The Rigged Hilbert Space of the Free Hamiltonian

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(October 23, 2003)

Abstract

We explicitly construct the Rigged Hilbert Space (RHS) of the free Hamiltonian H_0. The construction of the RHS of H_0 provides yet another opportunity to see that when continuous spectrum is present, the solutions of the Schrödinger equation lie in a RHS rather than just in a Hilbert space.

PACS numbers: 03.65.-w, 02.30.Hq

1 Introduction

There is a growing realization that the Rigged Hilbert Space (RHS) provides the methods needed to handle Dirac's bra-ket formalism and continuous spectrum. Moreover, there is an increasing number of Quantum Mechanics textbooks that include the RHS as part of their contents [1]–[7] (this list is non-exhaustive). However, there is still a lack of simple examples for which the RHS is explicitly constructed (one exception is Ref. [8]). Especially important is to construct the RHS generated by the Schrödinger equation, because claiming that Quantum Mechanics needs the RHS is tantamount to claiming that the solutions of the Schrödinger equation lie in a RHS (when continuous spectrum is present). The task of constructing the RHS generated by the Schrödinger equation was undertaken in Ref. [9]. The method proposed in [9] has been applied to two simple potentials [10, 11]. In this paper, we shall apply this method to the simplest example possible: the free Hamiltonian.

We note that the results of this paper follow immediately from those in Refs. [10, 11], by making the value of the potential zero. Nevertheless, we think that the example of the free Hamiltonian provides a very transparent way to understand the essentials of the method of [9], because the calculations are reduced to the minimum.

The time-independent Schrödinger equation for the free Hamiltonian H_0 reads, in the position representation, as

$$\langle \vec{x}|H_0|E\rangle = \frac{-\hbar^2}{2m}\nabla^2\langle \vec{x}|E\rangle = E\langle \vec{x}|E\rangle \, , \tag{1.1}$$

where ∇^2 is the three-dimensional Laplacian. In spherical coordinates $\vec{x} \equiv (r, \theta, \phi)$, Eq. (1.1) has the following form:

$$\langle r,\theta,\phi|H_0|E,l,m\rangle = \left(\frac{-\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}r + \frac{\hbar^2 l(l+1)}{2mr^2}\right)\langle r,\theta,\phi|E,l,m\rangle = E\langle r,\theta,\phi|E,l,m\rangle \, . \tag{1.2}$$

By separating the radial and angular dependences,

$$\langle r,\theta,\phi|E,l,m\rangle \equiv \langle r|E\rangle_l \, \langle \theta,\phi|l,m\rangle \equiv \frac{1}{r}\chi_l(r;E)Y_{l,m}(\theta,\phi), \tag{1.3}$$

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

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2mr^2}\right)\chi_l(r;E) = E\chi_l(r;E) \, . \tag{1.4}$$

In this paper, we shall restrict ourselves to the case of zero orbital angular momentum (the higher-order case can be treated analogously). We then write $\chi_{l=0}(r;E) \equiv \chi(r;E)$ and obtain

$$-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\chi(r;E) = E\chi(r;E) \, . \tag{1.5}$$

We shall write this equation as

$$h_0\chi(r;E) = E\chi(r;E) \, , \tag{1.6}$$

where

$$h_0 \equiv -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} \tag{1.7}$$

is the formal differential operator corresponding to the free Hamiltonian (for $l=0$). Our goal is to solve Eq. (1.6) and show that its solutions lie in a RHS rather than just in a Hilbert space.

The basic tool necessary to solve Eq. (1.6) is the Sturm-Liouville theory [12]. This theory provides the Hilbert space methods. As shown in many publications (cf. [9] and references therein), the Hilbert space methods do not provide us with all the tools needed in Quantum Mechanics when continuous spectrum is present. In particular, the Hilbert space cannot incorporate Dirac's bra-ket formalism. Therefore, an extension of the Hilbert space is needed. The extension that seems to be most suitable is the RHS (cf. [9] and references therein). In particular, the RHS incorporates Dirac's bra-ket formalism.

The structure of the paper is as follows. In Section 2, we construct the domain and the self-adjoint extension of the differential operator (1.7). In Section 3, we obtain the free Green function, whose expression is used in Section 4 to calculate the spectrum of H_0. Section 5 is devoted to the eigenfunction expansion and the direct integral decomposition of the Hilbert space. In Section 6, we construct the RHS of H_0. The Dirac basis vector expansion for H_0 is obtained in Section 7, and the energy representation of the RHS of H_0 is constructed in Section 8. Finally, the results of the paper are summarized in the diagram of Eq. (8.5).

2 Self-Adjoint Extension

The first step is to define a linear operator on a Hilbert space corresponding to the formal differential operator (1.7). In the radial position representation, the Hilbert space that belongs to the RHS of the free Hamiltonian is realized by the space $L^2([0,\infty), dr)$ of square integrable functions $f(r)$ defined on the interval $[0,\infty)$ (see the diagram (8.5) below).

The domain $\mathcal{D}(H_0)$ of the free Hamiltonian must be a proper dense linear subspace of $L^2([0,\infty), dr)$. The action of h_0 must be well defined on $\mathcal{D}(H_0)$, 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. The boundary conditions that select the possible self-adjoint extensions of h_0 are given by (see [13], page 1306)

$$f(0) + \alpha\, f'(0) = 0\,, \quad -\infty < \alpha \leq \infty\,. \tag{2.1}$$

Among all these boundary conditions, we choose $f(0) = 0$. Therefore, the requirements that are to be fulfilled by the elements of the domain of H_0 are

$$f(r) \in L^2([0,\infty), dr)\,, \tag{2.2a}$$
$$h_0 f(r) \in L^2([0,\infty), dr)\,, \tag{2.2b}$$
$$f(r) \in AC^2[0,\infty)\,, \tag{2.2c}$$
$$f(0) = 0\,, \tag{2.2d}$$

where $AC^2[0,\infty)$ denotes the space of functions whose derivative is absolutely continuous (for details on absolutely continuous functions, consult Refs. [13, 9]). The requirements in

Eq. (2.2) yield the domain of H_0:

$$\mathcal{D}(H_0) = \{f(r) \mid f(r), h_0 f(r) \in L^2([0,\infty), dr),\ f(r) \in AC^2[0,\infty),\ f(0)=0\}\,. \tag{2.3}$$

