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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 (RHS) 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 RHS. The RHS is able to associate an eigenket with 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 wavefunction. Thus the RHS treats discrete energies (discrete spectrum) and scattering energies (continuous spectrum) on the same footing.

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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 Antoine [1], Bohm [2] and 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 the 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 Galindo and Pascual [5], and Melsheimer [6] came to the same conclusion.

Earlier attempts to go beyond the Hilbert space framework are reported in [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 [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 the authors [10–16] took the Schrödinger equation as the dynamical equation.

A RHS is a triplet of spaces

$$\Phi \subset \mathcal{H} \subset \Phi^\times \quad (1.1)$$

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

$$\Phi \subset \mathcal{D}(H) \subset \mathcal{H}. \quad (1.2)$$

If a Schrödinger Hamiltonian is defined on the whole Hilbert space and has only a 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 while dealing with unbounded operators that have continuous spectrum.

The reason why the RHS is the extension of the Hilbert space that we need is two-fold. On the one hand, one of the key assumptions of quantum mechanics is that the quantity

$$(\varphi, H\varphi) \quad (1.3)$$

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

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

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 wavefunctions is the space Φ 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 $|E_n\rangle$ and denote the ket corresponding to an energy E in the continuous spectrum by $|E\rangle$, then we should have

$$H|E_n\rangle = E_n|E_n\rangle \quad (1.5a)$$

$$H|E\rangle = E|E\rangle. \quad (1.5b)$$

These eigenkets are normalized according to the following rule:

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

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

$$\varphi = \sum_n |E_n\rangle(E_n|\varphi) + \int dE|E\rangle\langle E|\varphi). \quad (1.7)$$

The solutions of equation (1.5a) are square normalizable, i.e., they lie in the Hilbert space. However, the solutions of equation (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 with 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 Φ^\times in (1.1). The action of the Hamiltonian, which is in principle defined only on the elements of Φ (or on the elements of $\mathcal{D}(H)$), can be extended to the elements $|F\rangle$ of Φ^\times by defining the following conjugate operator H^\times :

$$\langle\varphi|H^\times|F\rangle := \langle H^\dagger\varphi|F\rangle \quad \forall\varphi \in \Phi \quad |F\rangle \in \Phi^\times. \quad (1.8)$$

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

$$\langle\varphi|H^\times|E\rangle = \langle H^\dagger\varphi|E\rangle = E\langle\varphi|E\rangle \quad \forall\varphi \in \Phi. \quad (1.9)$$

When the arbitrary $\varphi \in \Phi$ 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 wavefunctions must be square normalizable. The subspace Φ is the set of physical wavefunctions, i.e., the set of square integrable functions for which any expectation value and any uncertainty can be computed. The dual space Φ^\times contains the eigenkets associated with energies in the continuous part of the spectrum of H . These eigenkets are defined as functionals over the space Φ , and they can be used to expand any $\varphi \in \Phi$ as in equation (1.7). The eigen-equation (1.5b) holds within the RHS in the sense of equation (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 Φ^\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 equation (1.5a) in the discrete case, and by equation (1.5b) in the continuous case) that belongs to a basis that expands any physical wavefunction as in equation (1.7).

The main shortcoming of the RHS theory is that it does not provide a prescription to construct the space Φ 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 Φ 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 [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 [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 towards the construction of a RHS associated with 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

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

where Δ is the three-dimensional Laplacian and

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

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 equation (2.1) as

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

By splitting radial and angular dependences,

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

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

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

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

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

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

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

In order to construct the domain $\mathcal{D}(H)$ of the Hamiltonian, we first need 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 with the formal differential operator (2.7) are determined by the following condition (cf [18], p 1306):

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

Among all the possibilities in equation (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

$$f(r) \in L^2([0, \infty), dr) \quad (2.9a)$$

$$f(r) \in AC^2[0, \infty) \quad (2.9b)$$

$$(hf)(r) \in L^2([0, \infty), dr) \quad (2.9c)$$

$$f(0) = 0 \quad (2.9d)$$

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 sub-interval of $[0, \infty)$. Thus the domain of our Hamiltonian is

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

It follows that the Hamiltonian defined by

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

is a well-defined self-adjoint linear operator.

3. Resolvent and Green function

The second step towards the construction of a 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,

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

The Green function $G(r, s; E)$ can be computed using the prescription provided by the following theorem (cf theorem XIII.3.16 of [18] and also [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 $\text{Im}(E) \neq 0$. 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

$$G(r, s; E) = \begin{cases} \frac{2m}{\hbar^2} \frac{\chi(r; E)\Theta(s; E)}{W(\chi, \Theta)} & r < s \\ \frac{2m}{\hbar^2} \frac{\chi(s; E)\Theta(r; E)}{W(\chi, \Theta)} & r > s \end{cases} \quad (3.2)$$

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

$$W(\chi, \Theta) = \chi\Theta' - \chi'\Theta. \quad (3.3)$$

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:

$$\sqrt{\cdot} : \{E \in \mathbb{C} \mid -\pi < \arg(E) \leq \pi\} \mapsto \{E \in \mathbb{C} \mid -\pi/2 < \arg(E) \leq \pi/2\}. \quad (3.4)$$

