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Completeness in quantum mechanics and the Weyl–Titchmarsh–Kodaira theorem

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Abstract

We discuss the completeness of (generalized) eigenfunctions in quantum mechanics using the classical theory developed by Weyl, Titchmarsh, and Kodaira. As applications, we rigorously prove the completeness of generalized eigenfunctions for the step and well potentials.

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1. Introduction

Since its formulation at the beginning of the 20th century, the interpretation of quantum mechanics represented a great challenge, as the very abstract formalism of this theory seemed to contradict well-established intuition and common sense. As is well known, the standard interpretation of quantum mechanics, formulated by Niels Bohr and Werner Heisenberg in 1927 [13], solved these apparent contradictions: it put quantum mechanics in a logical consistent footing and it gave a full scheme explaining the results of every experimental situation.

In this interpretation (the so-called Copenhagen Interpretation of Quantum Mechanics) the *completeness of eigenfunctions* for a given (self-adjoint) operator—representing for example the energy—plays a prominent role, since it allows for a faithful correspondence between the properties of a given physical system and its mathematical description (see for instance Dirac [9, p 36]). Now, 'completeness' in standard Hilbert space theory is a very precise notion. It asserts that the set of eigenfunctions for a self-adjoint operator on a Hilbert space $\mathcal{H}$ forms a *complete set*: every element of $\mathcal{H}$ can be expanded as a series in terms of that. As observed by Dirac [9], *this is not enough for quantum mechanics*. In fact, it is explicitly stated in his classical treatise (Dirac, [9, pp 37–40]) that the 'eigenkets' needed to express completeness in quantum mechanics are not always elements of a fixed Hilbert space.

Thus, two obvious questions arise: can we rigorously construct a reasonable space of bra and ket vectors? Can we prove completeness of energy eigenstates in physically interesting cases? The first problem has been treated by several researchers. We specially mention the work of Antoine [1] and Roberts [17] on the use of rigged Hilbert spaces (or 'Gelfand triplets') in quantum mechanics, and the more general theory of partial inner product spaces introduced by Antoine and Grossmann [2, 4]. An interesting discussion on 'quantum mechanics beyond Hilbert space' has been given by Antoine in [3], and rigged Hilbert spaces have also appeared recently in several papers by de la Madrid, Gadella, Gomez and Bohm [7, 8, 10].

On the other hand, it seems to us that the second problem has been treated less thoroughgoingly in the physics literature, in spite of its obvious importance. We mention that an explicit proof of completeness (under some mild integrability assumptions on the potentials) has been given by Newton in the classical paper [16], and also that some proofs—of varied levels of rigor—of the completeness of the hydrogen atom appear in [12, 14, 15]. Now, completeness, as understood by Dirac [9], can be thought of as a generalization of the standard theory of Fourier expansions, and such a generalization has been developed in the context of Sturm–Liouville problems by several mathematicians since the beginning of the 20th century (see Weyl [21], Kodaira [12] and Titchmarsh [20], and also Stone [18]). In this paper we stress on the fact that this Weyl–Titchmarsh–Kodaira theory basically solves the completeness problem, a point of view previously considered by Newton in [16]. Specifically, we use [12, 20, 21] to present rigorous proofs of the completeness of the 'generalized eigenstates' associated with a Hamiltonian of a free particle moving under the influence of the step and well potentials in one-dimensional quantum mechanics. We consider these cases to be of interest, because they illustrate how formal proofs proceed in the case of continuous spectrum and also when bound states are present.

The remainder of this paper is organized in two sections. Section 2 is a review of the Weyl–Titchmarsh–Kodaira theorem [5, 6, 12, 19–21]. We have included a rather detailed discussion of this result since it is not usually cited in the literature. Our examples of the step and well potentials are developed in section 3.

2. The Weyl–Titchmarsh–Kodaira completeness theorem

In this section we summarize some aspects of the Weyl–Kodaira–Titchmarsh theory, using as our main sources Kodaira's classical paper [12] on the completeness of eigenfunction expansions for the Schrödinger operator, the standard treatises [5, 6] and the recent textbook [19].

We begin with the Sturm–Liouville operator

$$L = -\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + q(x), \tag{1}$$

in which we assume that the variable x belongs to an interval (a, b) with $-\infty \leqslant a < b \leqslant +\infty$, and that $p(x)$ and $q(x)$ are real-valued functions on (a, b) satisfying the following conditions:

(a) $p(x) > 0$ for all $x \in (a, b)$;
(b) $p(x)$ and $p'(x)$ are continuous;
(c) $q(x) \in L^1_{\mathrm{loc}}(a, b)$, that is, $q(x)$ is integrable over finite subintervals of (a, b).

The Weyl–Titchmarsh–Kodaira theorem can be proven under less restrictive conditions on the function $p(x)$, see [5, p 224] and [19], but we will not require this higher level of generality.

Definition 1. *Let l_0 be an arbitrary complex number, and c some real number between a and b. If every solution $u(x)$ of $L(u) = l_0\, u$ is in $L^2(a, c]$ (respectively, in $L^2[c, b)$) we say that the operator L is of limit circle type at a (respectively, of limit circle type at b). Otherwise, we say that L is of limit point type at a (respectively, of limit point type at b).*

This definition depends only on the operator L and not on the complex number l_0. Indeed, a theorem due to Weyl (see [12, p 922], [5, p 225] and [19, chapter 9]) states that if every solution $u(x)$ of $L(u) = l_0\, u$ is in $L^2(a, c]$ for some complex number l_0 (respectively, in $L^2[c, b)$), then *for arbitrary* $l \in \mathbb{C}$, every solution $u(x)$ of $L(u) = lu$ is in $L^2(a, c]$ (respectively, in $L^2[c, b)$).