On $\mathcal{D}(H_0)$ the formal differential operator h_0 is self-adjoint. In choosing (2.3) as the domain of our formal differential operator h_0, we define a linear operator H_0 by

$$H_0 f(r) := h_0 f(r) = -\frac{\hbar^2}{2m}\frac{d^2}{dr^2} f(r)\,, \quad f(r) \in \mathcal{D}(H_0)\,. \tag{2.4}$$

3 Resolvent and Green Function

The expression of the free Green function $G_0(r,s;E)$ is given in terms of eigenfunctions of the differential operator h_0 subject to certain boundary conditions (cf. Theorem 1 in Appendix A). We shall divide the complex energy plane in three regions, and calculate $G_0(r,s;E)$ for each region separately. In all our calculations, we shall use the following branch of the square root function:

$$\sqrt{\cdot} : \{E \in \mathbb{C} \mid -\pi < \arg(E) \leq \pi\} \longmapsto \{E \in \mathbb{C} \mid -\pi/2 < \arg(E) \leq \pi/2\}\,. \tag{3.1}$$

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

For $\mathrm{Re}(E) < 0$, $\mathrm{Im}(E) \neq 0$, the free Green function (see Theorem 1 in Appendix A) is given by

$$G_0(r,s;E) = \left\{ \begin{array}{ll} -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\,\frac{\widetilde{\chi}(r;E)\,\widetilde{f}(s;E)}{2} & r<s \\ -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\,E}}\,\frac{\widetilde{\chi}(s;E)\,\widetilde{f}(r;E)}{2} & r>s \end{array} \right. \qquad \mathrm{Re}(E) < 0\,,\ \mathrm{Im}(E) \neq 0\,. \tag{3.2}$$

The eigenfunction $\widetilde{\chi}(r;E)$ satisfies the Schrödinger equation, Eq. (1.6), and the boundary conditions

$$\widetilde{\chi}(0;E) = 0\,, \tag{3.3a}$$

$$\widetilde{\chi}(r;E) \text{ is square integrable at } 0\,, \tag{3.3b}$$

which yield

$$\widetilde{\chi}(r;E) = e^{\sqrt{-\frac{2m}{\hbar^2}E}\,r} - e^{-\sqrt{-\frac{2m}{\hbar^2}E}\,r}\,, \quad 0 < r < \infty\,. \tag{3.4}$$

The eigenfunction $\widetilde{f}(r;E)$ satisfies the Schrödinger equation, Eq. (1.6), and the boundary condition

$$\widetilde{f}(r;E) \text{ is square integrable at } \infty\,, \tag{3.5}$$

which yield

$$\widetilde{f}(r;E) = e^{-\sqrt{-\frac{2m}{\hbar^2}E}\,r}\,, \quad 0 < r < \infty\,. \tag{3.6}$$

The Wronskian of $\widetilde{\chi}$ and $\widetilde{f}$ can be easily calculated:

$$W(\widetilde{\chi}, \widetilde{f}) = -2\sqrt{-\frac{2m}{\hbar^2}E}\,. \tag{3.7}$$

3.2 Region Re$(E) > 0$, Im$(E) > 0$

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

$$G_0(r,s;E) = \begin{cases} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}\, \chi(r;E)\, f^+(s;E) & r<s \\ -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}\, \chi(s;E)\, f^+(r;E) & r>s \end{cases} \qquad \mathrm{Re}(E) > 0,\ \mathrm{Im}(E) > 0\,. \quad (3.8)$$

The eigenfunction $\chi(r;E)$ satisfies Eq. (1.6) and the boundary conditions (3.3), which yield

$$\chi(r;E) = \sin(\sqrt{\frac{2m}{\hbar^2}E}\, r)\,, \quad 0<r<\infty\,. \qquad (3.9)$$

The eigenfunction $f^+(r;E)$ satisfies Eq. (1.6) subject to the boundary condition (3.5), which yield

$$f^+(r;E) = e^{i\sqrt{\frac{2m}{\hbar^2}E}\, r}\,, \quad 0<r<\infty\,. \qquad (3.10)$$

The expression of the Wronskian of χ and f^+ follows immediately from Eqs. (3.9) and (3.10):

$$W(\chi, f^+) = -\sqrt{\frac{2m}{\hbar^2}E}\,. \qquad (3.11)$$

3.3 Region Re$(E) > 0$, Im$(E) < 0$

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

$$G_0(r,s;E) = \begin{cases} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}\, \chi(r;E)\, f^-(s;E) & r<s \\ -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}\, \chi(s;E)\, f^-(r;E) & r>s \end{cases} \qquad \mathrm{Re}(E) > 0,\ \mathrm{Im}(E) < 0\,. \quad (3.12)$$

The eigenfunction $\chi(r;E)$ is given by (3.9), although now E belongs to the fourth quadrant of the energy plane. The eigenfunction $f^-(r;E)$ satisfies Eq. (1.6) and the boundary condition (3.5), which yield

$$f^-(r;E) = e^{-i\sqrt{\frac{2m}{\hbar^2}E}\, r}\,, \quad 0<r<\infty\,. \qquad (3.13)$$

The Wronskian of χ and f^- is given by

$$W(\chi, f^-) = -\sqrt{\frac{2m}{\hbar^2}E}\,. \qquad (3.14)$$

4 Spectrum of H_0

In this section, we obtain the spectrum of H_0, which we shall denote by $\mathrm{Sp}(H_0)$. We know that H_0 is self-adjoint, and therefore its spectrum is real. In order to obtain the set of real numbers that belong to $\mathrm{Sp}(H_0)$, we apply Theorem 4 of Appendix A. From Theorem 4 and from the previous section, it is clear that we should study the positive and the negative real lines separately. As expected, we shall obtain that $\mathrm{Sp}(H_0) = [0, \infty)$.

