E)}\,.
\end{aligned}
\tag{2.76}
$$

As actual computations show, the ket $|E\rangle$ in (2.76) is a generalized eigenfunctional of $H$ if $\mathbf{\Phi}$ is included in the maximal invariant subspace of $H$,

$$
\mathbf{\Phi} \subset \mathcal{D}\,. \tag{2.77}
$$

Due to the non-square integrability of the eigenfunction $\sigma(r;E)$, we need to impose further restrictions on the elements of $\mathcal{D}$ in order to make the eigenfunctional $|E\rangle$ in Eq. (2.76) continuous,

$$
\int_0^\infty dr\ |(r+1)^n(h+1)^m\varphi(r)|^2 < \infty, \quad n,m = 0,1,2,\ldots \tag{2.78}
$$

The imposition of conditions (2.78) upon the space $\mathcal{D}$ leads to the space of wave functions of the square barrier potential,

$$
\mathbf{\Phi} = \{\varphi \in \mathcal{D} \,|\, \int_0^\infty dr\ |(r+1)^n(h+1)^m\varphi(r)|^2 < \infty, \quad n,m = 0,1,2,\ldots\}\,. \tag{2.79}
$$

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

$$
\|\varphi\|_{n,m} := \sqrt{\int_0^\infty dr\ |(r+1)^n(h+1)^m\varphi(r)|^2}\,, \quad n,m = 0,1,2,\ldots \tag{2.80}
$$

The quantities (2.80) fulfill the conditions to be a norm (cf. Proposition 1 of Appendix D) and can be used to define a countably normed topology $\tau_{\mathbf{\Phi}}$ on $\mathbf{\Phi}$ (see [5]),

$$
\varphi_\alpha \xrightarrow[\alpha\to\infty]{\tau_{\mathbf{\Phi}}} \varphi \quad \text{iff} \quad \|\varphi_\alpha - \varphi\|_{n,m} \xrightarrow[\alpha\to\infty]{} 0\,, \quad n,m = 0,1,2,\ldots \tag{2.81}
$$

One can see that the space $\mathbf{\Phi}$ is stable under the action of $H$ and that $H$ is $\tau_{\mathbf{\Phi}}$-continuous (cf. Proposition 2 of Appendix D).

Once we have constructed the space $\mathbf{\Phi}$, we can construct its topological dual $\mathbf{\Phi}^\times$ as the space of $\tau_{\mathbf{\Phi}}$-continuous antilinear functionals on $\mathbf{\Phi}$ (see [5]) and therewith the RHS of the square barrier potential (for $l=0$)

$$
\mathbf{\Phi} \subset L^2([0,\infty),dr) \subset \mathbf{\Phi}^\times\,. \tag{2.82}
$$

The ket $|E\rangle$ in Eq. (2.76) is a well-defined antilinear functional on $\mathbf{\Phi}$, i.e., $|E\rangle$ belongs to $\mathbf{\Phi}^\times$ (cf. Proposition 3 of Appendix D). The ket $|E\rangle$ is a generalized eigenvector of the Hamiltonian $H$ (cf. Proposition 3 of Appendix D),

$$
H^\times|E\rangle = E|E\rangle\,, \tag{2.83}
$$

i.e.,

$$\langle\varphi|H^{\times}|E\rangle = \langle H\varphi|E\rangle = E\langle\varphi|E\rangle\,, \quad \forall\varphi\in\mathbf{\Phi}\,. \tag{2.84}$$

On the space $\mathbf{\Phi}$, all the expectation values of the Hamiltonian and all the algebraic operations involving $H$ are well-defined, and the generalized eigenvalue equation (2.84) holds. As we shall see in the next section, the functions $\varphi$ of $\mathbf{\Phi}$ can be expanded by a Dirac basis vector expansion.

### 2.7. Dirac Basis Vector Expansion

We are now in a position to derive the Dirac basis vector expansion. This derivation consists of the restriction of the Weyl-Kodaira expansions (2.55) and (2.59) to the space $\mathbf{\Phi}$. If we denote $\langle r|\varphi\rangle\equiv\varphi(r)$ and $\langle E|r\rangle\equiv\overline{\sigma(r;E)}$, and if we define the action of the left ket $\langle E|$ on $\varphi\in\mathbf{\Phi}$ as $\langle E|\varphi\rangle:=\widehat{\varphi}(E)$, then Eq. (2.55) becomes

$$\langle E|\varphi\rangle = \int_0^{\infty} dr\,\langle E|r\rangle\langle r|\varphi\rangle\,, \quad \varphi\in\mathbf{\Phi}\,. \tag{2.85}$$

If we denote $\langle r|E\rangle\equiv\sigma(r;E)$, then Eq. (2.59) becomes

$$\langle r|\varphi\rangle = \int_0^{\infty} dE\,\langle r|E\rangle\langle E|\varphi\rangle\,, \quad \varphi\in\mathbf{\Phi}\,. \tag{2.86}$$

This equation is the Dirac basis vector expansion of the square barrier potential. In fact, when we formally write (1.3) in the position representation, we get to (2.86).

In Eq. (2.86), the wave function $\langle r|\varphi\rangle$ is spanned in a "Fourier-type" expansion by the eigenfunctions $\langle r|E\rangle$. In this expansion, each eigenfunction $\langle r|E\rangle$ is weighted by $\langle E|\varphi\rangle = \widehat{\varphi}(E)$, which is the value of the wave function in the energy representation at the point $E$. Thus any function $\varphi(r)=\langle r|\varphi\rangle$ of $\mathbf{\Phi}$ can be written as a linear superposition of the monoenergetic eigenfunctions $\sigma(r;E)=\langle r|E\rangle$.