We denote by $AC_{\text{loc}}(a, b)$ the space of all functions $u : (a, b) \to \mathbb{R}$ such that u can be written as the integral of a locally integrable function, so that, in particular, if $u \in AC_{\text{loc}}(a, b)$ then its derivative u' exists almost everywhere [19]. We consider L as a linear operator on $L^2(a, b)$ by specifying its domain as follows:

$$\mathcal{D}(L) = \{u \in L^2(a, b) : u, u' \in AC_{\text{loc}}(a, b) \text{ and } Lu \in L^2(\mathbb{R})\}. \tag{2}$$

The operator L with domain $D(L)$ (we abbreviate this phrase by writing simply $(L, D(L))$ in what follows) is symmetric and closed. *Moreover*, L is of limit point type at a and at b, *if and only if* it is self-adjoint (see [12, p 923]). Thus, in view of the applications we have in mind, we hereafter consider only the limit point case.

Definition 2. *A system of fundamental solutions to $L(u) = lu$, $l \in \mathbb{C}$, is a pair of solutions $s_1(x, l)$, $s_2(x, l)$ such that*

(1) $[s_1, s_2] = p(x)(s_1(x, l)s_2'(x, l) - s_2(x, l)s_1'(x, l)) = 1$, in which $s_k'(x, l)$ denotes the derivative with respect to x;
(2) $s_k(x, \bar{l}) = \overline{s_k(x, l)}$, $k = 1, 2$;
(3) $s_k(x, l)$ and $s_k'(x, l)$ are analytic (as functions of l) on the whole complex plane.

Since we are considering exclusively the limit point case, the functions s_1 and s_2 cannot be both elements of $L^2((a, b))$. We also point out that such a system of solutions is certainly not unique. A particular choice of a system of fundamental solutions is obtained, for example, by solving $L(u) = lu$, $l \in \mathbb{C}$, with boundary conditions

$$s_1(c) = s_2'(c) = 0, \qquad s_2(c) = s_1'(c) = 1,$$

for an arbitrary point $c \in (a, b)$. That this boundary value problem possesses a unique solution is stated for example in [19, chapter 9]. Moreover, we have the following easy proposition.

Proposition 1. *If $u(x)$ solves the Schrödinger equation*

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}u + q(x)u = lu, \qquad l \in \mathbb{C}, \tag{3}$$

in which $q \in L^1_{\text{loc}}(a, b)$, then u and u' are continuous.

Thus, if the function $q(x)$ in (1) is discontinuous (as in the well and step potential examples) and we wish to find s_1, s_2 explicitly, this proposition tells us that s_1, s_2 must satisfy some matching conditions at the discontinuity points of $q(x)$ in addition to the properties appearing in definition 2.

The fundamental solutions s_1, s_2 are *generalized eigenfunctions* in the sense of Gelfand and Vilenkin [11]. That is, they can be considered as 'weak eigenfunctions of the eigenvalue problem $L(u) = lu$, $l \in \mathbb{C}$: for any $\phi \in \mathcal{D}(L)$, the identity

$$\langle s_i, L\phi\rangle = \langle s_i, l\phi\rangle, \qquad i = 1, 2,$$

holds, in which $\langle\ \rangle$ indicates L^2 pairing. Theorem 2 (equation (12) below) tells us precisely what it means for these generalized eigenfunctions to be a complete set.

Now we consider the self-adjoint operator $(L, D(L))$ and define the *characteristic functions*

$$f_b(l) = -\lim_{x\to b} \frac{s_2(x,l)}{s_1(x,l)}, \tag{4}$$

$$f_a(l) = -\lim_{x\to a} \frac{s_2(x,l)}{s_1(x,l)}. \tag{5}$$

An important observation due to Weyl (see [12, p 925]) is the fact that the characteristic functions are *uniquely determined* by the conditions

$$\int_c^b |s_2(x,l) + f_b(l)s_1(x,l)|^2\,\mathrm{d}x < +\infty$$

and

$$\int_a^d |s_2(x,l) + f_a(l)s_1(x,l)|^2\,\mathrm{d}x < +\infty,$$

in which $c, d \in (a, b)$. We also have the conjugation properties $f_a(\bar{l}) = \overline{f_a(l)}$ and $f_b(\bar{l}) = \overline{f_b(l)}$, and we also note that $f_a(l) \neq f_b(l)$ for $\mathrm{Im}(l) \neq 0$ since L is self-adjoint. We quote from [5, p 229]

Theorem 1. *The characteristic functions $f_a(l)$ and $f_b(l)$ are analytic on $\mathrm{Im}(l) \neq 0$, and if they have poles on the real axis, the poles are simple.*

With these preliminaries, we can state the Weyl–Titchmarsh–Kodaira theorem as discussed in Kodaira's classic paper [12, p 925] (see also [5, 19]). Let us define the *characteristic matrix* $M(l) = (M_{jk}(l))$ as

$$M_{11}(l) = \frac{f_a(l) f_b(l)}{f_a(l) - f_b(l)}, \tag{6}$$

$$M_{12}(l) = M_{21}(l) = \frac{1}{2}\frac{f_a(l) + f_b(l)}{f_a(l) - f_b(l)}, \tag{7}$$

$$M_{22}(l) = \frac{1}{f_a(l) - f_b(l)}. \tag{8}$$

This matrix allows us to define a matrix measure $(\rho_{i,j}(\lambda))$ which, in turn, determines a 'generalized Fourier transform', as the following theorem shows.

Theorem 2. *Let $(L, D(L))$ be the self-adjoint operator introduced above; assume that L has the spectral representation*

$$L = \int_{-\infty}^{+\infty} \lambda\,\mathrm{d}E(\lambda), \tag{9}$$

and let us consider the characteristic matrix $M(l) = (M_{jk}(l))$ defined in (6)–(8).