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

We first take Λ from Theorem 4 of Appendix A to be $(-\infty, 0)$. We choose a basis for the space of solutions of the equation $h_0\sigma = E\sigma$ as

$$\widetilde{\sigma}_1(r;E) = e^{\sqrt{-\frac{2m}{\hbar^2}E}\,r}\,, \tag{4.1a}$$

$$\widetilde{\sigma}_2(r;E) = \widetilde{f}(r;E)\,. \tag{4.1b}$$

Obviously,

$$\widetilde{\chi}(r;E) = \widetilde{\sigma}_1(r;E) - \widetilde{\sigma}_2(r;E)\,, \tag{4.2}$$

which along with Eq. (3.2) leads to

$$G_0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}}\,\frac{1}{2}\,[\widetilde{\sigma}_1(r;E) - \widetilde{\sigma}_2(r;E)]\,\widetilde{\sigma}_2(s;E)\,,\ r<s\,,\ \mathrm{Re}(E)<0\,, \mathrm{Im}(E)\neq 0\,. \tag{4.3}$$

Because

$$\overline{\widetilde{\sigma}_2(s;\overline{E})} = \widetilde{\sigma}_2(s;E)\,, \tag{4.4}$$

we can write Eq. (4.3) as

$$G_0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}}\,\frac{1}{2}\,\left[\widetilde{\sigma}_1(r;E)\overline{\widetilde{\sigma}_2(s;\overline{E})} - \widetilde{\sigma}_2(r;E)\overline{\widetilde{\sigma}_2(s;\overline{E})}\right]\,,$$
$$r<s\,,\ \mathrm{Re}(E)<0\,, \mathrm{Im}(E)\neq 0\,. \tag{4.5}$$

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

$$G_0(r,s;E) = \sum_{i,j=1}^{2} \theta_{ij}^-(E)\widetilde{\sigma}_i(r;E)\overline{\widetilde{\sigma}_j(s;\overline{E})}\,, \qquad r<s\,. \tag{4.6}$$

By comparing Eqs. (4.5) and (4.6) we see that

$$\theta_{ij}^-(E) = \begin{pmatrix} 0 & -\frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}}\frac{1}{2} \\ 0 & \frac{2m/\hbar^2}{\sqrt{-2m/\hbar^2\, E}}\frac{1}{2} \end{pmatrix}\,, \quad \mathrm{Re}(E)<0\,,\ \mathrm{Im}(E)\neq 0\,. \tag{4.7}$$

The functions $\theta_{ij}^-(E)$ are analytic in a neighborhood of $\Lambda = (-\infty, 0)$. Therefore, the interval $(-\infty, 0)$ is in the resolvent set, $\mathrm{Re}(H_0)$, of the operator H_0.

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

In this case, we choose the following basis for the space of solutions of $h_0\sigma = E\sigma$:

$$\sigma_1(r;E) = \chi(r;E)\,, \tag{4.8a}$$

$$\sigma_2(r;E) = \cos(\sqrt{\frac{2m}{\hbar^2}E}\,r)\,. \tag{4.8b}$$

Eqs. (3.10), (3.13) and (4.8) lead to

$$f^+(r;E) = i\sigma_1(r;E) + \sigma_2(r;E) \tag{4.9}$$

and to

$$f^-(r;E) = -i\sigma_1(r;E) + \sigma_2(r;E)\,. \tag{4.10}$$

By substituting Eq. (4.9) into Eq. (3.8) we get to

$$G_0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}\,\sigma_1(s;E)\left[i\sigma_1(r;E)+\sigma_2(r;E)\right],\ r>s\,,\ \mathrm{Re}(E)>0, \mathrm{Im}(E)>0\,. \tag{4.11}$$

By substituting Eq. (4.10) into Eq. (3.12) we get to

$$G_0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}\,\sigma_1(s;E)\left[-i\sigma_1(r;E)+\sigma_2(r;E)\right],\ r>s\,,\ \mathrm{Re}(E)>0, \mathrm{Im}(E)<0\,. \tag{4.12}$$

Because

$$\overline{\sigma_1(s;\overline{E})} = \sigma_1(s;E)\,, \tag{4.13}$$

Eq. (4.11) leads to

$$G_0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}\left[i\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})}+\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right], \\ \mathrm{Re}(E)>0, \mathrm{Im}(E)>0,\ r>s\,, \tag{4.14}$$

whereas Eq. (4.12) leads to

$$G_0(r,s;E) = -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}\left[-i\sigma_1(r;E)\overline{\sigma_1(s;\overline{E})}+\sigma_2(r;E)\overline{\sigma_1(s;\overline{E})}\right], \\ \mathrm{Re}(E)>0, \mathrm{Im}(E)<0\,,\ r>s\,. \tag{4.15}$$

The expression of the resolvent in terms of the basis σ_1, σ_2 can be written as (see Theorem 4 in Appendix A)

$$G_0(r,s;E) = \sum_{i,j=1}^{2} \theta_{ij}^+(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})}\,, \qquad r>s\,. \tag{4.16}$$

By comparing (4.16) to (4.14) we get to

$$\theta_{ij}^+(E) = \begin{pmatrix} -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}i & -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \\ 0 & 0 \end{pmatrix}, \quad \mathrm{Re}(E)>0\,,\ \mathrm{Im}(E)>0\,. \tag{4.17}$$

By comparing (4.16) to (4.15) we get to

$$\theta_{ij}^+(E) = \begin{pmatrix} \frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}}i & -\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\, E}} \\ 0 & 0 \end{pmatrix}, \quad \mathrm{Re}(E)>0\,,\ \mathrm{Im}(E)<0\,. \tag{4.18}$$

From Eqs. (4.17) and (4.18) we can see that the measures ϱ_{12}, ϱ_{21} and ϱ_{22} in Theorem 4 of Appendix A are zero, and that the measure ϱ_{11} is given by

$$\begin{aligned}
\varrho_{11}((E_1,E_2)) &= \lim_{\delta\to 0}\lim_{\varepsilon\to 0+}\frac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}\left[\theta_{11}^{+}(E-i\varepsilon)-\theta_{11}^{+}(E+i\varepsilon)\right]dE \\
&= \int_{E_1}^{E_2}\frac{1}{\pi}\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,dE\,, \qquad (4.19)
\end{aligned}$$

which leads to

$$\varrho(E)\equiv\varrho_{11}(E)=\frac{1}{\pi}\frac{2m/\hbar^2}{\sqrt{2m/\hbar^2\,E}}\,,\quad E\in(0,\infty)\,. \qquad (4.20)$$

The function $\theta_{11}^{+}(E)$ has a branch cut along $(0,\infty)$, and therefore $(0,\infty)$ is included in $\mathrm{Sp}(H_0)$. Because $\mathrm{Sp}(H_0)$ is a closed set, $\mathrm{Sp}(H_0)=[0,\infty)$.