Although the Weyl-Kodaira expansions (2.55) and (2.59) are valid for every element of the Hilbert space, the Dirac basis vector expansions (2.85) and (2.86) are only valid for functions $\varphi\in\mathbf{\Phi}$ because only those functions fulfill both

$$\overline{\widehat{\varphi}(E)} = \langle\varphi|E\rangle \tag{2.87}$$

and

$$\langle\varphi|H^{\times}|E\rangle = \langle H\varphi|E\rangle = E\langle\varphi|E\rangle\,. \tag{2.88}$$

Another way to rephrase the Dirac basis vector expansion is the Nuclear Spectral (Gelfand-Maurin) theorem. Instead of using the general statement of [5], we prove this theorem using the Sturm-Liouville theory (see Proposition 4 of Appendix E). The Nuclear Spectral Theorem allows us to write the scalar product of any two functions $\varphi,\psi$ of $\mathbf{\Phi}$ in terms of the action of the kets $|E\rangle$ on $\varphi,\psi$:

$$(\varphi,\psi) = \int_0^{\infty} dE\,\langle\varphi|E\rangle\langle E|\psi\rangle\,, \quad \forall\varphi,\psi\in\mathbf{\Phi}\,. \tag{2.89}$$

It also allows us to write the matrix elements of the Hamiltonian and all of its powers between two elements $\varphi, \psi$ of $\mathbf{\Phi}$ in terms of the action of the kets $|E\rangle$ on $\varphi, \psi$:

$$(\varphi, H^n \psi) = \int_0^\infty dE\, E^n \langle \varphi|E\rangle\langle E|\psi\rangle \,, \quad \forall \varphi, \psi \in \mathbf{\Phi} \,, n = 1, 2, \ldots \tag{2.90}$$

### 2.8. Energy Representation of the RHS

In this section, we construct the energy representation of the RHS. Since the unitary operator $U$ transforms from the position representation into the energy representation, the action of $U$ on the RHS provides the energy representation of the RHS.

We have already shown that in the energy representation the Hamiltonian $H$ acts as the multiplication operator $\widehat{E}$. The energy representation of the space $\mathbf{\Phi}$ is defined as

$$\widehat{\mathbf{\Phi}} := U\mathbf{\Phi} \,. \tag{2.91}$$

It is very easy to see that $\widehat{\mathbf{\Phi}}$ is a linear subspace of $L^2([0,\infty), dE)$. In order to endow $\widehat{\mathbf{\Phi}}$ with a topology $\tau_{\widehat{\mathbf{\Phi}}}$, we carry the topology on $\mathbf{\Phi}$ into $\widehat{\mathbf{\Phi}}$,

$$\tau_{\widehat{\mathbf{\Phi}}} := U\tau_{\mathbf{\Phi}} \,. \tag{2.92}$$

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

$$U^\times \mathbf{\Phi}^\times = (U\mathbf{\Phi})^\times = \widehat{\mathbf{\Phi}}^\times \,. \tag{2.93}$$

If we denote $|\widehat{E}\rangle \equiv U^\times |E\rangle$, then we can prove that $|\widehat{E}\rangle$ is the antilinear Schwartz delta functional, i.e., $|\widehat{E}\rangle$ is the antilinear functional that associates to each function $\widehat{\varphi}$ the complex conjugate of its value at the point $E$ (see Proposition 5 of Appendix F),

$$\begin{aligned} |\widehat{E}\rangle : \widehat{\mathbf{\Phi}} &\longmapsto \mathbb{C} \\ \widehat{\varphi} &\longmapsto \langle \widehat{\varphi}|\widehat{E}\rangle := \overline{\widehat{\varphi}(E)} \,. \end{aligned} \tag{2.94}$$

Therefore, the Schwartz delta functional appears in the (spectral) energy representation of the RHS associated to the Hamiltonian. If we write the action of the Schwartz delta functional as an integral operator, then the Dirac $\delta$-function appears as the kernel of that integral operator.

It is very helpful to show the different realizations of the RHS through the following diagram:

$$\begin{array}{cccccccc} H;\ \varphi(r) & \mathbf{\Phi} & \subset & L^2([0,\infty), dr) & \subset & \mathbf{\Phi}^\times & |E\rangle & \text{position repr.} \\ & \downarrow U & & \downarrow U & & \downarrow U^\times & & \\ \widehat{E};\ \widehat{\varphi}(E) & \widehat{\mathbf{\Phi}} & \subset & L^2([0,\infty), dE) & \subset & \widehat{\mathbf{\Phi}}^\times & |\widehat{E}\rangle & \text{energy repr.} \end{array} \tag{2.95}$$

On the top line of the diagram (2.95), 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.

### 2.9. Meaning of the $\delta$-Normalization of the Eigenfunctions

In this section, we show that the $\delta$-normalization of the eigenfunctions is related to the measure $d\mu(E)$ that is used to compute the scalar product of the wave functions in the energy representation,

$$(\varphi, \psi) = \int_0^\infty \overline{\varphi(E)}\psi(E)d\mu(E)\,. \tag{2.96}$$

We will see that if the measure in (2.96) is the Lebesgue measure $dE$, then the eigenfunctions are $\delta$-normalized, and that if the measure is $\rho(E)dE$, then the eigenfunctions are $\rho$-normalized.