(1) Then, for every $\lambda \in \mathbb{R}$, there exists the limit

$$\rho_{jk}(\lambda) = \lim_{\delta\to 0^+}\lim_{\epsilon\to 0^+} \frac{1}{\pi}\int_\delta^{\lambda+\delta} \mathrm{Im}(M_{jk}(t + \mathrm{i}\epsilon))\,\mathrm{d}t, \qquad j, k = 1, 2. \tag{10}$$

(2) *The matrix* $P(\lambda) = (\rho_{ij}(\lambda))$ *is continuous on the right and it satisfies the following monotonicity property: for* $\mu < \lambda$*, the matrix* $P(\lambda) - P(\mu)$ *is positive semi-definite.*

(3) *Set* $E(\Delta) = E(\lambda) - E(\mu)$ *for any finite interval* $\Delta = (\mu, \lambda]$*. Then, for any* $u \in L^2(a, b)$*, the spectral projection* $E(\Delta)u(x)$ *can be represented as*

$$E(\Delta)u(x) = \int_a^b u(y)\,\mathrm{d}y \int_\Delta \sum_{j,k=1}^{2} s_j(x,\lambda)s_k(y,\lambda)\,\mathrm{d}\rho_{jk}(\lambda). \tag{11}$$

This integral converges absolutely, and moreover,

$$\int_a^b \mathrm{d}y \left| \int_\Delta \sum_{j,k=1}^{2} s_j(x,\lambda)s_k(y,\lambda)\,\mathrm{d}\rho_{jk}(\lambda) \right|^2 < \infty.$$

(4) *For any* $u \in L^2(a, b)$ *we have the representation*

$$u(x) = \int_a^b u(y)\,\mathrm{d}y \int_{-\infty}^{+\infty} \sum_{j,k=1}^{2} s_j(x,\lambda)s_k(y,\lambda)\,\mathrm{d}\rho_{jk}(\lambda), \tag{12}$$

in which the limits are taken in the sense of $L^2(a, b)$*.*

Equation (12) allows us to obtain a generalized Fourier transform $u \mapsto \mathcal{F}(u)$ from $L^2(a, b)$ onto a Hilbert space $\overline{\mathcal{H}}$ which we now define. Consider the space of vector-valued measurable functions $\phi(\lambda) = (\phi_1(\lambda), \phi_2(\lambda))$ such that $\phi_j \in L^2(\mathbb{R})$, for $j \in \{1, 2\}$, and set

$$\|\phi\|^2_{\overline{\mathcal{H}}} = \int_{-\infty}^{+\infty} \sum_{j,k=1}^{2} \phi_j(\lambda)\overline{\phi_k(\lambda)}\,\mathrm{d}\rho_{jk}(\lambda).$$

Item (ii) in theorem 2 implies that $\|\phi\|^2_{\overline{\mathcal{H}}} \geqslant 0$, and we can define the Hilbert space $\overline{\mathcal{H}}$ as

$$\overline{\mathcal{H}} = \{\phi = (\phi_1, \phi_2) : \|\phi\|_{\overline{\mathcal{H}}} < \infty\}.$$

This is the space which allows us to define a generalized Fourier transform. Indeed, if we set

$$\widetilde{u}_k(\lambda) = \int_a^b s_k(y,\lambda)u(y)\,\mathrm{d}y, \qquad k \in \{1, 2\},$$

then the vector-valued function $(\mathcal{F}(u))(\lambda) = (\widetilde{u}_1(\lambda), \widetilde{u}_2(\lambda))$ is well defined as an element of $\overline{\mathcal{H}}$. We can then re-write equation (12) as

$$u(x) = \int_{-\infty}^{+\infty} \sum_{j,k=1}^{2} s_j(x,\lambda)\widetilde{u}_k(\lambda)\,\mathrm{d}\rho_{jk}(\lambda), \tag{13}$$

in which the convergence is assumed to be in the L^2 sense. Then, the following theorem holds [12, p 928].

Theorem 3. *The transformation* $\mathcal{F}$ *is a unitary transformation from* $L^2(a, b)$ *onto* $\overline{\mathcal{H}}$*, and its inverse is given by*

$$\mathcal{F}^{-1}(\phi_1, \phi_2)(x) = \int_{-\infty}^{+\infty} \sum_{j,k=1}^{2} s_j(x,\lambda)\phi_k(\lambda)\,\mathrm{d}\rho_{jk}(\lambda).$$

Remark 4. It is not always easy to compute either the entries of the characteristic matrix M or the spectral measure ρ_{ij}. One way to do this is by using Green's functions; see for instance

[7]. On the one hand [6, theorem XIII.5.18], there exist analytic functions $\theta_{ij}^{\pm}$ such that the Green's function of the eigenvalue problem (3) is given by

$$G(x,x',l)=\begin{cases}\sum_{i,j=1,2}\theta_{ij}^{-}(l)S_i(x,l)\overline{S_j(x',\bar{l})} & x<x'\\ \sum_{i,j=1,2}\theta_{ij}^{+}(l)S_i(x,l)\overline{S_j(x',\bar{l})} & x>x',\end{cases} \tag{14}$$

in which S_1, S_2 are fundamental solutions as in definition 2, but we do not insist that they satisfy the normalization condition $[S_1,S_2]=1$. In this case we have

$$\rho_{jk}((a,b))=\lim_{\delta\to0}\lim_{\epsilon\to0+}\frac{1}{2\pi\mathrm{i}}\int_{a+\delta}^{b-\delta}[\theta_{jk}^{-}(s-\mathrm{i}\epsilon)-\theta_{jk}^{-}(s+\mathrm{i}\epsilon)]\,\mathrm{d}s \tag{15}$$

$$=\lim_{\delta\to0}\lim_{\epsilon\to0+}\frac{1}{2\pi\mathrm{i}}\int_{a+\delta}^{b-\delta}\left[\theta_{jk}^{+}(s-\mathrm{i}\epsilon)-\theta_{jk}^{+}(s+\mathrm{i}\epsilon)\right]\mathrm{d}s. \tag{16}$$

On the other hand, it is well known [7, 12, 19] that

$$G(x,x';l)=\frac{(2m/\hbar^2)}{W(S_1,S_2)}\begin{cases}S_2(x,l)S_1(x',l) & x<x'\\ S_2(x',l)S_1(x,l) & x>x',\end{cases} \tag{17}$$

so that by uniqueness, we can compute $\rho_{ij}((a,b))$ straightforwardly comparing (14) and (17).