5 Diagonalization and Eigenfunction Expansion

In the present section, we diagonalize H_0 and construct the expansion of the wave functions in terms of the eigenfunctions of the differential operator h_0.

By Theorem 2 of Appendix A, there is a unitary map $\widetilde{U}_0$ defined by

$$\begin{aligned}
\widetilde{U}_0 : L^2([0,\infty),dr) &\longmapsto L^2((0,\infty),\varrho(E)dE) \\
f(r) &\longmapsto \widetilde{f}(E)=\widetilde{U}_0 f(E)=\int_0^{\infty}dr\,f(r)\overline{\chi(r;E)}\,, \qquad (5.1)
\end{aligned}$$

that brings $\mathcal{D}(H_0)$ onto the space

$$\mathcal{D}(\widetilde{H}_0)=\{\widetilde{f}(E)\in L^2((0,\infty),\varrho(E)dE)\mid \int_0^{\infty}dE\,E^2|\widetilde{f}(E)|^2\varrho(E)<\infty\}\,. \qquad (5.2)$$

The unitary operator $\widetilde{U}_0$ provides a ϱ-normalization (cf. Ref. [11]). In order to obtain a δ-normalization, the measure $\varrho(E)$ must be absorbed in the definition of the eigenfunctions (cf. Ref. [11]). This is why we define

$$\sigma(r;E):=\sqrt{\varrho(E)}\,\chi(r;E)\,, \qquad (5.3)$$

which is the δ-normalized eigensolution of the differential operator h_0. If we define

$$\widehat{f}(E):=\sqrt{\varrho(E)}\widetilde{f}(E)\,,\quad \widetilde{f}(E)\in L^2((0,\infty),\varrho(E)dE)\,, \qquad (5.4)$$

and construct the unitary operator

$$\begin{aligned}
\widehat{U}_0 : L^2((0,\infty),\varrho(E)dE) &\longmapsto L^2((0,\infty),dE) \\
\widetilde{f} &\longmapsto \widehat{f}(E)=\widehat{U}_0\widetilde{f}(E):=\sqrt{\varrho(E)}\widetilde{f}(E)\,, \qquad (5.5)
\end{aligned}$$

then the operator that δ-diagonalizes our Hamiltonian is $U_0:=\widehat{U}_0\widetilde{U}_0$,

$$\begin{aligned}
U_0 : L^2([0,\infty),dr) &\longmapsto L^2((0,\infty),dE) \\
f &\longmapsto U_0 f:=\widehat{f}\,. \qquad (5.6)
\end{aligned}$$

The action of U_0 can be written as an integral operator:

$$\widehat{f}(E) = U_0 f(E) = \int_0^\infty dr f(r)\overline{\sigma(r;E)}\,, \quad f(r) \in L^2([0,\infty), dr)\,. \tag{5.7}$$

The image of $\mathcal{D}(H_0)$ under the action of U_0 is

$$\mathcal{D}(\widehat{H}_0) := U\mathcal{D}(H_0) = \{\widehat{f}(E) \in L^2((0,\infty), dE) \,|\, \int_0^\infty E^2 |\widehat{f}(E)|^2 dE < \infty\}\,. \tag{5.8}$$

Therefore, we have constructed a unitary operator

$$\begin{array}{rcl} U_0 : \mathcal{D}(H) \subset L^2([0,\infty), dr) & \longmapsto & \mathcal{D}(\widehat{H}_0) \subset L^2((0,\infty), dE) \\ f & \longmapsto & \widehat{f} = U_0 f \end{array} \tag{5.9}$$

that transforms from the position representation into the energy representation (see diagram (8.5) below). The operator U_0 diagonalizes the free Hamiltonian in the sense that $\widehat{H}_0 \equiv U_0 H_0 U_0^{-1}$ is the multiplication operator. The inverse operator of U_0 is given by (see Theorem 3 of Appendix A)

$$f(r) = U_0^{-1}\widehat{f}(r) = \int_0^\infty dE\, \widehat{f}(E)\sigma(r;E)\,, \quad \widehat{f}(E) \in L^2((0,\infty), dE)\,. \tag{5.10}$$

The operator U_0^{-1} transforms from the energy representation into the position representation (see diagram (8.5) below). The expressions (5.7) and (5.10) provide the eigenfunction expansion of any square integrable function in terms of the δ-normalized eigensolutions $\sigma(r;E)$ of h_0.

6 Construction of the RHS of the Free Hamiltonian

The Sturm-Liouville theory only provides a domain $\mathcal{D}(H_0)$ on which the Hamiltonian H_0 is self-adjoint and a unitary operator U_0 that diagonalizes H_0. This unitary operator induces a direct integral decomposition of the Hilbert space (cf. Ref. [9] and references therein),

$$\begin{array}{rcl} \mathcal{H} & \longmapsto & U_0\mathcal{H} \equiv \widehat{\mathcal{H}} = \oplus \displaystyle\int_{\mathrm{Sp}(H_0)} \mathcal{H}(E) dE \\ f & \longmapsto & U_0 f \equiv \{\widehat{f}(E)\}, \quad \widehat{f}(E) \in \mathcal{H}(E)\,. \end{array} \tag{6.1}$$

As shown in Refs. [17, 9, 10, 11], the direct integral decomposition does not provide us with all the tools needed in Quantum Mechanics. This is why we extend the Hilbert space to the RHS.