For the sake of simplicity, in this section we label the wave functions in the position and in the energy representation with the same symbol. With this notation, Eq. (2.86) reads

$$\varphi(r) = \int_0^\infty dE\, \varphi(E)\sigma(r;E)\,, \tag{2.97a}$$

$$\psi(r) = \int_0^\infty dE\, \psi(E)\sigma(r;E)\,. \tag{2.97b}$$

Since $\varphi(r), \psi(r) \in L^2([0,\infty), dr)$, their scalar product is well-defined,

$$(\varphi, \psi) = \int_0^\infty dr\, \overline{\varphi(r)}\psi(r)\,. \tag{2.98}$$

Plugging (2.97) into (2.98), we obtain

$$(\varphi, \psi) = \int_0^\infty dE \int_0^\infty dE'\, \overline{\varphi(E)}\psi(E') \int_0^\infty dr\, \overline{\sigma(r;E)}\sigma(r;E')\,. \tag{2.99}$$

If we use the Lebesgue measure $dE$, then the scalar product (2.96) can be written as

$$(\varphi, \psi) = \int_0^\infty dE\, \overline{\varphi(E)}\psi(E)\,. \tag{2.100}$$

Comparison of (2.99) and (2.100) leads to

$$\int_0^\infty dr\, \overline{\sigma(r;E)}\sigma(r;E') = \delta(E-E')\,, \tag{2.101}$$

i.e., the eigenfunctions $\sigma(r;E)$ are $\delta$-normalized.

We now consider the case in which the eigenfunctions are $\rho$-normalized. If we use the measure $d\mu(E) = \rho(E)dE$, then the scalar product of $\varphi$ and $\psi$ is given by

$$(\varphi, \psi) = \int_0^\infty \overline{\varphi_\rho(E)}\psi_\rho(E)\rho(E)\, dE\,, \tag{2.102}$$

where $\varphi_\rho(E) := \varphi(E)/\sqrt{\rho(E)}$ and $\psi_\rho(E) := \psi(E)/\sqrt{\rho(E)}$. If we define $\sigma_\rho(r;E) := \sigma(r;E)/\sqrt{\rho(E)}$, then Eq. (2.97) reads

$$\varphi(r) = \int_0^\infty \varphi_\rho(E)\sigma_\rho(r;E)\rho(E)\,dE\,, \tag{2.103a}$$

$$\psi(r) = \int_0^\infty \psi_\rho(E)\sigma_\rho(r;E)\rho(E)\,dE\,. \tag{2.103b}$$

Plugging Eq. (2.103) into (2.98), we obtain

$$(\varphi,\psi) = \int_0^\infty dE \int_0^\infty dE' \, \overline{\varphi_\rho(E)}\psi_\rho(E')\rho(E)\rho(E') \int_0^\infty dr\, \overline{\sigma_\rho(r;E)}\sigma_\rho(r;E')\,. \tag{2.104}$$

Comparison of (2.104) and (2.102) leads to

$$\int_0^\infty dr\, \overline{\sigma_\rho(r;E)}\sigma_\rho(r;E') = \frac{1}{\rho(E)}\delta(E-E')\,, \tag{2.105}$$

i.e., the eigenfunctions $\sigma_\rho(r;E)$ are $\rho$-normalized.

## 3. CONCLUSION

In this paper, we have constructed the Rigged Hilbert Space

$$\mathbf{\Phi} \subset L^2([0,\infty), dr) \subset \mathbf{\Phi}^\times \tag{3.1}$$

of the square barrier Hamiltonian and its energy representation

$$\widehat{\mathbf{\Phi}} \subset L^2([0,\infty), dE) \subset \widehat{\mathbf{\Phi}}^\times\,. \tag{3.2}$$

The spectrum of the Hamiltonian $H$ is the positive real semiaxis. For each value $E$ of the spectrum of $H$, we have constructed a Dirac ket $|E\rangle$ that is a generalized eigenfunctional of $H$ whose corresponding generalized eigenvalue is $E$. In the energy representation, $|E\rangle$ acts as the antilinear Schwartz delta functional. On the space $\mathbf{\Phi}$, all algebraic operations involving the Hamiltonian $H$ are well-defined. In particular, the expectation values of the Hamiltonian in any element of $\mathbf{\Phi}$ are well-defined. Any element of $\mathbf{\Phi}$ can be expanded in terms of the eigenkets $|E\rangle$ by a Dirac basis vector expansion. The elements of $\mathbf{\Phi}$ are represented by well-behaved functions, in contrast to the elements of the Hilbert space, which are represented by sets of equivalent functions that can vary arbitrarily on any set of zero Lebesgue measure. Therefore, it seems natural to conclude that a physically acceptable wave function is not any element of the Hilbert space but rather an element of the subspace $\mathbf{\Phi}$.

The monoenergetic eigensolutions $\sigma(r;E)$ of the time-independent Schrödinger equation are not square integrable, and therefore they cannot represent an acceptable wave function. Those eigensolutions has been used to define the eigenkets $|E\rangle$ that expand the physical wave functions $\varphi \in \mathbf{\Phi}$ in a Dirac basis vector expansion. The eigenkets $|E\rangle$ belong to the space $\mathbf{\Phi}^\times$. The eigensolutions $\sigma(r;E) = \langle r|E\rangle$ have been also used to construct the unitary operator $U$ that transforms from the position representation into the energy representation.

In our quest for the RHS of the square barrier potential, we have found a systematic method to construct the RHS of a large class of spherically symmetric potentials:

1. Expression of the formal differential operator.

2. Hilbert space $\mathcal{H}$ of square integrable functions on which the formal differential operator acts.

3. A domain $\mathcal{D}(H)$ of the Hilbert space on which the formal differential operator is self-adjoint.

4. Green functions (resolvent) of that self-adjoint operator.

5. Diagonalization of the self-adjoint operator, eigenfunction expansion of the elements of $\mathcal{H}$ in terms of the eigensolutions of the formal differential operator, and direct integral decomposition of $\mathcal{H}$ induced by the self-adjoint operator.