3. Applications: completeness of the energy

3.1. The step potential

Let a, $V_0>0$ and consider the Hamiltonian

$$H=-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+V(x), \tag{18}$$

defined on $L^2(\mathbb{R})$, where $V(x)=V_0$ for $-a\leqslant x\leqslant a$ and $V(x)=0$ elsewhere. Here we assume that $\mathcal{D}(H)$ is the maximal domain of self-adjointness, that is,

$$\mathcal{D}(H)=\{f,f'\in AC_{\mathrm{loc}}(\mathbb{R}):Hf\in L^2(\mathbb{R})\}$$

as in (2). We consider the eigenvalue problem

$$H\varphi(x,k)=l\varphi(x,k), \tag{19}$$

where $k^2=\frac{2m}{\hbar^2}l$. We set $\eta(k):=\left(\frac{2mV_0}{\hbar^2}-k^2\right)^{1/2}$, and we define

$$\theta(k):=ka+\tan^{-1}\left(\frac{k}{\eta(k)}\tanh(\eta(k)a)\right)\quad\text{and}\quad\phi(k):=ka-\tan^{-1}\left(\frac{\eta(k)}{k}\tanh(\eta(k)a)\right).$$

Then a set of fundamental solutions for the eigenvalue equation (19) is given by

$$s_1(x,k)=\begin{cases}A(k)\sin(kx-\theta(k)) & x<-a\\ B(k)\sinh(\eta(k)x) & |x|\leqslant a\\ A(k)\sin(kx+\theta(k)) & x>a,\end{cases}$$

in which the matching conditions imposed by proposition 1 led us to define $A(k)=\frac{1}{\eta(k)}\left(\sinh^2(ka)+\left(\frac{\eta(k)}{k}\right)^2\cosh^2(ka)\right)^{1/2}$ and $B(k)=1/\eta(k)$, and

$$s_2(x,k)=\begin{cases}C(k)\cos(kx-\phi(k)) & x<-a\\ D(k)\cosh(\eta(k)x) & |x|\leqslant a\\ C(k)\cos(kx+\phi(k)) & x>a,\end{cases}$$

where, again because of proposition 1,

$$C(k) = \left(\cosh^2(\eta(k)a) + \left(\frac{\eta(k)}{k}\right)^2 \sinh^2(\eta(k)a)\right)^{1/2}$$

and $D(k) = 1$.

We now apply the Weyl–Titchmarsh–Kodaira theory. Recalling (4), (5), we have that the characteristic functions are defined as

$$f_\infty(k) = -\lim_{x\to\infty} \frac{s_2(x,k)}{s_1(x,k)} \qquad \text{and} \qquad f_{-\infty}(k) = -\lim_{x\to-\infty} \frac{s_2(x,k)}{s_1(x,k)}. \tag{20}$$

In our case we have

$$f_\infty(k) = \begin{cases} \mathrm{i}\frac{C(k)}{A(k)}\,\mathrm{e}^{\mathrm{i}(\phi(k)-\theta(k))}, & \mathrm{Im}(k) > 0 \\ -\mathrm{i}\frac{C(k)}{A(k)}\,\mathrm{e}^{-\mathrm{i}(\phi(k)-\theta(k))}, & \mathrm{Im}(k) < 0 \end{cases} \tag{21}$$

and

$$f_{-\infty}(k) = \begin{cases} -\mathrm{i}\frac{C(k)}{A(k)}\,\mathrm{e}^{\mathrm{i}(\phi(k)-\theta(k))}, & \mathrm{Im}(k) > 0 \\ \mathrm{i}\frac{C(k)}{A(k)}\,\mathrm{e}^{-\mathrm{i}(\phi(k)-\theta(k))}, & \mathrm{Im}(k) < 0. \end{cases} \tag{22}$$

We note that $f_\infty(k) = -f_{-\infty}(k)$ for $k \neq 0$.

Next, we compute the characteristic matrix $M(k) = M_{ij}(k)$ following (6)–(8). We find that

$$M_{11}(k) = \frac{f_\infty(k) f_{-\infty}(k)}{f_{-\infty}(k) - f_\infty(k)} = \frac{\mathrm{i}}{2}\frac{C(k)}{A(k)}\,\mathrm{e}^{\mathrm{i}(\phi(k)-\theta(k))} \tag{23}$$

$$M_{12}(k) = M_{21}(k) = \frac{1}{2}\frac{f_{-\infty}(k) + f_\infty(k)}{f_{-\infty}(k) - f_\infty(k)} = 0 \tag{24}$$

$$M_{22}(k) = \frac{1}{f_{-\infty}(k) - f_\infty(k)} = \frac{\mathrm{i}}{2}\frac{A(k)}{C(k)}\,\mathrm{e}^{-\mathrm{i}(\phi(k)-\theta(k))}, \tag{25}$$

and we can state two 'Fourier transform'-type results as corollaries of the general theorems of the previous section.

Theorem 5. *Let H be the second-order differential operator on $L^2(\mathbb{R})$ defined by (18) with the matrix measure $(\rho_{ij}(\lambda))$, $\lambda \in \mathbb{R}$. Set for $u \in L^2(\mathbb{R})$,*

$$\widetilde{u}_j(\lambda) = \int_{-\infty}^{\infty} s_j(y,\lambda) u(y)\,\mathrm{d}y, \qquad j \in \{1,2\}.$$

Then $\lambda \mapsto \widetilde{u}_1(\lambda)$ is an odd function and $\lambda \mapsto \widetilde{u}_2(\lambda)$ is an even function. Furthermore, the map $\mathcal{F}u = (\widetilde{u}_1, \widetilde{u}_2)$ is a unitary operator from $L^2(\mathbb{R})$ onto $L^2([0,\infty), \mathrm{d}\rho_{1,1}) \oplus L^2([0,\infty), \mathrm{d}\rho_{2,2})$.