We first need to construct a dense invariant domain $\mathbf{\Phi}_0$ on which all the powers and all the expectation values of H_0 are well defined, and on which the Dirac kets act as antilinear functionals. Before building $\mathbf{\Phi}_0$, we need to build the maximal invariant subspace $\mathcal{D}_0$ of H_0,

$$\mathcal{D}_0 := \bigcap_{n=0}^{\infty} \mathcal{D}(H_0^n)\,. \tag{6.2}$$

It is easy to check that

$$\mathcal{D}_0 = \{\varphi \in L^2([0,\infty),dr) \mid \ h_0^n\varphi(r) \in L^2([0,\infty),dr),\ h_0^n\varphi(0)=0, n=0,1,2,\ldots,$$
$$\varphi(r) \in C^\infty([0,\infty))\}\,. \tag{6.3}$$

We can now construct the subspace $\mathbf{\Phi}_0$ on which the eigenkets $|E\rangle$ of H_0 are well defined as antilinear functionals. This subspace is given by

$$\mathbf{\Phi}_0 = \{\varphi \in \mathcal{D}_0 \mid \int_0^\infty dr\ |(r+1)^n(h_0+1)^m\varphi(r)|^2 < \infty, \quad n,m=0,1,2,\ldots\}\,. \tag{6.4}$$

On $\mathbf{\Phi}_0$, we define the family of norms

$$\|\varphi\|_{n,m} := \sqrt{\int_0^\infty dr\ |(r+1)^n(h_0+1)^m\varphi(r)|^2}\ , \quad n,m=0,1,2,\ldots \tag{6.5}$$

The quantities (6.5) fulfill the conditions to be a norm (see Proposition 1 of Appendix B), and can be used to define a countably normed topology $\tau_{\mathbf{\Phi}_0}$ on $\mathbf{\Phi}_0$ (for the definition of a countably normed topology, consult Ref. [9] and references therein),

$$\varphi_\alpha \xrightarrow[\alpha\to\infty]{\tau_{\mathbf{\Phi}_0}} \varphi \quad \text{iff} \quad \|\varphi_\alpha - \varphi\|_{n,m} \xrightarrow[\alpha\to\infty]{} 0\,, \quad n,m=0,1,2,\ldots \tag{6.6}$$

The space $\mathbf{\Phi}_0$ is stable under the action of H_0, and H_0 is $\tau_{\mathbf{\Phi}_0}$-continuous (see Proposition 2 of Appendix B).

Once we have constructed the space $\mathbf{\Phi}_0$, we can construct its topological dual $\mathbf{\Phi}_0^\times$ as the space of $\tau_{\mathbf{\Phi}_0}$-continuous antilinear functionals on $\mathbf{\Phi}_0$ and therewith the RHS of the free Hamiltonian (see diagram (8.5) below):

$$\mathbf{\Phi}_0 \subset L^2([0,\infty),dr) \subset \mathbf{\Phi}_0^\times\,. \tag{6.7}$$

For each $E \in \mathrm{Sp}(H_0)$, we can now associate a ket $|E\rangle$ to the generalized eigenfunction $\sigma(r;E)$ through

$$\begin{aligned} |E\rangle : \mathbf{\Phi}_0 \ &\longmapsto \ \mathbb{C} \\ \varphi \ &\longmapsto \ \langle\varphi|E\rangle := \int_0^\infty \overline{\varphi(r)}\sigma(r;E)\,dr = \overline{(U_0\varphi)(E)}\,. \end{aligned} \tag{6.8}$$

The ket $|E\rangle$ in Eq. (6.8) is a well-defined antilinear functional on $\mathbf{\Phi}_0$, i.e., $|E\rangle$ belongs to $\mathbf{\Phi}_0^\times$ (see Proposition 3 of Appendix B). The ket $|E\rangle$ is a generalized eigenvector of the free Hamiltonian H_0 (see Proposition 3 of Appendix B):

$$H_0^\times|E\rangle = E|E\rangle\,; \tag{6.9}$$

that is,

$$\langle\varphi|H_0^\times|E\rangle = \langle H_0^\dagger\varphi|E\rangle = E\langle\varphi|E\rangle\,, \quad \forall\varphi \in \mathbf{\Phi}_0\,. \tag{6.10}$$

7 The Dirac Basis Vector Expansion for H_0

We are now in a position to derive the Dirac basis vector expansion for the free Hamiltonian. This derivation consists of the restriction of the Weyl-Kodaira expansions (5.7) and (5.10) to the space $\mathbf{\Phi}_0$. 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 bra $\langle E|$ on $\varphi \in \mathbf{\Phi}_0$ as $\langle E|\varphi\rangle := \widehat{\varphi}(E)$, then Eq. (5.7) becomes

$$\langle E|\varphi\rangle = \int_0^\infty dr\, \langle E|r\rangle\langle r|\varphi\rangle\,, \quad \varphi \in \mathbf{\Phi}_0\,. \tag{7.1}$$

If we denote $\langle r|E\rangle \equiv \sigma(r;E)$, then Eq. (5.10) becomes

$$\langle r|\varphi\rangle = \int_0^\infty dE\, \langle r|E\rangle\langle E|\varphi\rangle\,, \quad \varphi \in \mathbf{\Phi}_0\,. \tag{7.2}$$

This equation is the Dirac basis vector expansion of the wave function φ in terms of the free eigenkets $|E\rangle$. We can also prove the Nuclear Spectral Theorem for the free Hamiltonian (see Proposition 4 of Appendix B),

$$(\varphi, H_0^n\psi) = \int_0^\infty dE\, E^n \langle\varphi|E\rangle\langle E|\psi\rangle\,, \quad \forall\varphi,\psi \in \mathbf{\Phi}_0\,, n = 1,2,\ldots \tag{7.3}$$

8 Energy Representation of the RHS of H_0

We have already seen that in the energy representation, the Hamiltonian H_0 acts as the multiplication operator $\widehat{H}_0$. The energy representation of the space $\mathbf{\Phi}_0$ is defined as

$$\widehat{\mathbf{\Phi}}_0 := U_0\mathbf{\Phi}_0\,. \tag{8.1}$$

Obviously $\widehat{\mathbf{\Phi}}_0$ is a linear subspace of $L^2([0,\infty),dE)$. In oder to endow $\widehat{\mathbf{\Phi}}_0$ with a topology $\tau_{\widehat{\mathbf{\Phi}}_0}$, we carry the topology on $\mathbf{\Phi}_0$ into $\widehat{\mathbf{\Phi}}_0$,

$$\tau_{\widehat{\mathbf{\Phi}}_0} := U_0\tau_{\mathbf{\Phi}_0}\,. \tag{8.2}$$

With this topology, the space $\widehat{\mathbf{\Phi}}_0$ is a linear topological space. If we denote the dual space of $\widehat{\mathbf{\Phi}}_0$ by $\widehat{\mathbf{\Phi}}_0^\times$, then we have

$$U_0^\times\mathbf{\Phi}_0^\times = (U_0\mathbf{\Phi}_0)^\times = \widehat{\mathbf{\Phi}}_0^\times\,. \tag{8.3}$$