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

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

$$G(r, s; E) = \begin{cases} -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2 E}} \frac{\tilde{\chi}(r; E)\tilde{\Theta}(s; E)}{2\tilde{\mathcal{J}}_3(E)} & r < s \\ -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2 E}} \frac{\tilde{\chi}(s; E)\tilde{\Theta}(r; E)}{2\tilde{\mathcal{J}}_3(E)} & r > s \end{cases} \quad \text{Re}(E) < 0 \quad \text{Im}(E) \neq 0. \quad (3.5)$$

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

$$\tilde{\chi}(0; E) = 0 \quad (3.6a)$$

$$\tilde{\chi}(r; E) \in AC^2([0, \infty)) \quad (3.6b)$$

$$\tilde{\chi}(r; E) \text{ is square integrable at } 0 \quad (3.6c)$$

which yield

$$\tilde{\chi}(r; E) = \begin{cases} \frac{i}{2} \left(\exp\left(\sqrt{-\frac{2m}{\hbar^2}(E + V_1)}r\right) - \exp\left(-\sqrt{-\frac{2m}{\hbar^2}(E + V_1)}r\right) \right) & 0 < r < a \\ \tilde{\mathcal{J}}_1(E) \exp\left(\sqrt{-\frac{2m}{\hbar^2}(E - V_2)}r\right) + \tilde{\mathcal{J}}_2(E) \exp\left(-\sqrt{-\frac{2m}{\hbar^2}(E - V_2)}r\right) & a < r < b \\ \tilde{\mathcal{J}}_3(E) \exp\left(\sqrt{-\frac{2m}{\hbar^2}Er}\right) + \tilde{\mathcal{J}}_4(E) \exp\left(-\sqrt{-\frac{2m}{\hbar^2}Er}\right) & b < r < \infty. \end{cases} \quad (3.7)$$

The expressions of the functions $\tilde{\mathcal{J}}_1(E)$ – $\tilde{\mathcal{J}}_4(E)$ can be found in appendix A.

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

$$\tilde{\Theta}(r; E) \in AC^2([0, \infty)) \quad (3.8a)$$

$$\tilde{\Theta}(r; E) \text{ is square integrable at } \infty \quad (3.8b)$$

which yield

$$\begin{aligned} & \tilde{\Theta}(r; E) \\ = & \begin{cases} \tilde{\mathcal{A}}_1(E) \exp\left(\sqrt{-\frac{2m}{\hbar^2}(E + V_1)} r\right) + \tilde{\mathcal{A}}_2(E) \exp\left(-\sqrt{-\frac{2m}{\hbar^2}(E + V_1)} r\right) & 0 < r < a \\ \tilde{\mathcal{A}}_3(E) \exp\left(\sqrt{-\frac{2m}{\hbar^2}(E - V_2)} r\right) + \tilde{\mathcal{A}}_4(E) \exp\left(-\sqrt{-\frac{2m}{\hbar^2}(E - V_2)} r\right) & a < r < b \\ \exp\left(-\sqrt{-\frac{2m}{\hbar^2}} E r\right) & b < r < \infty. \end{cases} \end{aligned} \quad (3.9)$$

The expressions of the functions $\tilde{\mathcal{A}}_1(E)$ – $\tilde{\mathcal{A}}_4(E)$ can be found in appendix A.

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

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

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

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

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

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),

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

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 $\text{Re}(E) > 0$, $\text{Im}(E) < 0$

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

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

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 equation (3.11)—hence the same symbol as in the section 3.2—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),

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

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 towards the construction of the RHS is to obtain the (Hilbert space) spectrum $\text{Sp}(H)$ 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 $\text{Sp}(H)$ 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 [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*

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

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 $\mathbf{E}(\Lambda)L^2([0, \infty), dr)$ onto $L^2(\Lambda, \{\rho_{ij}\})$, $\mathbf{E}(\Lambda)$ being the spectral projection associated with Λ .

The spectral measures $\{\rho_{ij}\}$ are provided by the following theorem (cf theorem XIII.5.18 of [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 $\text{Re}(H) := \mathbb{C} - \text{Sp}(H)$. 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*

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

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

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

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

$$\sigma_1(r; E) = \begin{cases} \tilde{\mathcal{B}}_1(E) \exp\left(\sqrt{-\frac{2m}{\hbar^2}(E+V_1)}r\right) + \tilde{\mathcal{B}}_2(E) \exp\left(-\sqrt{-\frac{2m}{\hbar^2}(E+V_1)}r\right) & 0 < r < a \\ \tilde{\mathcal{B}}_3(E) \exp\left(\sqrt{-\frac{2m}{\hbar^2}(E-V_2)}r\right) + \tilde{\mathcal{B}}_4(E) \exp\left(-\sqrt{-\frac{2m}{\hbar^2}(E-V_2)}r\right) & a < r < b \\ \exp\left(\sqrt{-\frac{2m}{\hbar^2}}Er\right) & b < r < \infty \end{cases} \quad (4.4a)$$