Proof. In order to compute the density functions $\rho_{ij}(\lambda)$, we apply (10) to the characteristic matrix $M_{ij}(k)$ that we found above; we shall always assume that $\mathrm{Im}(k) > 0$. First we see that

$$\frac{C(k)}{A(k)} = \frac{(\eta^2 + k^2)\cosh^2(\eta a) - k^2}{(\eta^2 + k^2)\sinh^2(\eta a) + k^2} = \frac{(2mV_0/\hbar^2)\cosh^2(\eta a) - k^2}{(2mV_0/\hbar^2)\sinh^2(\eta a) + k^2}.$$

Then we note that $C(k)/A(k)$ and $A(k)/C(k)$ are continuous with finite limit when $k \to 0$. Therefore, for $s \in [0,t]$ the sequence of functions

$$M_{1,1}(s + \mathrm{i}\epsilon) = \mathrm{i}\frac{C(s+\mathrm{i}\epsilon)}{2A(s+\mathrm{i}\epsilon)}\,\mathrm{e}^{\mathrm{i}(\phi(s+\mathrm{i}\epsilon)-\theta(s+\mathrm{i}\epsilon)}$$

are continuous and uniformly bounded on ϵ. Moreover, from the fact that the pointwise limit $\lim_{\epsilon\to 0^+} M_{1,1}(s+\mathrm{i}\epsilon) = \mathrm{i}\frac{C(s)}{2A(s)}\,\mathrm{e}^{\mathrm{i}(\phi(s)-\theta(s))}$, it follows that

$$m_1(s) := \lim_{\epsilon\to 0^+} \mathrm{Im}(M_{1,1}(s+\mathrm{i}\epsilon)) = \frac{C(s)}{2A(s)}\mathrm{Im}(\mathrm{i}\,\mathrm{e}^{\mathrm{i}(\phi(s)-\theta(s))}).$$

Thus,

$$m_1(s) = \frac{C(s)}{2A(s)}\cos(\phi(s)-\theta(s)),$$

since $C(k)/A(k)$ is real when $k = s \in \mathbb{R}$. But then,

$$\rho_{11}(t) = \frac{1}{\pi}\int_0^t \mathrm{Im}(M_{11}(s))\,\mathrm{d}s = \frac{1}{\pi}\int_0^t m_1(s)\,\mathrm{d}s$$

and

$$\mathrm{d}\rho_{11}(t) = \frac{1}{2\pi}\left(\frac{C(t)}{A(t)}\cos(\phi(t)-\theta(t))\right)\mathrm{d}t = \frac{1}{\pi}m_1(t)\,\mathrm{d}t.$$

On the other hand,

$$m_2(t) := \mathrm{Im}(M_{22}(t)) = \frac{1}{2\pi}\frac{A(t)}{C(t)}\cos(\phi(t)-\theta(t)),$$

and so by the same reasoning as above we obtain that

$$\mathrm{d}\rho_{22}(t) = \frac{1}{2\pi}\left(\frac{A(t)}{C(t)}\cos(\phi(t)-\theta(t))\right)\mathrm{d}t = \frac{1}{\pi}m_2(t)\,\mathrm{d}t.$$

Next we remark that the function $\lambda \mapsto s_1(y,\lambda)$ is an odd function and $\lambda \mapsto s_2(y,\lambda)$ an even function, and consequently $\widetilde{u}_1(\lambda)$ and $\widetilde{u}_2(\lambda)$ are odd and even functions respectively since they are defined in terms of the fundamental solutions $s_1(y,\lambda)$, $s_2(y,\lambda)$ for the eigenvalue equation (19). Thus, both functions $\widetilde{u}_1(\lambda)$ and $\widetilde{u}_2(\lambda)$ can be assumed to be defined only on the half line $[0,\infty)$. Then by theorem 3 the generalized Fourier transform $\mathcal{F}u = (\widetilde{u}_1, \widetilde{u}_2)$ maps $L^2(\mathbb{R})$ onto $L^2([0,\infty), \mathrm{d}\rho_{1,1}) \oplus L^2([0,\infty), \mathrm{d}\rho_{2,2})$ as a unitary operator. □

Theorem 6. *Let $(\rho_{i,j}(\lambda))$ be the matrix measure associated with the self-adjoint operator H. Then for every $u \in L^2(\mathbb{R})$ the asymptotic expansion holds:*

$$u(x) = \frac{2}{\pi}\left(\int_0^\infty s_1(x,t)\widetilde{u}_1(t)m_1(t)\,\mathrm{d}t + \int_0^\infty s_2(x,t)\widetilde{u}_2(t)m_2(t)\,\mathrm{d}t\right). \qquad (26)$$

Furthermore,

$$\int_{-\infty}^\infty |u(s)|^2 ds = \frac{2}{\pi}\int_0^\infty (|\widetilde{u}_1(t)|^2 m_1(t) + |\widetilde{u}_2(t)|^2 m_2(t))\,\mathrm{d}t. \qquad (27)$$

Proof. From the inversion formula (13) in addition to the fact that $m_i(-t) = m_i(t)$ and $\mathrm{d}\rho_{i,i}(-t) = -m_i(t)\,\mathrm{d}t$ for $t \in \mathbb{R}$, this shows the first identity. Now the second statement follows from the preceding theorem. □

3.2. The well potential

We now study the completeness of the (generalized) eigenstates of the Hamiltonian of quantum mechanics for a particle moving in a one-dimensional well potential.

Let $a, V_0 > 0$ and consider the Hamiltonian

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x), \tag{28}$$

where $V(x) = -V_0$ for $-a \leqslant x \leqslant a$ and $V(x) = 0$ elsewhere. Here we assume that $\mathcal{D}(H)$ is the maximal domain of self-adjointness, that is,

$$\mathcal{D}(H) = \{f, f' \in AC_{\mathrm{loc}}(\mathbb{R}) : Hf \in L^2(\mathbb{R})\},$$

as in (2). We consider the eigenvalue problem

$$H\varphi(x,k) = l\varphi(x,k), \tag{29}$$

and we define $k = (2ml)^{1/2}/\hbar$ and $q = (2m(l+V_0))^{1/2}/\hbar$.