6. Subspace $\mathbf{\Phi}$ of $\mathcal{D}(H)$ on which all the expectation values of $H$ are well-defined and on which the Dirac kets act as antilinear functionals.

7. Rigged Hilbert space $\mathbf{\Phi} \subset \mathcal{H} \subset \mathbf{\Phi}^{\times}$.

## ACKNOWLEDGMENTS

One of the authors (R. de la Madrid) wishes to thank Prof. J.-P. Antoine and T. Kuna for introducing him to the Sturm-Liouville theory and Profs. R. De la Llave, A. Galindo, L. Caffarelli and J. Bona for illuminating discussions. Many thanks are due to N. Harshman and C. Koeninger for invaluable advise on English style.

Financial support from the U.E. TMR Contract number ERBFMRX-CT96-0087 "The Physics of Quantum Information", from the Welch Foundation, from La Junta de Castilla y León Project PC02 1999, from DGCYT PB98-0370, and from DGICYT PB98-0370 is gratefully acknowledged.

## APPENDIX A: SELF-ADJOINT EXTENSION

In this appendix, we list the possible self-adjoint extensions associated to the differential operator $h$. We first need some definitions (cf. [21]).

**Definition 1** By $AC^2([0,\infty))$ we denote 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 $f^{(2)}$ exists almost everywhere, and is integrable over any compact subinterval of $[0,\infty)$. At 0 $f'$ is continuous from the right.

The space $AC^2([0,\infty))$ is the largest space of functions on which the differential operator $h$ can be defined.

**Definition 2** We define the spaces

$$\mathcal{H}_h^2([0,\infty)) := \{f \in AC^2([0,\infty)) \mid f, hf \in L^2([0,\infty), dr)\} \tag{A1}$$
$$\mathcal{H}^2([0,\infty)) := \{f \in AC^2([0,\infty) \mid f, f^{(2)} \in L^2([0,\infty), dr)\} \tag{A2}$$
$$\mathcal{H}_0^2([0,\infty)) := \{f \in \mathcal{H}^2([0,\infty)) \mid f \text{ vanishes outside some compact subset of } (0,\infty)\}\,. \tag{A3}$$

Using these spaces, we can define the necessary operators to calculate the self-adjoint extensions associated to $h$.

**Definition 3** If $h$ is the formal differential operator (2.5), we define the operators $H_0$ and $H_1$ on $L^2([0,\infty), dr)$ by the formulas

$$\mathcal{D}(H_0) = \mathcal{H}_0^2([0,\infty)), \quad H_0 f := hf, \quad f \in \mathcal{D}(H_0)\,. \tag{A4}$$
$$\mathcal{D}(H_1) = \mathcal{H}_h^2([0,\infty)), \quad H_1 f := hf, \quad f \in \mathcal{D}(H_1)\,. \tag{A5}$$

The operators $H_0$ and $H_1$ are sometimes called the *minimal* and the *maximal* operators associated to the differential operator $h$, respectively. The domain $\mathcal{D}(H_1)$ is the largest domain of the Hilbert space $L^2([0,\infty), dr)$ on which the action of the differential operator $h$ can be defined and remains inside $L^2([0,\infty), dr)$. Further, $H_0^\dagger = H_1$.

The self-adjoint extensions of $H_0$ are given by the restrictions of the operator $H_1$ to domains determined by the conditions (see [21], page 1306)

$$f(0) + \alpha\, f'(0) = 0\,, \quad -\infty < \alpha \le \infty\,. \tag{A6}$$

These boundary conditions lead to the domains

$$\mathcal{D}_\alpha(H) = \{f \in \mathcal{D}(H_1) \mid f(0) + \alpha\, f'(0) = 0\}\,, \quad -\infty < \alpha \le \infty\,. \tag{A7}$$

On these domains, the formal differential operator $h$ is self-adjoint. The boundary condition that fits spherically symmetric potentials is $f(0) = 0$, i.e., $\alpha = 0$. This condition selects our domain (2.12),

$$\mathcal{D}(H) = \mathcal{D}_{\alpha=0}(H) = \{f \in \mathcal{D}(H_1) \mid f(0) = 0\}\,. \tag{A8}$$

## APPENDIX B: RESOLVENT AND GREEN FUNCTION

The following theorem provides the procedure to compute the Green function of the Hamiltonian $H$ (cf. Theorem XIII.3.16 of Ref. [21]):

**Theorem 1** Let $H$ be the self-adjoint operator (2.13) derived from the real formal differential operator (2.5) by the imposition of the boundary condition (2.10d). Let $\Im E \neq 0$. Then there is exactly one solution $\chi(r;E)$ of $(h-E)\sigma = 0$ square-integrable at 0 and satisfying the boundary condition (2.10d), 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

$$G(r,s;E) = \begin{cases} \frac{2m}{\hbar^2}\frac{\chi(r;E)\,\Theta(s;E)}{W(\chi,\Theta)} & r<s \\ \frac{2m}{\hbar^2}\frac{\chi(s;E)\,\Theta(r;E)}{W(\chi,\Theta)} & r>s\,, \end{cases} \tag{B1}$$