If we denote $|\widehat{E}\rangle \equiv U_0^\times|E\rangle$, then we can prove that $|\widehat{E}\rangle$ is the antilinear Schwartz delta functional (see Proposition 5 of Appendix B),

$$\begin{aligned} |\widehat{E}\rangle : \widehat{\mathbf{\Phi}} &\longmapsto \mathbb{C} \\ \widehat{\varphi} &\longmapsto \langle\widehat{\varphi}|\widehat{E}\rangle := \overline{\widehat{\varphi}(E)}\,. \end{aligned} \tag{8.4}$$

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

$$\begin{array}{lccccccl} H_0;\ \varphi(r) & \mathbf{\Phi}_0 & \subset & L^2([0,\infty),dr) & \subset & \mathbf{\Phi}_0^\times & |E\rangle & \text{position repr.} \\ & \downarrow U_0 & & \downarrow U_0 & & \downarrow U_0^\times & & \\ \widehat{H}_0;\ \widehat{\varphi}(E) & \widehat{\mathbf{\Phi}}_0 & \subset & L^2([0,\infty),dE) & \subset & \widehat{\mathbf{\Phi}}_0^\times & |\widehat{E}\rangle & \text{energy repr.} \end{array}$$

On the top line, we have the position representation of the Hamiltonian, the wave functions, the kets, and the RHS. On the bottom line, we have their energy representation counterparts.

9 Conclusions

We have constructed the RHS of H_0 (for the zero angular momentum case), and its energy representation. We have associated an eigenket $|E\rangle$ to each energy E in the spectrum of H_0, and shown that $|E\rangle$ belongs to $\mathbf{\Phi}_0^{\times}$. We have seen that the energy representation of $|E\rangle$ is given by the antilinear Schwartz delta functional. We have also shown that the Dirac basis vector expansion holds within the RHS of H_0.

Thus, we conclude that the natural setting for the solutions of the Schrödinger equation of H_0 is the Rigged Hilbert Space rather than just the Hilbert space.

Acknowledgment

C. Koeninger's advise on English style is gratefully acknowledged. This work was financially supported by the E.U. TMR Contract No. ERBFMRX-CT96-0087 "The Physics of Quantum Information."

A Appendix A: The Sturm-Liouville Theory

The following theorem provides the procedure to compute the Green function of H_0 (cf. Theorem XIII.3.16 of Ref. [13] and also Refs. [9, 10, 11] for some applications):

Theorem 1 Let H_0 be the self-adjoint operator (2.4) derived from the real formal differential operator (1.7) by the imposition of the boundary condition (2.2d). Let $\mathrm{Im}(E) \neq 0$. Then there is exactly one solution $\chi(r;E)$ of $(h_0 - E)\sigma = 0$ square-integrable at 0 and satisfying the boundary condition (2.2d), and exactly one solution $f(r;E)$ of $(h_0 - E)\sigma = 0$ square-integrable at infinity. The resolvent $(E - H_0)^{-1}$ is an integral operator whose kernel $G_0(r,s;E)$ is given by

$$G_0(r,s;E) = \left\{ \begin{array}{ll} \frac{2m}{\hbar^2}\,\frac{\chi(r;E)\,f(s;E)}{W(\chi,f)} & r < s \\ \frac{2m}{\hbar^2}\,\frac{\chi(s;E)\,f(r;E)}{W(\chi,f)} & r > s\,, \end{array} \right. \tag{A.1}$$

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

$$W(\chi,f) = \chi f' - \chi' f\,. \tag{A.2}$$

The theorem that provides the operator U_0 that diagonalizes H_0 is the following (cf. Theorem XIII.5.13 of Ref. [13] and also Refs. [9, 10, 11] for some applications):

Theorem 2 (Weyl-Kodaira) Let h_0 be the formally self-adjoint differential operator (1.7) defined on the interval $[0,\infty)$. Let H_0 be the self-adjoint operator (2.4). 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 $h_0\sigma = E\sigma$. Then there exists a positive 2×2 matrix measure $\{\varrho_{ij}\}$ defined on Λ, such that

1. the limit
$$(U_0 f)_i(E) = \lim_{c\to 0}\lim_{d\to\infty}\left[\int_c^d f(r)\overline{\sigma_i(r;E)}dr\right] \tag{A.3}$$
exists in the topology of $L^2(\Lambda,\{\varrho_{ij}\})$ for each f in $L^2([0,\infty),dr)$ and defines an isometric isomorphism U_0 of $\mathsf{E}(\Lambda)L^2([0,\infty),dr)$ onto $L^2(\Lambda,\{\varrho_{ij}\})$, where $\mathsf{E}(\Lambda)$ is the spectral projection associated with Λ;

2. for each Borel function G defined on the real line and vanishing outside Λ,
$$U_0\mathcal{D}(G(H_0)) = \{[f_i]\in L^2(\Lambda,\{\varrho_{ij}\})\mid [Gf_i]\in L^2(\Lambda,\{\varrho_{ij}\})\} \tag{A.4}$$
and
$$(U_0G(H_0)f)_i(E) = G(E)(U_0f)_i(E), \quad i=1,2,\ E\in\Lambda,\ f\in\mathcal{D}(G(H_0))\,. \tag{A.5}$$

The theorem that provides the inverse of the operator U_0 is the following (cf. Theorem XIII.5.14 of Ref. [13] and also Refs. [9, 10, 11] for some applications):

Theorem 3 (Weyl-Kodaira) Let H_0, Λ, $\{\varrho_{ij}\}$, etc., be as in Theorem 2. Let E_0 and E_1 be the end points of Λ. Then

1. the inverse of the isometric isomorphism U_0 of $\mathsf{E}(\Lambda)L^2([0,\infty),dr)$ onto $L^2(\Lambda,\{\varrho_{ij}\})$ is given by the formula
$$(U_0^{-1}F)(r) = \lim_{\mu_0\to E_0}\lim_{\mu_1\to E_1}\int_{\mu_0}^{\mu_1}\left(\sum_{i,j=1}^{2}F_i(E)\sigma_j(r;E)\varrho_{ij}(dE)\right) \tag{A.6}$$
where $F=[F_1,F_2]\in L^2(\Lambda,\{\varrho_{ij}\})$, 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 Λ, then $G(H_0)$ has the representation
$$G(H_0)f(r) = \int_0^\infty f(s)K(H_0,r,s)ds\,, \tag{A.7}$$
where
$$K(H_0,r,s) = \sum_{i,j=1}^{2}\int_e G(E)\overline{\sigma_i(s;E)}\sigma_j(r;E)\varrho_{ij}(dE)\,. \tag{A.8}$$