Theorem 7. *A set of fundamental solutions of the eigenvalue equation (29) is given by*

$$S_l(x,E) = \begin{cases} I\,\mathrm{e}^{\mathrm{i}kx} + R(k)\,\mathrm{e}^{-\mathrm{i}kx} & x \leqslant -a \\ A(q)\,\mathrm{e}^{\mathrm{i}qx} + B(q)\,\mathrm{e}^{-\mathrm{i}qx} & |x| \leqslant a \\ T(k)\,\mathrm{e}^{\mathrm{i}kx} & x \geqslant a \end{cases} \tag{30}$$

and

$$S_r(x,E) = \begin{cases} T(k)\,\mathrm{e}^{-\mathrm{i}kx} & x \leqslant -a \\ A(q)\,\mathrm{e}^{-\mathrm{i}qx} + B(q)\,\mathrm{e}^{\mathrm{i}qx} & |x| \leqslant a \\ R(k)\,\mathrm{e}^{-\mathrm{i}kx} + \mathrm{e}^{-\mathrm{i}kx} & x \geqslant a, \end{cases} \tag{31}$$

where the coefficients $I, A(q), B(q), R(k), T(k)$ are to be found by using matching conditions at $x = \pm a$ guaranteeing that the Schrödinger equation is fulfilled in the whole real axis. The subscripts r and l stand for the square integrability of the wavefunction $S_{l,r}$ at $x = \pm\infty$ respectively.

The proof of theorem 7 is straightforward, except by the matching condition part. In order to obtain explicit expressions for the fundamental solutions S_l and S_r on the whole complex plane $l \in \mathbb{C}$, we have to define them by pieces, in the first and fourth quadrants, and in the $\mathrm{Re}(l) < 0$ half-plane.

(1) Scattering states: $\mathrm{Re}(l) > 0$.

(a) First quadrant: $\mathrm{Im}(l) \geqslant 0$. The fundamental solutions can be written as

$$S_l(x,l) = \begin{cases} \mathrm{e}^{\mathrm{i}kx} + R(k)\,\mathrm{e}^{-\mathrm{i}kx} & x \leqslant -a \\ A(q)\,\mathrm{e}^{\mathrm{i}qx} + B(q)\,\mathrm{e}^{-\mathrm{i}qx} & |x| \leqslant a \\ T(k)\,\mathrm{e}^{\mathrm{i}kx} & x \geqslant a \end{cases} \tag{32}$$

$$S_r(x,l) = \begin{cases} T(k)\,\mathrm{e}^{-\mathrm{i}kx} & x \leqslant -a \\ A(q)\,\mathrm{e}^{-\mathrm{i}qx} + B(q)\,\mathrm{e}^{\mathrm{i}qx} & |x| \leqslant a \\ R(k)\,\mathrm{e}^{\mathrm{i}kx} + \mathrm{e}^{-\mathrm{i}kx} & x \geqslant a. \end{cases} \tag{33}$$

Clearly, $S_{r,l}$ is integrable at $x = \pm\infty$ respectively. We show that the fundamental solutions in the other quadrants can be obtained from the above expressions by using reflection and complex conjugation, that is, discrete symmetries of the Schrödinger equation.

(b) Fourth quadrant: $\mathrm{Im}(l) \leqslant 0$. We note that this region is the complex conjugated of the above one in the complex l-plane. We therefore obtain the fundamental solutions by taking complex conjugation in equations (32) and (33), namely

$$S_l(x,l) = \begin{cases} \mathrm{e}^{-\mathrm{i}kx} + \overline{R}(k)\,\mathrm{e}^{\mathrm{i}kx} & x \leqslant -a \\ \overline{A}(q)\,\mathrm{e}^{-\mathrm{i}qx} + \overline{B}(q)\,\mathrm{e}^{\mathrm{i}qx} & |x| \leqslant a \\ \overline{T}(k)\,\mathrm{e}^{-\mathrm{i}kx} & x \geqslant a \end{cases} \tag{34}$$

and

$$S_r(x,l) = \begin{cases} \overline{T}(k)\,\mathrm{e}^{\mathrm{i}kx} & x \leqslant -a \\ \overline{A}(q)\,\mathrm{e}^{\mathrm{i}qx} + \overline{B}(q)\,\mathrm{e}^{-\mathrm{i}qx} & |x| \leqslant a \\ \overline{R}(k)\,\mathrm{e}^{-\mathrm{i}kx} + \mathrm{e}^{\mathrm{i}kx} & x \geqslant a. \end{cases} \tag{35}$$

(2) Bound states: $\mathrm{Re}(l) < 0$. In this case we perform the transformation $k \longrightarrow \mathrm{i}K$, with $K = \sqrt{-2ml}/\hbar$, in equations (32) and (33). In other words, for a real value of $l < 0$ we make an analytical continuation of the variable k. The fundamental solutions read

$$S_l(x,l) = \begin{cases} \mathrm{e}^{-Kx} + R(\mathrm{i}K)\,\mathrm{e}^{Kx} & x \leqslant -a \\ A(q)\,\mathrm{e}^{\mathrm{i}qx} + B(q)\,\mathrm{e}^{-\mathrm{i}qx} & |x| \leqslant a \\ T(\mathrm{i}K)\,\mathrm{e}^{-Kx} & x \geqslant a \end{cases} \tag{36}$$

and

$$S_r(x,l) = \begin{cases} T(\mathrm{i}K)\,\mathrm{e}^{Kx} & x \leqslant -a \\ A(q)\,\mathrm{e}^{-\mathrm{i}qx} + B(q)\,\mathrm{e}^{\mathrm{i}qx} & |x| \leqslant a \\ R(\mathrm{i}K)\,\mathrm{e}^{-Kx} + \mathrm{e}^{Kx} & x \geqslant a. \end{cases} \tag{37}$$