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

$$W(\chi,\Theta) = \chi\Theta' - \chi'\Theta\,. \tag{B2}$$

If we define

$$\widetilde{k} := \sqrt{-\frac{2m}{\hbar^2}\,E}\,, \tag{B3a}$$

$$\widetilde{Q} := \sqrt{-\frac{2m}{\hbar^2}\,(E-V_0)}\,, \tag{B3b}$$

then the functions $\widetilde{\mathcal{J}}(E)$ of Eq. (2.19) are given by

$$\widetilde{\mathcal{J}}_1(E) = \frac{1}{2}e^{-\widetilde{Q}a}\left[\left(1+\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{\widetilde{k}a} + \left(-1+\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{-\widetilde{k}a}\right], \tag{B4a}$$

$$\widetilde{\mathcal{J}}_2(E) = \frac{1}{2}e^{\widetilde{Q}a}\left[\left(1-\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{\widetilde{k}a} + \left(-1-\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{-\widetilde{k}a}\right], \tag{B4b}$$

$$\widetilde{\mathcal{J}}_3(E) = \frac{1}{2}e^{-\widetilde{k}b}\left[\left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}b}\widetilde{\mathcal{J}}_1(E) + \left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\widetilde{Q}b}\widetilde{\mathcal{J}}_2(E)\right], \tag{B4c}$$

$$\widetilde{\mathcal{J}}_4(E) = \frac{1}{2}e^{\widetilde{k}b}\left[\left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}b}\widetilde{\mathcal{J}}_1(E) + \left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\widetilde{Q}b}\widetilde{\mathcal{J}}_2(E)\right], \tag{B4d}$$

and the functions $\widetilde{\mathcal{A}}(E)$ of Eq. (2.22) by

$$\widetilde{\mathcal{A}}_3(E) = \frac{1}{2}e^{-\widetilde{Q}b}\left(1-\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{-\widetilde{k}b}, \tag{B5a}$$

$$\widetilde{\mathcal{A}}_4(E) = \frac{1}{2}e^{\widetilde{Q}b}\left(1+\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{-\widetilde{k}b}, \tag{B5b}$$

$$\widetilde{\mathcal{A}}_1(E) = \frac{1}{2}e^{-\widetilde{k}a}\left[\left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}a}\widetilde{\mathcal{A}}_3(E) + \left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\widetilde{Q}a}\widetilde{\mathcal{A}}_4(E)\right], \tag{B5c}$$

$$\widetilde{\mathcal{A}}_2(E) = \frac{1}{2}e^{\widetilde{k}a}\left[\left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}a}\widetilde{\mathcal{A}}_3(E) + \left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\sqrt{-\widetilde{Q}a}}\widetilde{\mathcal{A}}_4(E)\right]. \tag{B5d}$$

The expression for the Wronskian of $\widetilde{\chi}$ and $\widetilde{\Theta}_-$ is

$$W(\widetilde{\chi},\widetilde{\Theta}_-) = -2\widetilde{k}\widetilde{\mathcal{J}}_3(E)\,. \tag{B6}$$

If we define

$$k := \sqrt{\frac{2m}{\hbar^2}\,E}\,, \tag{B7a}$$

$$Q := \sqrt{\frac{2m}{\hbar^2}\,(E-V_0)}\,, \tag{B7b}$$

then the functions $\mathcal{J}(E)$ of Eq. (2.24) are given by

$$\mathcal{J}_1(E) = \frac{1}{2} e^{-iQa} \left( \sin(ka) + \frac{k}{iQ} \cos(ka) \right), \tag{B8a}$$

$$\mathcal{J}_2(E) = \frac{1}{2} e^{iQa} \left( \sin(ka) - \frac{k}{iQ} \cos(ka) \right), \tag{B8b}$$

$$\mathcal{J}_3(E) = \frac{1}{2} e^{-ikb} \left[ \left(1+\frac{Q}{k}\right) e^{iQb} \mathcal{J}_1(E) + \left(1-\frac{Q}{k}\right) e^{-iQb} \mathcal{J}_2(E) \right], \tag{B8c}$$

$$\mathcal{J}_4(E) = \frac{1}{2} e^{ikb} \left[ \left(1-\frac{Q}{k}\right) e^{iQb} \mathcal{J}_1(E) + \left(1+\frac{Q}{k}\right) e^{-iQb} \mathcal{J}_2(E) \right], \tag{B8d}$$

and the functions $\mathcal{A}^+(E)$ of Eq. (2.25) by

$$\mathcal{A}_3^+(E) = \frac{1}{2} e^{-iQb} \left(1+\frac{k}{Q}\right) e^{ikb}, \tag{B9a}$$

$$\mathcal{A}_4^+(E) = \frac{1}{2} e^{iQb} \left(1-\frac{k}{Q}\right) e^{ikb}, \tag{B9b}$$

$$\mathcal{A}_1^+(E) = \frac{1}{2} e^{-ika} \left[ \left(1+\frac{Q}{k}\right) e^{iQa} \mathcal{A}_3^+(E) + \left(1-\frac{Q}{k}\right) e^{-iQa} \mathcal{A}_4^+(E) \right], \tag{B9c}$$

$$\mathcal{A}_2^+(E) = \frac{1}{2} e^{ika} \left[ \left(1-\frac{Q}{k}\right) e^{iQa} \mathcal{A}_3^+(E) + \left(1+\frac{Q}{k}\right) e^{-iQa} \mathcal{A}_4^+(E) \right]. \tag{B9d}$$

The Wronskian of $\chi$ and $\Theta_+$ is

$$W(\chi,\Theta_+) = 2ik\mathcal{J}_4(E)\,. \tag{B10}$$

The functions $\mathcal{A}^-(E)$ of Eq. (2.27) are given by

$$\mathcal{A}_3^-(E) = \frac{1}{2} e^{-iQb} \left(1-\frac{k}{Q}\right) e^{-ikb}, \tag{B11a}$$

$$\mathcal{A}_4^-(E) = \frac{1}{2} e^{iQb} \left(1+\frac{k}{Q}\right) e^{-ikb}, \tag{B11b}$$

$$\mathcal{A}_1^-(E) = \frac{1}{2} e^{-ika} \left[ \left(1+\frac{Q}{k}\right) e^{iQa} \mathcal{A}_3^-(E) + \left(1-\frac{Q}{k}\right) e^{-iQa} \mathcal{A}_4^-(E) \right], \tag{B11c}$$

$$\mathcal{A}_2^-(E) = \frac{1}{2} e^{ika} \left[ \left(1-\frac{Q}{k}\right) e^{iQa} \mathcal{A}_3^-(E) + \left(1+\frac{Q}{k}\right) e^{-iQa} \mathcal{A}_4^-(E) \right]. \tag{B11d}$$