$$\sigma_2(r; E) = \tilde{\Theta}(r; E). \quad (4.4b)$$

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

$$\tilde{\chi}(r; E) = \tilde{\mathcal{J}}_3(E)\sigma_1(r; E) + \tilde{\mathcal{J}}_4(E)\sigma_2(r; E) \quad (4.5)$$

which along with equation (3.5) leads to

$$G(r, s; E) = -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2}E} \frac{1}{2} \left[\sigma_1(r; E) + \frac{\tilde{\mathcal{J}}_4(E)}{\tilde{\mathcal{J}}_3(E)} \sigma_2(r; E) \right] \sigma_2(s; E) \quad (4.6)$$

$r < s \quad \text{Re}(E) < 0 \quad \text{Im}(E) \neq 0.$

Since

$$\overline{\sigma_2(s; \bar{E})} = \sigma_2(s; E) \quad (4.7)$$

we can write equation (4.6) as

$$G(r, s; E) = -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2}E} \frac{1}{2} \left[\sigma_1(r; E) \overline{\sigma_2(s; \bar{E})} + \frac{\tilde{\mathcal{J}}_4(E)}{\tilde{\mathcal{J}}_3(E)} \sigma_2(r; E) \overline{\sigma_2(s; \bar{E})} \right] \quad (4.8)$$

$r < s \quad \text{Re}(E) < 0 \quad \text{Im}(E) \neq 0.$

By comparing equations (4.2) and (4.8) we see that

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

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

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

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 Høegre [20] for different values of V_1, V_2 in equation (2.2). In general, there is a finite number of bound states whose energies E_1, \dots, E_N are in the interval $(-V_1, 0)$. The corresponding normalized wavefunctions read [18]

$$\phi_n(r) = N_n \tilde{\Theta}(r; E_n) \quad n = 1, \dots, N \quad (4.11)$$

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 ,

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

Therefore E_1, \dots, 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 be) as the normalization obtained in [21–23]. To see this, we denote the momentum of those bound states by $k_n = i|k_n| = i\tilde{k}_n$, $n = 1, \dots, N$. Then we have that

$$\tilde{\Theta}(r; \tilde{k}_n) = \tilde{\Theta}(r; -ik_n) = \Theta_+(r; k_n) \quad (4.13)$$

and that

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

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

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

Since the eigenfunction $\phi_n(r)$ of equation (4.11) is normalized to one, from equations (4.12)–(4.14) it follows that

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

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

$$\sigma_1(r; E) = \chi(r; E) \quad (4.17a)$$

$$\sigma_2(r; E)$$

$$= \begin{cases} \cos \left(\sqrt{\frac{2m}{\hbar^2}} (E + V_1)r \right) & 0 < r < a \\ \mathcal{C}_1(E) \exp \left(i\sqrt{\frac{2m}{\hbar^2}} (E - V_2)r \right) + \mathcal{C}_2(E) \exp \left(-i\sqrt{\frac{2m}{\hbar^2}} (E - V_2)r \right) & a < r < b \\ \mathcal{C}_3(E) \exp \left(i\sqrt{\frac{2m}{\hbar^2}} Er \right) + \mathcal{C}_4(E) \exp \left(-i\sqrt{\frac{2m}{\hbar^2}} Er \right) & b < r < \infty. \end{cases} \quad (4.17b)$$

The functions \mathcal{C}_1 – \mathcal{C}_4 , whose expressions are given by equation (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 equation (3.11).

Equations (3.12), (3.14) and (4.17) lead to

$$\Theta_+(r; E) = -\frac{C_4(E)}{W(E)}\sigma_1(r; E) + \frac{J_4(E)}{W(E)}\sigma_2(r; E) \quad (4.18a)$$

$$\Theta_-(r; E) = \frac{C_3(E)}{W(E)}\sigma_1(r; E) - \frac{J_3(E)}{W(E)}\sigma_2(r; E) \quad (4.18b)$$

where

$$W(E) = J_4(E)C_3(E) - J_3(E)C_4(E). \quad (4.19)$$

By substituting equation (4.18a) into equation (3.10) we get

$$G(r, s; E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2 E}} \frac{1}{2iJ_4(E)} \left[-\frac{C_4(E)}{W(E)}\sigma_1(r; E) + \frac{J_4(E)}{W(E)}\sigma_2(r; E) \right] \sigma_1(s; E) \\ \operatorname{Re}(E) > 0 \quad \operatorname{Im}(E) > 0 \quad r > s. \quad (4.20)$$

By substituting equation (4.18b) into equation (3.13) we get

$$G(r, s; E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2 E}} \frac{1}{2iJ_3(E)} \left[\frac{C_3(E)}{W(E)}\sigma_1(r; E) - \frac{J_3(E)}{W(E)}\sigma_2(r; E) \right] \sigma_1(s; E) \\ \operatorname{Re}(E) > 0 \quad \operatorname{Im}(E) < 0 \quad r > s. \quad (4.21)$$