The spectral measures are provided by the following theorem (cf. Theorem XIII.5.18 of Ref. [13] and also Refs. [9, 10, 11] for some applications):

Theorem 4 (Titchmarsh-Kodaira) Let Λ be an open interval of the real axis and O be an open set in the complex plane containing Λ. Let $\mathrm{Re}(H_0)$ be the resolvent set of H_0. Let $\{\sigma_1(r;E),\, \sigma_2(r;E)\}$ be a set of functions which form a basis for the solutions of the equation $h_0\sigma = E\sigma$, $E \in O$, and which are continuous on $(0,\infty)\times O$ and analytically dependent on E for E in O. Suppose that the kernel $G_0(r,s;E)$ for the resolvent $(E-H_0)^{-1}$ has a representation

$$G_0(r,s;E) = \begin{cases} \sum_{i,j=1}^{2} \theta_{ij}^{-}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})}\,, & r<s\,, \\ \sum_{i,j=1}^{2} \theta_{ij}^{+}(E)\sigma_i(r;E)\overline{\sigma_j(s;\overline{E})}\,, & r>s\,, \end{cases} \tag{A.9}$$

for all E in $\mathrm{Re}(H_0)\cap O$, and that $\{\varrho_{ij}\}$ is a positive matrix measure on Λ associated with H_0 as in Theorem 2. Then the functions $\theta_{ij}^{\pm}$ are analytic in $\mathrm{Re}(H_0)\cap O$, and given any bounded open interval $(E_1,E_2)\subset\Lambda$, we have for $1\le i,j\le 2$,

$$\begin{aligned} \varrho_{ij}((E_1,E_2)) &= \lim_{\delta\to 0}\lim_{\varepsilon\to 0+} \tfrac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}[\theta_{ij}^{-}(E-i\varepsilon)-\theta_{ij}^{-}(E+i\varepsilon)]dE \\ &= \lim_{\delta\to 0}\lim_{\varepsilon\to 0+} \tfrac{1}{2\pi i}\int_{E_1+\delta}^{E_2-\delta}[\theta_{ij}^{+}(E-i\varepsilon)-\theta_{ij}^{+}(E+i\varepsilon)]dE\,. \end{aligned} \tag{A.10}$$

B Appendix B: Auxiliary Propositions

In this appendix, we list the propositions invoked throughout the paper.

Proposition 1 The quantities

$$\|\varphi\|_{n,m} := \sqrt{\int_0^\infty dr\ |(r+1)^n(h_0+1)^m\varphi(r)|^2}\,, \quad \varphi\in\mathbf{\Phi}_0\,,\ n,m=0,1,2,\ldots, \tag{B.1}$$

are norms.

Proof It is very easy to show that the quantities (B.1) fulfill the conditions to be a norm:

$$\|\varphi+\psi\|_{n,m} \le \|\varphi\|_{n,m}+\|\psi\|_{n,m}\,, \tag{B.2a}$$
$$\|\alpha\varphi\|_{n,m} = |\alpha|\,\|\varphi\|_{n,m}\,, \tag{B.2b}$$
$$\|\varphi\|_{n,m}\ge 0\,, \tag{B.2c}$$
$$\text{If } \|\varphi\|_{n,m}=0, \text{ then } \varphi=0\,. \tag{B.2d}$$

The only condition that is somewhat difficult to prove is (B.2d): if $\|\varphi\|_{n,m}=0$, then

$$(1+r)^n(h_0+1)^m\varphi(r)=0\,, \tag{B.3}$$

which yields

$$(h_0+1)^m\varphi(r)=0\,. \tag{B.4}$$

If $m=0$, then Eq. (B.4) implies $\varphi(r)=0$. If $m=1$, then Eq. (B.4) implies that -1 is an eigenvalue of H_0 whose corresponding eigenvector is φ. Since -1 is not an eigenvalue of H_0, φ must be the zero vector. If $m>1$, the proof is similar.

Proposition 2 The space $\mathbf{\Phi}_0$ is stable under the action of H_0, and H_0 is $\tau_{\mathbf{\Phi}_0}$-continuous.

Proof In order to see that H_0 is $\tau_{\mathbf{\Phi}_0}$-continuous, we just have to realize that

$$\begin{aligned} \|H_0\varphi\|_{n,m} &= \|(H_0+I)\varphi-\varphi\|_{n,m} \\ &\leq \|(H_0+I)\varphi\|_{n,m}+\|\varphi\|_{n,m} \\ &= \|\varphi\|_{n,m+1}+\|\varphi\|_{n,m}\,. \end{aligned} \tag{B.5}$$

We now prove that $\mathbf{\Phi}_0$ is stable under the action of H_0. Let $\varphi\in\mathbf{\Phi}_0$. Saying that $\varphi\in\mathbf{\Phi}_0$ is equivalent to saying that $\varphi\in\mathcal{D}_0$ and that the norms $\|\varphi\|_{n,m}$ are finite for every $n,m=0,1,2,\ldots$ Since $H_0\varphi$ is also in $\mathcal{D}_0$, and since the norms $\|H_0\varphi\|_{n,m}$ are also finite (see Eq. (B.5)), the vector $H_0\varphi$ is also in $\mathbf{\Phi}_0$.

Proposition 3 The function

$$\begin{aligned} |E\rangle : \mathbf{\Phi}_0 &\longmapsto \mathbb{C} \\ \varphi &\longmapsto \langle\varphi|E\rangle := \int_0^\infty \overline{\varphi(r)}\sigma(r;E)dr = \overline{(U_0\varphi)(E)}\,. \end{aligned} \tag{B.6}$$

is an antilinear functional on $\mathbf{\Phi}_0$ and a generalized eigenvector of (the restriction to $\mathbf{\Phi}_0$ of) H_0.