The Wronskian of $\chi$ and $\Theta_-$ is

$$W(\chi,\Theta_-) = -2ik\mathcal{J}_3(E)\,. \tag{B12}$$

## APPENDIX C: DIAGONALIZATION AND EIGENFUNCTION EXPANSION

The theorem that provides the operator $U$ that diagonalizes $H$ is (cf. Theorem XIII.5.13 of Ref. [21])

**Theorem 2** (Weyl-Kodaira) Let $h$ be the formally self-adjoint differential operator (2.5) defined on the interval $[0,\infty)$. Let $H$ be the self-adjoint operator (2.13). Let $\Lambda$ 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 $\Lambda$, $\{\sigma_1(r;E),\, \sigma_2(r;E)\}$ forms a basis for the space of solutions of $h\sigma = E\sigma$. Then there exists a positive $2\times 2$ matrix measure $\{\rho_{ij}\}$ defined on $\Lambda$, such that

1. the limit

$$(Uf)_i(E) = \lim_{c\to 0}\lim_{d\to\infty}\left[\int_c^d f(r)\overline{\sigma_i(r;E)}dr\right] \tag{C1}$$

   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 $E(\Lambda)L^2([0,\infty),dr)$ onto $L^2(\Lambda,\{\rho_{ij}\})$;

2. for each Borel function $G$ defined on the real line and vanishing outside $\Lambda$,

$$U\mathcal{D}(G(H)) = \{[f_i]\in L^2(\Lambda,\{\rho_{ij}\})\mid [Gf_i]\in L^2(\Lambda,\{\rho_{ij}\})\} \tag{C2}$$

   and

$$(UG(H)f)_i(E) = G(E)(Uf)_i(E), \quad i=1,2,\, E\in\Lambda,\, f\in\mathcal{D}(G(H))\,. \tag{C3}$$

The theorem that provides the inverse of the operator $U$ is (cf. Theorem XIII.5.14 of Ref. [21])

**Theorem 3** (Weyl-Kodaira) Let $H$, $\Lambda$, $\{\rho_{ij}\}$, etc., be as in Theorem 2. Let $E_0$ and $E_1$ be the end points of $\Lambda$. Then

1. the inverse of the isometric isomorphism $U$ of $E(\Lambda)L^2([0,\infty),dr)$ onto $L^2(\Lambda,\{\rho_{ij}\})$ is given by the formula

$$(U^{-1}F)(r) = \lim_{\mu_0\to E_0}\lim_{\mu_1\to E_1}\int_{\mu_0}^{\mu_1}\left(\sum_{i,j=1}^{2}F_i(E)\sigma_j(r;E)\rho_{ij}(dE)\right) \tag{C4}$$

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

2. if $G$ is a bounded Borel function vanishing outside a Borel set $e$ whose closure is compact and contained in $\Lambda$, then $G(H)$ has the representation

$$G(H)f(r) = \int_0^\infty f(s)K(H,r,s)ds\,, \tag{C5}$$

where

$$K(H,r,s) = \sum_{i,j=1}^{2} \int_e G(E)\overline{\sigma_i(s;E)}\sigma_j(r;E)\rho_{ij}(dE)\,. \tag{C6}$$

The spectral measures are provided by the following theorem (cf. Theorem XIII.5.18 of Ref. [21]):

**Theorem 4** (Titchmarsh-Kodaira) Let $\Lambda$ be an open interval of the real axis and $O$ be an open set in the complex plane containing $\Lambda$. 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

$$G(r,s;E) = \left\{ \begin{array}{ll} \sum_{i,j=1}^{2} \theta_{ij}^{-}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})}\,, & r<s\,, \\ \sum_{i,j=1}^{2} \theta_{ij}^{+}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})}\,, & r>s\,, \end{array} \right. \tag{C7}$$

for all $E$ in $\mathrm{Re}(H)\cap O$, and that $\{\rho_{ij}\}$ is a positive matrix measure on $\Lambda$ 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 $1\leq i,j\leq 2$,

$$\begin{array}{rcl} \rho_{ij}((E_1,E_2)) & = & \lim_{\delta\to 0}\lim_{\epsilon\to 0+}\frac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}[\theta_{ij}^{-}(E-i\epsilon)-\theta_{ij}^{-}(E+i\epsilon)]dE \\ & = & \lim_{\delta\to 0}\lim_{\epsilon\to 0+}\frac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}[\theta_{ij}^{+}(E-i\epsilon)-\theta_{ij}^{+}(E+i\epsilon)]dE\,. \end{array} \tag{C8}$$

The functions $\widetilde{\mathcal{B}}(E)$ of Eq. (2.28a) are given by

$$\widetilde{\mathcal{B}}_3(E) = \frac{1}{2}e^{-\widetilde{Q}b}\left(1+\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{\widetilde{k}b}, \tag{C9a}$$

$$\widetilde{\mathcal{B}}_4(E) = \frac{1}{2}e^{\widetilde{Q}b}\left(1-\frac{\widetilde{k}}{\widetilde{Q}}\right)e^{\widetilde{k}b}, \tag{C9b}$$

$$\widetilde{\mathcal{B}}_1(E) = \frac{1}{2}e^{-\widetilde{k}a}\left[\left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}a}\widetilde{\mathcal{B}}_3(E)+\left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\widetilde{Q}a}\widetilde{\mathcal{B}}_4(E)\right], \tag{C9c}$$

$$\widetilde{\mathcal{B}}_2(E) = \frac{1}{2}e^{\widetilde{k}a}\left[\left(1-\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{\widetilde{Q}a}\widetilde{\mathcal{B}}_3(E)+\left(1+\frac{\widetilde{Q}}{\widetilde{k}}\right)e^{-\widetilde{Q}a}\widetilde{\mathcal{B}}_4(E)\right]. \tag{C9d}$$