Since

$$\overline{\sigma_1(s; \bar{E})} = \sigma_1(s; E) \quad (4.22)$$

equation (4.20) can be written as

$$G(r, s; E) = \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2 E}} \frac{1}{2iJ_4(E)} \left[-\frac{C_4(E)}{W(E)}\sigma_1(r; E)\overline{\sigma_1(s; \bar{E})} + \frac{J_4(E)}{W(E)}\sigma_2(r; E)\overline{\sigma_1(s; \bar{E})} \right] \\ \operatorname{Re}(E) > 0 \quad \operatorname{Im}(E) > 0 \quad r > s \quad (4.23)$$

whereas equation (4.21) can be written as

$$G(r, s; E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2 E}} \frac{1}{2iJ_3(E)} \left[\frac{C_3(E)}{W(E)}\sigma_1(r; E)\overline{\sigma_1(s; \bar{E})} - \frac{J_3(E)}{W(E)}\sigma_2(r; E)\overline{\sigma_1(s; \bar{E})} \right] \\ \operatorname{Re}(E) > 0 \quad \operatorname{Im}(E) < 0 \quad r > s. \quad (4.24)$$

By comparing (4.2) to (4.23) we get

$$\theta_{ij}^+(E) = \begin{pmatrix} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2 E}} \frac{1}{2i} \frac{-C_4(E)}{J_4(E)W(E)} & 0 \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2 E}} \frac{1}{2i} \frac{1}{W(E)} & 0 \end{pmatrix} \quad \operatorname{Re}(E) > 0 \quad \operatorname{Im}(E) > 0. \quad (4.25)$$

By comparing (4.2) to (4.24) we get

$$\theta_{ij}^+(E) = \begin{pmatrix} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2 E}} \frac{1}{2i} \frac{C_3(E)}{J_3(E)W(E)} & 0 \\ \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2 E}} \frac{1}{2i} \frac{1}{W(E)} & 0 \end{pmatrix} \quad \operatorname{Re}(E) > 0 \quad \operatorname{Im}(E) < 0. \quad (4.26)$$

From equations (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

$$\rho_{11}((E_1, E_2)) = \lim_{\delta \rightarrow 0} \lim_{\epsilon \rightarrow 0^+} \frac{1}{2\pi i} \int_{E_1+\delta}^{E_2-\delta} [\theta_{11}^+(E - i\epsilon) - \theta_{11}^+(E + i\epsilon)] dE \\ = \int_{E_1}^{E_2} \frac{1}{4\pi} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2 E}} \frac{1}{J_3(E)J_4(E)} dE \quad (4.27)$$

which leads to

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

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

$$\text{Sp}(H) = \{E_1, \dots, E_N\} \cup [0, \infty). \quad (4.29)$$

Therefore, the spectrum of H has a discrete part $\Lambda_b = \{E_1, \dots, E_N\}$ and a continuous part $\Lambda_c = [0, \infty)$.

5. Direct integral decomposition

The fourth step towards 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 with the discrete spectrum and another Hilbert space associated with the continuous spectrum.

We first apply theorem 2 to the discrete part of the spectrum. By that theorem, there is a unitary operator U_b from $\mathcal{H}_b := \mathbf{E}(\Lambda_b)L^2([0, \infty), dr)$ onto $\hat{\mathcal{H}}_b := \mathbb{C}^N$ defined by

$$U_b : \mathcal{H}_b \mapsto \hat{\mathcal{H}}_b \quad f_b(r) \mapsto U_b f_b = \{(\phi_1, f_b), \dots, (\phi_N, f_b)\}. \quad (5.1)$$

In this equation, \mathcal{H}_b is the Hilbert space spanned by the bound states ϕ_1, \dots, ϕ_N , $\hat{\mathcal{H}}_b$ is the space of N -tuples of the form $\{(\phi_n, f_b)\}_{n=1}^N$ (hence $\hat{\mathcal{H}}_b$ is isomorphic to \mathbb{C}^N), $f_b = \mathbf{E}(\Lambda_b)f$, i.e., f_b is the component of f along the space \mathcal{H}_b :

$$f_b(r) = \sum_{n=1}^N (\phi_n, f) \phi_n(r) \quad (5.2)$$

and (ϕ_n, f_b) is the scalar product of the n th bound state $\phi_n(r)$ of equation (4.11) with f_b ,

$$(\phi_n, f_b) = \int_0^\infty dr \overline{\phi_n(r)} f_b(r) \quad n = 1, \dots, N. \quad (5.3)$$

On the space $\hat{\mathcal{H}}_b$, the Hamiltonian acts as the following $N \times N$ diagonal matrix:

$$\hat{H}_b := U_b H_b U_b^{-1} = \begin{pmatrix} E_1 & 0 & \dots & 0 \\ 0 & E_2 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & E_N \end{pmatrix} \quad (5.4)$$

where H_b is the restriction of H to \mathcal{H}_b .