Now we use the matching conditions at $x = \pm a$ and we find all of the coefficients appearing in (32)–(37). The reflection and transmission coefficients are given by

$$\begin{aligned} T(k) &= \frac{\mathrm{e}^{-2\mathrm{i}ka}}{\left[\cos 2qa - \frac{\mathrm{i}}{2}\left(\frac{k}{q} + \frac{q}{k}\right)\sin 2qa\right]} \\ R(k) &= \frac{\mathrm{i}}{2}\left(\frac{q}{k} - \frac{k}{q}\right)\sin 2qa \frac{\mathrm{e}^{-2\mathrm{i}ka}}{\left[\cos 2qa - \frac{\mathrm{i}}{2}\left(\frac{k}{q} + \frac{q}{k}\right)\sin 2qa\right]}. \end{aligned} \tag{38}$$

We do not display the coefficients $A(q)$ and $B(q)$ explicitly because they are not relevant for our analysis of completeness. For instance, we recall from section 2 that the characteristic matrix depends only on the asymptotic behavior of the solutions S_l and S_r near $\pm\infty$. As a consistency test, we note that the reflection and transmission coefficients fulfill the condition

$$|R(k)|^2 + |T(k)|^2 = 1, \tag{39}$$

an identity which guarantees the conservation of the probability current.

We also observe that $S_r(x,l)$ is the reflection of $S_l(x,l)$ about $x = 0$, that is, $S_r(x,l) = S_l(-x,l)$. The Wronskian of S_r and S_l is given by $W(S_r, S_l) = 2\mathrm{i}kT(k)$ and, if we compare the solutions from the first quadrant, which we will identify by a superscript '+', with the one corresponding to the fourth quadrant, denoted by a '−' superscript, we find the relations

$$\overline{S_l^+(x,\bar{l})} = S_l^-(x,l) \tag{40}$$

and

$$\overline{S_r^+(x,\bar{l})} = S_r^-(x,l), \tag{41}$$

which we will use later.

From now on we will use E instead of l to denote the (generalized) eigenvalue of equation (29), in order to emphasize its physical meaning of the eigenvalue as energy, although E continues being a complex number. Now we are prepared to use the techniques of the previous section in order to obtain the completeness of our generalized eigenfunctions. In this particular example, it is simpler to compute the spectral measure by using the Green's function, as explained in remark 4. We have

$$G(x,x';E) = \frac{2m/\hbar^2}{W(S_r,S_l)} \begin{cases} S_r(x,E)S_l(x',E) & x < x' \\ S_r(x',E)S_l(x,E) & x > x' \end{cases} \tag{42}$$

and we choose our fundamental solutions to be

$$\sigma_1(x,E) = S_l^+(x,E) \qquad \sigma_2(x,E) = S_r^+(x,E). \tag{43}$$

After a straightforward computation we find

$$T\overline{S_l^+(x',\bar{E})} - \frac{T\bar{R}}{\bar{T}}\overline{S_r^+(x',\bar{E})} = TS_l^-(x',E) - \frac{T\bar{R}}{\bar{T}}S_r^-(x',E), \tag{44}$$

and we conclude that the following identities hold:

$$T\overline{S_l^+(x',\bar{E})} - \frac{T\bar{R}}{\bar{T}}\overline{S_r^+(x',\bar{E})} = S_r^+(x',E), \tag{45}$$

$$-\frac{\bar{T}R}{T}\sigma_1(x,E) + \bar{T}\sigma_2(x,E) = S_l^-(x,E). \tag{46}$$

From these identities we can compute the Green's function using equation (42). We obtain

$$G(x,x';E) = \frac{m\,\mathrm{i}}{\hbar^2 k}\left[-\sigma_1(x,E)\overline{\sigma_1(x',\bar{E})} + \frac{\bar{R}}{\bar{T}}\sigma_1(x,E)\overline{\sigma_2(x',\bar{E})}\right] \tag{47}$$

for $\mathrm{Re}(E) > 0$, $\mathrm{Im}(E) > 0$, $x > x'$, and

$$G(x,x';E) = \frac{m\,\mathrm{i}}{\hbar^2 k}\left[-\frac{R}{T}\sigma_1(x,E)\overline{\sigma_2(x',\bar{E})} + \sigma_2(x,E)\overline{\sigma_2(x',\bar{E})}\right] \tag{48}$$

for $\mathrm{Re}(E) > 0$, $\mathrm{Im}(E) < 0$, $x > x'$.

Now we recall remark 4. The Green's function $G'(x,x';E)$ is given by the expression

$$G(x,x';E) = \begin{cases} \sum_{ij}\theta_{ij}^-(E)\sigma_i(x,E)\overline{\sigma_j(x',\bar{E})} & x < x' \\ \sum_{i,j}\theta_{ij}^+(E)\sigma_i(x,E)\overline{\sigma_j(x',\bar{E})} & x > x'. \end{cases} \tag{49}$$

Comparing equations (47) and (48) to equation (49), we get ($\mathrm{Re}(E) > 0$)

$$\begin{aligned} \theta_{i,j}^+(E) &= \begin{pmatrix} -m\,\mathrm{i}/\hbar^2 k & m\,\mathrm{i}/\hbar^2 k\bar{R}/\bar{T} \\ 0 & 0 \end{pmatrix} \qquad \mathrm{Im}(E) > 0 \\ \theta_{i,j}^+(E) &= \begin{pmatrix} 0 & -m\,\mathrm{i}/\hbar^2 kR/T \\ 0 & m\,\mathrm{i}/\hbar^2 k \end{pmatrix} \qquad \mathrm{Im}(E) < 0 \end{aligned} \tag{50}$$

and now we use that (see remark 4) the elements of the matrix measure $\rho_{ij}(E)$ are given by the integral

$$\rho_{ij}([E_1,E_2]) = \lim_{\delta\to 0}\lim_{\epsilon\to 0^+}\frac{1}{2\pi\mathrm{i}}\int_{E_1+\delta}^{E_2-\delta}\mathrm{d}E\left[\theta_{ij}^+(E-\mathrm{i}\epsilon) - \theta_{ij}^+(E+\mathrm{i}\epsilon)\right]. \tag{51}$$