The functions $\mathcal{C}(E)$ of Eq. (2.35b) are given by

$$\mathcal{C}_1(E) = \frac{1}{2} e^{-iQa} \left( \cos(ka) - \frac{k}{iQ} \sin(ka) \right) , \tag{C10a}$$

$$\mathcal{C}_2(E) = \frac{1}{2} e^{iQa} \left( \cos(ka) + \frac{k}{iQ} \sin(ka) \right) , \tag{C10b}$$

$$\mathcal{C}_3(E) = \frac{1}{2} e^{-ikb} \left[ \left( 1 + \frac{Q}{k} \right) e^{iQb} \mathcal{C}_1(E) + \left( 1 - \frac{Q}{k} \right) e^{-iQb} \mathcal{C}_2(E) \right] , \tag{C10c}$$

$$\mathcal{C}_4(E) = \frac{1}{2} e^{ikb} \left[ \left( 1 - \frac{Q}{k} \right) e^{iQb} \mathcal{C}_1(E) + \left( 1 + \frac{Q}{k} \right) e^{-iQb} \mathcal{C}_2(E) \right] . \tag{C10d}$$

## APPENDIX D: CONSTRUCTION OF THE RHS

**Proposition 1** The quantities

$$\|\varphi\|_{n,m} := \sqrt{\int_0^\infty dr \ |(r+1)^n (h+1)^m \varphi(r)|^2}, \quad \varphi \in \mathbf{\Phi} \, , \, n,m = 0,1,2,\ldots , \tag{D1}$$

are norms.

*Proof* It is very easy to show that the quantities (D1) fulfill the conditions to be a norm,

$$\begin{aligned} &\|\varphi + \psi\|_{n,m} \leq \|\varphi\|_{n,m} + \|\psi\|_{n,m} \, , && \text{(D2a)} \\ &\|\alpha\varphi\|_{n,m} = |\alpha| \, \|\varphi\|_{n,m} \, , && \text{(D2b)} \\ &\|\varphi\|_{n,m} \geq 0 \, , && \text{(D2c)} \\ &\text{If } \|\varphi\|_{n,m} = 0, \text{ then } \varphi = 0 \, . && \text{(D2d)} \end{aligned}$$

The only condition that is somewhat difficult to prove is (D2d): if $\|\varphi\|_{n,m} = 0$, then

$$(1+r)^n (h+1)^m \varphi(r) = 0 \, , \tag{D3}$$

which yields

$$(h+1)^m \varphi(r) = 0 \, . \tag{D4}$$

If $m = 0$, then Eq. (D4) implies $\varphi(r) = 0$. If $m = 1$, then Eq. (D4) implies that $-1$ is an eigenvalue of $H$ whose corresponding eigenvector is $\varphi$. Since $-1$ is not an eigenvalue of $H$, $\varphi$ must be the zero vector. If $m > 1$, the proof is similar.

**Proposition 2** The space $\mathbf{\Phi}$ is stable under the action of $H$, and $H$ is $\tau_{\mathbf{\Phi}}$-continuous.

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

$$\begin{aligned} \|H\varphi\|_{n,m} &= \|(H+I)\varphi - \varphi\|_{n,m} \\ &\leq \|(H+I)\varphi\|_{n,m} + \|\varphi\|_{n,m} \\ &= \|\varphi\|_{n,m+1} + \|\varphi\|_{n,m} \, . \end{aligned} \tag{D5}$$

We now prove that $\mathbf{\Phi}$ is stable under the action of $H$. Let $\varphi \in \mathbf{\Phi}$. To say that $\varphi \in \mathbf{\Phi}$ is equivalent to say that $\varphi \in \mathcal{D}$ and that the norms $\|\varphi\|_{n,m}$ are finite for every $n, m = 0, 1, 2, \ldots$ Since $H\varphi$ is also in $\mathcal{D}$, and since the norms $\|H\varphi\|_{n,m}$ are also finite (see Eq. (D5)), the vector $H\varphi$ is also in $\mathbf{\Phi}$.

**Proposition 3** The function

$$
\begin{aligned}
|E\rangle : \mathbf{\Phi} &\longmapsto \mathbb{C} \\
\varphi &\longmapsto \langle \varphi | E \rangle := \int_0^\infty \overline{\varphi(r)} \sigma(r; E) dr = \overline{(U\varphi)(E)} \, .
\end{aligned}
\tag{D6}
$$

is an antilinear functional on $\mathbf{\Phi}$ that is a generalized eigenvector of (the restriction to $\mathbf{\Phi}$ of) $H$.