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

$$\tilde{U}_c : \mathcal{H}_c \mapsto L^2((0, \infty), \rho(E) dE) \quad (5.5)$$

$$f_c(r) \mapsto \tilde{f}_c(E) = (\tilde{U}_c f_c)(E) = \int_0^\infty dr f_c(r) \overline{\chi(r; E)}$$

where $f_c = \mathbf{E}(\Lambda_c)f$, i.e., f_c is the component of f along the Hilbert space \mathcal{H}_c . The space \mathcal{H}_c is the Hilbert space that corresponds to the continuous part of the spectrum—hence the subscript c.

If we write

$$\mathcal{D}(H) = \mathcal{H}_b \oplus \mathcal{D}(H_c) \quad (5.6)$$

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

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

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

$$\begin{aligned} U_c : \mathcal{H}_c &\longmapsto \hat{\mathcal{H}}_c \\ f_c &\longmapsto \hat{f}_c(E) = (U_c f_c)(E) = \int_0^\infty dr f_c(r) \overline{\phi(r; E)} \end{aligned} \quad (5.8)$$

where $\hat{\mathcal{H}}_c = L^2([0, \infty), dE)$. 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_b and U_c are provided by the following theorem (cf theorem XIII.5.14 of [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 $\mathbb{E}(\Lambda)L^2([0, \infty), dr)$ onto $L^2(\Lambda, \{\rho_{ij}\})$ is given by the formula*

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

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_b is given by

$$(U_b^{-1} \hat{f}_b)(r) = \sum_{n=1}^N (\phi_n, f_b) \phi_n(r) \quad (5.10)$$

where $\hat{f}_b = \{(\phi_1, f_b), \dots, (\phi_N, f_b)\}$ is an N -tuple of complex numbers. The operator U_b^{-1} transforms from $\hat{\mathcal{H}}_b$ onto \mathcal{H}_b .

According to theorem 4, the inverse of U_c is given by

$$f_c(r) = (U_c^{-1} \hat{f}_c)(r) = \int_0^\infty dE \hat{f}_c(E) \phi(r; E) \quad \hat{f}_c(E) \in L^2([0, \infty), dE). \quad (5.11)$$

The operator U_c^{-1} transforms from $\hat{\mathcal{H}}_c$ into \mathcal{H}_c .

Using the operators U_b and U_c we can construct an operator U defined as

$$\begin{aligned} U : \mathcal{H} &\longmapsto \hat{\mathcal{H}} = \oplus_{n=1}^N \hat{\mathcal{H}}(E_n) \oplus \int_0^\infty \hat{\mathcal{H}}(E) dE \\ f &\longmapsto Uf := [U_b f, U_c f] = [\hat{f}_b, \{\hat{f}_c(E)\}] \end{aligned} \quad (5.12)$$

where \mathcal{H} is realized by $\mathcal{H}_b \oplus \mathcal{H}_c$, and $\hat{\mathcal{H}}$ is realized by $\hat{\mathcal{H}}_b \oplus \hat{\mathcal{H}}_c$. The Hilbert space $\hat{\mathcal{H}}(E_n)$, which is associated with each energy E_n in the discrete spectrum, and the Hilbert space $\hat{\mathcal{H}}(E)$, which is associated with each energy E in the continuous spectrum, are realized by the Hilbert space of complex numbers \mathbb{C} . On $\hat{\mathcal{H}}$, the operator H acts as the multiplication operator:

$$Hf \longmapsto UHf \equiv \sum_{n=1}^N E_n (\phi_n, f_b) + \{E \hat{f}_c(E)\} \quad f \in \mathcal{D}(H). \quad (5.13)$$

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

$$(\hat{f}, \hat{g})_{\hat{\mathcal{H}}} = \sum_{n=1}^N (f_b, \phi_n)(\phi_n, g_b) + \int_0^\infty dE \overline{\hat{f}_c(E)} \hat{g}_c(E) \quad (5.14)$$

where $\hat{f}_b = \{(\phi_1, f_b), \dots, (\phi_N, f_b)\}$ and $\hat{g}_b = \{(\phi_1, g_b), \dots, (\phi_N, g_b)\}$.

Therefore, U induces a direct integral decomposition of the Hilbert space associated with the Hamiltonian H (see [4, 27]). 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 :

$$f(r) = f_b(r) + f_c(r) = \sum_{n=1}^N (\phi_n, f) \phi_n(r) + \int_0^\infty dE \hat{f}(E) \phi(r; E) \quad (5.15)$$

$$\hat{f} \equiv \hat{f}_b + \hat{f}_c(E) = \{(\phi_n, f)\}_{n=1}^N + \int_0^\infty dr f(r) \overline{\phi(r; E)}. \quad (5.16)$$

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 with the discrete spectrum. In this case, the Hilbert space \mathcal{H}_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}_b :

$$\Phi_b = \mathcal{H}_b = \Phi_b^\times. \quad (6.1)$$

The eigenket $|E_n\rangle$ associated with any energy E_n in the discrete spectrum is defined by

$$\begin{aligned} |E_n\rangle : \Phi_b &\longmapsto \mathbb{C} \\ \varphi_b &\longmapsto (\varphi_b | E_n) := (\varphi_b, \phi_n) = \int_0^\infty dr \overline{\varphi_b(r)} \phi_n(r). \end{aligned} \quad (6.2)$$

Clearly, the function $|E_n\rangle$ is an antilinear functional over Φ_b , i.e., $|E_n\rangle \in \Phi_b^\times$. Besides being an eigenvector of the Hamiltonian in the usual sense, $|E_n\rangle$ is also an eigenvector of H_b in the RHS sense of equation (1.8):

$$(\varphi_b | H_b^\times | E_n) = E_n (\varphi_b | E_n) \quad \forall \varphi_b \in \Phi_b. \quad (6.3)$$

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 draw a parallel with the continuous case.