Proof From the definition (B.6), it is pretty easy to see that $|E\rangle$ is an antilinear functional. In order to show that $|E\rangle$ is continuous, we define

$$\mathcal{M}(E) := \sup_{r\in[0,\infty)} |\sigma(r;E)|\ . \tag{B.7}$$

Because

$$\begin{aligned} |\langle\varphi|E\rangle| &= |\overline{U\varphi(E)}| \\ &= \left|\int_0^\infty dr\,\overline{\varphi(r)}\sigma(r;E)\right| \\ &\leq \int_0^\infty dr\,|\overline{\varphi(r)}||\sigma(r;E)| \\ &\leq \mathcal{M}(E)\int_0^\infty dr\,|\varphi(r)| \\ &= \mathcal{M}(E)\int_0^\infty dr\,\frac{1}{1+r}(1+r)|\varphi(r)| \\ &\leq \mathcal{M}(E)\left(\int_0^\infty dr\,\frac{1}{(1+r)^2}\right)^{1/2}\left(\int_0^\infty dr\ |(1+r)\varphi(r)|^2\right)^{1/2} \\ &= \mathcal{M}(E)\left(\int_0^\infty dr\,\frac{1}{(1+r)^2}\right)^{1/2}\|\varphi\|_{1,0} \\ &= \mathcal{M}(E)\|\varphi\|_{1,0}\,, \end{aligned} \tag{B.8}$$

the functional $|E\rangle$ is continuous when $\mathbf{\Phi}_0$ is endowed with the $\tau_{\mathbf{\Phi}_0}$ topology.

In order to prove that $|E\rangle$ is a generalized eigenvector of H_0, we make use of the conditions (6.3) and (6.5) satisfied by the elements of $\mathbf{\Phi}_0$:

$$\begin{aligned}
\langle\varphi|H_0^\times|E\rangle &= \langle H_0^\dagger\varphi|E\rangle \\
&= \int_0^\infty dr\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\overline{\varphi(r)}\right)\sigma(r;E) \\
&= -\frac{\hbar^2}{2m}\left[\frac{d\overline{\varphi(r)}}{dr}\sigma(r;E)\right]_0^\infty+\frac{\hbar^2}{2m}\left[\overline{\varphi(r)}\frac{d\sigma(r;E)}{dr}\right]_0^\infty \\
&\quad+\int_0^\infty dr\,\overline{\varphi(r)}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dr^2}\sigma(r;E)\right) \\
&= E\langle\varphi|E\rangle\,.
\end{aligned}\tag{B.9}$$

Similarly, one can also prove that

$$\langle\varphi|(H_0^\times)^n|E\rangle=E^n\langle\varphi|E\rangle\,.\tag{B.10}$$

Proposition 4 (Nuclear Spectral Theorem) Let

$$\mathbf{\Phi}_0\subset L^2([0,\infty),dr)\subset\mathbf{\Phi}_0^\times\tag{B.11}$$

be the RHS of H_0 such that $\mathbf{\Phi}_0$ remains invariant under H_0 and H_0 is a $\tau_{\mathbf{\Phi}_0}$-continuous operator on $\mathbf{\Phi}_0$. Then, for each E in the spectrum of H_0 there is a generalized eigenvector $|E\rangle$ such that

$$H_0^\times|E\rangle=E|E\rangle\tag{B.12}$$

and such that

$$(\varphi,\psi)=\int_{\mathrm{Sp}(H_0)}dE\,\langle\varphi|E\rangle\langle E|\psi\rangle\,,\quad\forall\varphi,\psi\in\mathbf{\Phi}_0\,,\tag{B.13}$$

and

$$(\varphi,H_0^n\psi)=\int_{\mathrm{Sp}(H_0)}dE\,E^n\langle\varphi|E\rangle\langle E|\psi\rangle\,,\quad\forall\varphi,\psi\in\mathbf{\Phi}_0\,,n=1,2,\ldots\tag{B.14}$$

Proof Let φ and ψ be in $\mathbf{\Phi}_0$. Since U_0 is unitary,

$$(\varphi,\psi)=(U_0\varphi,U_0\psi)=(\widehat{\varphi},\widehat{\psi})\,.\tag{B.15}$$

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,

$$(\widehat{\varphi},\widehat{\psi})=\int_{\mathrm{Sp}(H_0)}dE\,\overline{\widehat{\varphi}(E)}\widehat{\psi}(E)\,.\tag{B.16}$$

Because φ and ψ belong to $\mathbf{\Phi}_0$, the action of each eigenket $|E\rangle$ on them is well defined,

$$\langle\varphi|E\rangle=\overline{\widehat{\varphi}(E)}\,,\tag{B.17a}$$

$$\langle E|\psi\rangle=\widehat{\psi}(E)\,.\tag{B.17b}$$

By plugging Eq. (B.17) into Eq. (B.16) and Eq. (B.16) into Eq. (B.15), we obtain Eq. (B.13). The proof of (B.14) is similar:

$$\begin{aligned}
(\varphi, H_0^n \psi) &= (U_0\varphi, U_0 H_0^n U_0^{-1} U_0 \psi) \\
&= (\widehat{\varphi}, \widehat{H}_0^n \widehat{\psi}) \\
&= \int_{\mathrm{Sp}(H_0)} dE \, \overline{\widehat{\varphi}(E)} (\widehat{H}_0^n \widehat{\psi})(E) \\
&= \int_{\mathrm{Sp}(H_0)} dE \, E^n \overline{\widehat{\varphi}(E)} \widehat{\psi}(E) \\
&= \int_{\mathrm{Sp}(H_0)} dE \, E^n \langle \varphi | E \rangle \langle E | \psi \rangle \, .
\end{aligned} \tag{B.18}$$

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

Proof Because

$$\begin{aligned}
\langle \widehat{\varphi} | U_0^{\times} | E \rangle &= \langle U_0^{-1} \widehat{\varphi} | E \rangle \\
&= \langle \varphi | E \rangle \\
&= \int_0^\infty \overline{\varphi(r)} \sigma(r; E) dr \\
&= \overline{\widehat{\varphi}(E)} \, ,
\end{aligned} \tag{B.19}$$

the functional $U_0^{\times}|E\rangle = |\widehat{E}\rangle$ is the antilinear Schwartz delta functional.

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