*Proof* From the definition (D6), it is pretty easy to see that $|E\rangle$ is an antilinear functional. In order to show that $|E\rangle$ is continuous, we define

$$
\mathcal{M}(E) := \sup_{r \in [0,\infty)} |\sigma(r; E)| \ . \tag{D7}
$$

Since

$$
\begin{aligned}
|\langle \varphi | E \rangle| &= |\overline{U\varphi(E)}| \\
&= \left| \int_0^\infty dr \, \overline{\varphi(r)} \sigma(r; E) \right| \\
&\leq \int_0^\infty dr \, |\overline{\varphi(r)}| |\sigma(r; E)| \\
&\leq \mathcal{M}(E) \int_0^\infty dr \, |\varphi(r)| \\
&= \mathcal{M}(E) \int_0^\infty dr \, \frac{1}{1+r} (1+r) |\varphi(r)| \\
&\leq \mathcal{M}(E) \left( \int_0^\infty dr \, \frac{1}{(1+r)^2} \right)^{1/2} \left( \int_0^\infty dr \, |(1+r)\varphi(r)|^2 \right)^{1/2} \\
&= \mathcal{M}(E) \left( \int_0^\infty dr \, \frac{1}{(1+r)^2} \right)^{1/2} \|\varphi\|_{1,0} \\
&= \mathcal{M}(E) \|\varphi\|_{1,0} \, ,
\end{aligned}
\tag{D8}
$$

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

In order to prove that $|E\rangle$ is a generalized eigenvector of $H$, we make use of the conditions (2.75) and (2.78) satisfied by the elements of $\mathbf{\Phi}$,

$$
\begin{aligned}
\langle \varphi | H^\times | E \rangle &= \langle H\varphi | E \rangle \\
&= \int_0^\infty dr \left( -\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V(r) \right) \overline{\varphi(r)} \sigma(r; E) \\
&= -\frac{\hbar^2}{2m} \left[ \frac{d\overline{\varphi(r)}}{dr} \sigma(r; E) \right]_0^\infty + \frac{\hbar^2}{2m} \left[ \overline{\varphi(r)} \frac{d\sigma(r; E)}{dr} \right]_0^\infty
\end{aligned}
$$

$$
\begin{aligned}
&+\int_0^\infty dr\,\overline{\varphi(r)}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}+V(r)\right)\sigma(r;E) \\
&= E\langle\varphi|E\rangle\,.
\end{aligned}
\tag{D9}
$$

Similarly, one can also prove that

$$
\langle\varphi|(H^\times)^n|E\rangle = E^n\langle\varphi|E\rangle\,.
\tag{D10}
$$

## APPENDIX E: DIRAC BASIS VECTOR EXPANSION

**Proposition 4** (Nuclear Spectral Theorem) Let

$$
\mathbf{\Phi} \subset L^2([0,\infty),dr) \subset \mathbf{\Phi}^\times
\tag{E1}
$$

be the RHS of the square 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 $E$ in the spectrum of $H$ there is a generalized eigenvector $|E\rangle$ such that

$$
H^\times|E\rangle = E|E\rangle
\tag{E2}
$$

and such that

$$
(\varphi,\psi) = \int_{\mathrm{Sp}(H)} dE\,\langle\varphi|E\rangle\langle E|\psi\rangle\,, \quad \forall\varphi,\psi\in\mathbf{\Phi}\,,
\tag{E3}
$$

and

$$
(\varphi,H^n\psi) = \int_{\mathrm{Sp}(H)} dE\,E^n\langle\varphi|E\rangle\langle E|\psi\rangle\,, \quad \forall\varphi,\psi\in\mathbf{\Phi}\,, n=1,2,\ldots
\tag{E4}
$$

*Proof* Let $\varphi$ and $\psi$ be in $\mathbf{\Phi}$. Since $U$ is unitary,

$$
(\varphi,\psi) = (U\varphi,U\psi) = (\widehat{\varphi},\widehat{\psi})\,.
\tag{E5}
$$

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

$$
(\widehat{\varphi},\widehat{\psi}) = \int_{\mathrm{Sp}(H)} dE\,\overline{\widehat{\varphi}(E)}\widehat{\psi}(E)\,.
\tag{E6}
$$

Since $\varphi$ and $\psi$ belong to $\mathbf{\Phi}$, the action of each eigenket $|E\rangle$ on them is well-defined,

$$
\langle\varphi|E\rangle = \overline{\widehat{\varphi}(E)}\,,
\tag{E7a}
$$

$$
\langle E|\psi\rangle = \widehat{\psi}(E)\,.
\tag{E7b}
$$

Plugging Eq. (E7) into Eq. (E6) and Eq. (E6) into Eq. (E5), we get to Eq. (E3). The proof of (E4) is similar:

$$\begin{aligned}
(\varphi, H^n\psi) &= (U\varphi, UH^nU^{-1}U\psi) \\
&= (\widehat{\phi}, \widehat{E}^n\widehat{\psi}) \\
&= \int_{\mathrm{Sp}(H)} dE\, \overline{\widehat{\varphi}(E)}(\widehat{E}^n\widehat{\psi})(E) \\
&= \int_{\mathrm{Sp}(H)} dE\, E^n\overline{\widehat{\varphi}(E)}\widehat{\psi}(E) \\
&= \int_{\mathrm{Sp}(H)} dE\, E^n\langle\varphi|E\rangle\langle E|\psi\rangle\,.
\end{aligned} \tag{E8}$$

## APPENDIX F: ENERGY REPRESENTATION OF THE RHS

**Proposition 5** The energy representation of the eigenket $|E\rangle$ is the antilinear Schwartz delta functional $|\widehat{E}\rangle$.

*Proof* Since

$$\begin{aligned}
\langle\widehat{\varphi}|U^{\times}|E\rangle &= \langle U^{-1}\widehat{\varphi}|E\rangle \\
&= \langle\varphi|E\rangle \\
&= \int_0^\infty \overline{\varphi(r)}\sigma(r;E)dr \\
&= \overline{\widehat{\varphi}(E)}\,,
\end{aligned} \tag{F1}$$

the functional $U^{\times}|E\rangle = |\widehat{E}\rangle$ is the antilinear Schwartz delta functional.

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