Now, we construct the RHS associated with 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}_c of the operator H_c :

$$\mathcal{D}_c := \bigcap_{n=0}^{\infty} \mathcal{D}(H_c^n). \quad (6.4)$$

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

$$\mathcal{D}_c = \left\{ \varphi_c \in \mathcal{H}_c \mid h^n \varphi_c(r) \in \mathcal{H}_c, h^n \varphi_c(0) = 0, \varphi_c^{(n)}(a) = \varphi_c^{(n)}(b) = 0, n = 0, 1, 2, \dots; \right. \\ \left. \varphi_c(r) \in C^\infty([0, \infty)) \right\}. \quad (6.5)$$

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

$$|E\rangle : \Phi_c \mapsto \mathbb{C} \quad \varphi_c \mapsto \langle \varphi_c | E \rangle := \int_0^\infty dr \overline{\varphi_c(r)} \phi(r; E) = \overline{(U_c \varphi_c)(E)}. \quad (6.6)$$

A necessary condition for $|E\rangle$ to be well-defined is that Φ_c be included in \mathcal{D}_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 behaviour at infinity of the elements of \mathcal{D}_c ,

$$\int_0^\infty dr |(r+1)^n (h+1)^m \varphi_c(r)|^2 < \infty \quad n, m = 0, 1, 2, \dots \quad (6.7)$$

The imposition of (6.7) upon the space \mathcal{D}_c yields

$$\Phi_c = \left\{ \varphi_c \in \mathcal{D}_c \mid \int_0^\infty dr |(r+1)^n (h+1)^m \varphi_c(r)|^2 < \infty, n, m = 0, 1, 2, \dots \right\}. \quad (6.8)$$

On Φ_c , we define the family of norms

$$\|\varphi_c\|_{n,m} := \sqrt{\int_0^\infty dr |(r+1)^n (h+1)^m \varphi_c(r)|^2} \quad n, m = 0, 1, 2, \dots \quad (6.9)$$

These norms can be used to define a countably normed topology τ_{Φ_c} on Φ_c (see [4]):

$$\varphi_{c,\alpha} \xrightarrow[\alpha \rightarrow \infty]{\tau_{\Phi_c}} \varphi_c \quad \text{iff} \quad \|\varphi_{c,\alpha} - \varphi_c\|_{n,m} \xrightarrow[\alpha \rightarrow \infty]{} 0 \quad n, m = 0, 1, 2, \dots \quad (6.10)$$

Once we have constructed the space Φ_c , we can construct its topological dual Φ_c^\times as the space of τ_{Φ_c} -continuous antilinear functionals on Φ_c (see [4]) and therewith the RHS corresponding to the continuous part of the spectrum:

$$\Phi_c \subset \mathcal{H}_c \subset \Phi_c^\times. \quad (6.11)$$

In order to show that the RHS (6.11) is what we are looking for, we need to prove the following proposition (the proof is given 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) fulfil the conditions to be a norm.*
- (ii) *The space Φ_c is stable under the action of H_c , and H_c is τ_{Φ_c} -continuous.*
- (iii) *The ket $|E\rangle$ of equation (6.6) is a well-defined antilinear functional on Φ_c , i.e., $|E\rangle$ belongs to Φ_c^\times .*
- (iv) *The ket $|E\rangle$ is a generalized eigenvector of H_c ,*

$$H_c^\times |E\rangle = E |E\rangle \quad (6.12)$$

i.e.,

$$\langle \varphi_c | H_c^\times |E\rangle = \langle H_c^\dagger \varphi_c | E\rangle = E \langle \varphi_c | E\rangle \quad \forall \varphi_c \in \Phi_c. \quad (6.13)$$

Proposition 1 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

$$\Phi \subset \mathcal{H} \subset \Phi^\times \quad (6.14)$$

where

$$\Phi := \Phi_b \oplus \Phi_c \quad \mathcal{H} := \mathcal{H}_b \oplus \mathcal{H}_c \quad \Phi^\times := \Phi_b^\times \oplus \Phi_c^\times. \quad (6.15)$$

On the space Φ , 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 $|E_n\rangle$ and $|E\rangle$ satisfy the normalization (1.6). Since the spaces Φ_b and Φ_c are orthogonal to each other, we also have that

$$\langle \varphi | E_n \rangle = \langle \varphi_b | E_n \rangle \quad \langle \varphi | E \rangle = \langle \varphi_c | E \rangle. \quad (6.16)$$

As we shall see in the section 6.2, the kets $|E_n\rangle$ 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 equation (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 Φ_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 wavefunction φ as in equation (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 Φ .

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

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

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 $\varphi \in \Phi$, because only those functions fulfil both

$$\overline{\langle \varphi_c | E \rangle} = \langle \varphi | E \rangle \quad (6.18)$$

and

$$\langle \varphi | H^\times | E \rangle = \langle H^\dagger \varphi | E \rangle = E \langle \varphi | E \rangle. \quad (6.19)$$

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 [4], we prove the theorem using the machinery of the Sturm–Liouville theory (our proof is given in appendix B).

Proposition 2 (Nuclear spectral theorem). *Let*

$$\Phi \subset L^2([0, \infty), dr) \subset \Phi^\times \quad (6.20)$$

be the RHS of the square well-barrier Hamiltonian H such that Φ remains invariant under H and H is a τ_Φ -continuous operator on Φ . Then, for each energy in the spectrum of H there is a generalized eigenvector such that

$$H|E_n\rangle = E_n|E_n\rangle \quad E_n \in \{E_1, \dots, E_N\} \quad (6.21a)$$

$$H^\times|E\rangle = E|E\rangle \quad E \in [0, \infty) \quad (6.21b)$$

and such that

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

and

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

Thus this theorem allows us to write the scalar product (6.22) of any two functions φ, ψ of Φ and the matrix elements (6.23) in terms of the action of the kets $|E_n\rangle$ 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 (6.11) by applying to it the unitary operator U of equation (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}_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 $|E_n\rangle$ under U_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_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_c acts as the multiplication operator. The energy representation of the space Φ_c is defined as

$$\hat{\Phi}_c := U_c \Phi_c. \quad (6.24)$$

The space $\hat{\Phi}_c$ is a linear subspace of $L^2([0, \infty), dE)$. In order to endow $\hat{\Phi}_c$ with a topology $\tau_{\hat{\Phi}_c}$, we carry the topology on Φ_c into $\hat{\Phi}_c$:

$$\tau_{\hat{\Phi}_c} := U_c \tau_{\Phi_c}. \quad (6.25)$$

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

$$U_c^\times \Phi_c^\times = (U_c \Phi_c)^\times = \hat{\Phi}_c^\times. \quad (6.26)$$

From the following chain of equalities:

$$\langle \hat{\varphi}_c | U_c^\times | E \rangle = \langle U_c^{-1} \hat{\varphi}_c | E \rangle = \int_0^\infty dr \overline{\varphi_c(r)} \phi(r; E) = \overline{\varphi_c(E)} \quad (6.27)$$

it follows that the energy representation of the Dirac ket $|E\rangle$, that we denote by $|\hat{E}\rangle$, is the antilinear Schwartz delta functional, i.e., $|\hat{E}\rangle$ is the antilinear functional that associates with each function $\hat{\varphi}_c$ 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:

$$\begin{array}{ccccccc}
H; \varphi & \Phi_b \oplus \Phi_c & \subset & \mathcal{H}_b \oplus \mathcal{H}_c & \subset & \Phi_b^\times \oplus \Phi_c^\times & |E_n\rangle \oplus |E\rangle \\
& U_b \downarrow \oplus \downarrow U_c & & U_b \downarrow \oplus \downarrow U_c & & U_b^\times \downarrow \oplus \downarrow U_c^\times & \\
\hat{H}; \hat{\varphi} & \hat{\Phi}_b \oplus \hat{\Phi}_c & \subset & \hat{\mathcal{H}}_b \oplus \hat{\mathcal{H}}_c & \subset & \hat{\Phi}_b^\times \oplus \hat{\Phi}_c^\times & |\hat{E}_n\rangle \oplus |\hat{E}\rangle
\end{array} \quad (6.28)$$

On the top line of the diagram (6.28), we have the RHS, the Hamiltonian, the wavefunctions 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

$$k := \sqrt{\frac{2m}{\hbar^2} E}. \quad (6.29)$$

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

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

This eigensolution can be used to obtain the unitary operator V_c that transforms from the position into the momentum representation

$$\hat{f}_c(k) = (V_c f_c)(k) = \int_0^\infty dr f_c(r) \overline{\langle r|k\rangle} \quad f_c \in \mathcal{H}_c. \quad (6.31)$$

(The operator V_b corresponding to the discrete case is U_b .) On the k -representation, the Hamiltonian (continuous part) acts as multiplication by k^2 . To each $k \in [0, \infty)$, there corresponds an eigenket $|k\rangle$ that acts on Φ_c as the following integral operator:

$$\langle \varphi_c|k\rangle := \int_0^\infty dr \langle \varphi_c|r\rangle \langle r|k\rangle = \overline{(V_c \varphi_c)(k)} \quad \varphi_c \in \Phi_c. \quad (6.32)$$

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 equation (6.29) provides a Riemann surface in a natural way. For instance, we can define the Jost function

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

the eigensolution

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

and the Green function

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

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 equations (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:

$$\Phi_b \oplus \Phi_c \subset \mathcal{H}_b \oplus \mathcal{H}_c \subset \Phi_b^\times \oplus \Phi_c^\times. \quad (7.1)$$

The spectrum of the Hamiltonian has a discrete part $\{E_1, \dots, E_N\}$ 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 $|E_n\rangle$, which is given by equation (6.2), is an element of Φ_b^\times . If the energy E belongs to the continuous spectrum, its corresponding eigenket $|E\rangle$, which is given by equation (6.6), is an element of Φ_c^\times . Thus the RHS treats the discrete and the continuous spectra independently and on the same footing. Each element φ of $\Phi_b \oplus \Phi_c$ can be expanded by the eigenkets of the Hamiltonian as in equation (6.17). The elements of $\Phi_b \oplus \Phi_c$ 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 $\Phi_b \oplus \Phi_c$.

Therefore, the RHS (7.1) contains all the physically meaningful solutions of the Schrödinger equation—the physical wavefunctions are included in $\Phi_b \oplus \Phi_c$, whereas the monoenergetic solutions of the time independent Schrödinger equation are included in $\Phi_b^\times \oplus \Phi_c^\times$.

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

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

then the coefficients in equation (3.7) are given by

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

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

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

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

and the coefficients in equation (3.9) by

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

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

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

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

If we define

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

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

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

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

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

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

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

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

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

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

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

The coefficients in equation (3.14) are given by

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

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

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

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

The coefficients in equation (4.4a) are given by

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

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

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

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

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

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

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

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

$$\mathcal{C}_4(E) \equiv \mathcal{C}_4(k) = \frac{1}{2} e^{ikb} \left[\left(1 - \frac{Q_2}{k} \right) e^{iQ_2 b} \mathcal{C}_1(k) + \left(1 + \frac{Q_2}{k} \right) e^{-iQ_2 b} \mathcal{C}_2(k) \right]. \quad (\text{A9d})$$

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,

$$\|\varphi_c + \psi_c\|_{n,m} \leq \|\varphi_c\|_{n,m} + \|\psi_c\|_{n,m} \quad (\text{B1a})$$

$$\|\alpha\varphi_c\|_{n,m} = |\alpha| \|\varphi_c\|_{n,m} \quad (\text{B1b})$$

$$\|\varphi_c\|_{n,m} \geq 0 \quad (\text{B1c})$$

$$\text{if } \|\varphi_c\|_{n,m} = 0 \quad \text{then } \varphi_c = 0. \quad (\text{B1d})$$

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

$$(1+r)^n (h+1)^m \varphi_c(r) = 0 \quad (\text{B2})$$

which yields

$$(h+1)^m \varphi_c(r) = 0. \quad (\text{B3})$$

If $m = 0$, then equation (B3) implies $\varphi_c(r) = 0$. If $m = 1$, then equation (B3) implies that -1 is an eigenvalue of H_c whose corresponding eigenvector is φ_c . Since there is no discrete eigenvalue in the continuous part of the spectrum, φ_c must be the zero vector. The proof for $m > 1$ is similar.

(ii) In order to see that H_c is τ_{Φ_c} -continuous, we just have to realize that

$$\begin{aligned} \|H_c \varphi_c\|_{n,m} &= \|(H_c + I)\varphi_c - \varphi_c\|_{n,m} \\ &\leq \|(H_c + I)\varphi_c\|_{n,m} + \|\varphi_c\|_{n,m} \\ &= \|\varphi_c\|_{n,m+1} + \|\varphi_c\|_{n,m}. \end{aligned} \quad (\text{B4})$$

The stability of Φ_c under the action of H_c also follows from equation (B4).

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

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

Since

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

the functional $|E\rangle$ is continuous when Φ_c is endowed with the τ_{Φ_c} topology.

(iv) In order to prove that $|E\rangle$ is a generalized eigenvector of H_c , we make use of the conditions (6.5) and (6.7) satisfied by the elements of Φ_c :

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

Proof of proposition 2. Let φ and ψ be in Φ . Since U of equation (5.12) is unitary,

$$(\varphi, \psi) = (U\varphi, U\psi) = (\hat{\varphi}_b, \hat{\psi}_b)_{\mathcal{H}_b} + (\hat{\varphi}_c, \hat{\psi}_c)_{\mathcal{H}_c}. \tag{B8}$$

The scalar product of $\hat{\varphi}_b$ and $\hat{\psi}_b$ can be written as

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

The wavefunctions $\hat{\varphi}_c$ and $\hat{\psi}_c$ are in particular elements of $L^2([0, \infty), dE)$. Hence their scalar product is well-defined:

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

Since φ_c and ψ_c belong to Φ_c , the action of each eigenket $|E\rangle$ on them is well-defined,

$$\langle \varphi_c | E \rangle = \overline{\hat{\varphi}_c(E)} \tag{B11a}$$

$$\langle E | \psi_c \rangle = \hat{\psi}_c(E). \tag{B11b}$$

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

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