It follows from (50) that $\rho_{21} = 0$, while for ρ_{12} we have

$$\rho_{12}([E_1,E_2]) = \frac{-1}{2\pi\mathrm{i}}\frac{m\,\mathrm{i}}{\hbar^2}\int_{E_1}^{E_2}\mathrm{d}E\,\frac{1}{k}\left(\frac{R}{T} + \frac{\bar{R}}{\bar{T}}\right) = 0. \tag{52}$$

For the other matrix elements, we find

$$\rho_{11}([E_1, E_2]) = \frac{1}{2\pi\mathrm{i}} \int_{E_1}^{E_2} \left[-\left(-\frac{m\,\mathrm{i}}{\hbar^2 k} \right) \right] \mathrm{d}E = \frac{1}{2\pi}(k_2 - k_1), \tag{53}$$

$$\rho_{22}([E_1, E_2]) = \frac{1}{2\pi\mathrm{i}} \int_{E_1}^{E_2} \frac{m\,\mathrm{i}}{\hbar^2 k} \mathrm{d}E = \frac{1}{2\pi}(k_2 - k_1), \tag{54}$$

where we have used that $k_j = (2mE_j)^{1/2}/\hbar$, $j = 1, 2$.

On the other hand, for the second and third quadrants, that is for $\mathrm{Re}(E) < 0$, we proceed analogously by choosing fundamental solutions

$$\sigma_1(x, E) = S_l(x, E) \qquad \sigma_2(x, E) = S_r(x, E), \tag{55}$$

where we have used the expressions given by (48). In this case we have the relations

$$\begin{aligned} \overline{S_l(x, \bar{E})} &= S_l(x, E) \\ \overline{S_r(x, \bar{E})} &= S_r(x, E). \end{aligned} \tag{56}$$

Using the fundamental solutions appearing in (55) we find

$$G(x, x'; E) = \frac{2m}{\hbar^2} \left(\frac{1}{-2KT} \right) \sigma_2(x, E) \overline{\sigma_1(x', \bar{E})} \qquad x < x', \tag{57}$$

which leads us to the matrix (see equation (49))

$$\theta^-_{ij}(E) = \frac{-m}{\hbar^2 KT} \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad \mathrm{Re}(E) < 0. \tag{58}$$

This means that the only non-trivial matrix element of the measure is given by

$$\rho_{21}([E_1, E_2]) = \lim_{\rho\to 0} \lim_{\epsilon\to 0+} \frac{1}{2\pi\mathrm{i}} \int_{E_1+\delta}^{E_2-\delta} \mathrm{d}E \big[\theta^-_{21}(E - \mathrm{i}\epsilon) - \theta^-_{21}(E + \mathrm{i}\epsilon) \big]. \tag{59}$$

In order to compute this element, we divide the region $\mathrm{Re}(E) < 0$ into two pieces. We consider first $\mathrm{Re}(E) \in (-\infty, -V_0)$. In this region $\theta^-_{21}(E)$ is analytic on E, and it follows that ρ_{21} vanishes there.

If $\mathrm{Re}(E) \in (-V_0, 0)$, the situation is different. We note that we can find the poles of the transmission coefficient $T(k)$ (see equation (38)) by making the transformation $k = \mathrm{i}K$. They are given by the condition

$$\cot qa - \tan qa = \mathrm{i}(q/k + k/q), \tag{60}$$

that is,

$$\tan qa = -\mathrm{i}k/q \qquad \cot qa = \mathrm{i}k/q. \tag{61}$$

For $\mathrm{Re}(E) > 0$ there is no solution to the above equations. For $\mathrm{Re}(E) < -V_0$ both k and q are imaginary, in the limit $\mathrm{Im}(E) = 0$, and therefore there is no solution. Nevertheless, in the interval $-V_0 < E < 0$, k is pure imaginary but q is real. In this case, equation (61) leads to

$$\tan qa = \sqrt{\frac{2m}{h^2}}|E|/q \qquad \cot qa = -\sqrt{\frac{2m|E|}{h^2}}/q, \tag{62}$$

where we used that $k = \mathrm{i}\sqrt{\frac{2m(E)}{h^2}}$. Equation (62) corresponds to the conditions for the existence of bound states associated with the even and odd eigenstates of the well potential (see for instance reference [22]).

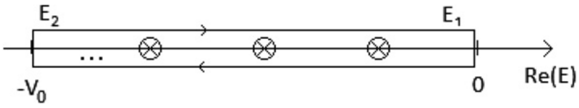

Figure 1. Integration contour corresponding to the integral of equation (63). The crosses circles represent the poles of the transmission coefficient.

The foregoing analysis implies that we need to apply the residue theorem in order to compute correctly ρ_{21} by means of equation (59). We consider the contour $C(\epsilon,\delta)$ of figure 1 and apply the residue theorem:

$$\int_{C(\epsilon,\delta)} \left[\theta_{21}^{-}(E-\mathrm{i}\epsilon)-\theta_{21}^{-}(E+\mathrm{i}\epsilon)\right] = 2\pi\mathrm{i}\sum_{j=1}^{N}\mathrm{Res}\left\{\theta_{21}^{-}(z), z_j\right\}, \tag{63}$$

in which we are assuming that $\theta_{21}^{-}(z)$ has N poles z_j, $j=1,\ldots,N$, given by the solutions to equation (62), lying in $[E_2,E_1]\subseteq[-V_0,0]$. On the other hand,

$$\int_{C(\epsilon,\delta)} \left[\theta_{21}^{-}(E-\mathrm{i}\epsilon)-\theta_{21}^{-}(E+\mathrm{i}\epsilon)\right] = \int_{C_1(\epsilon,\delta)\cup C_2(\epsilon,\delta)} \left[\theta_{21}^{-}(E-\mathrm{i}\epsilon)-\theta_{21}^{-}(E+\mathrm{i}\epsilon)\right]$$
$$+\int_{L_1\cup L_2}\left[\theta_{21}^{-}(E-\mathrm{i}\epsilon)-\theta_{21}^{-}(E+\mathrm{i}\epsilon)\right], \tag{64}$$

where $C_1(\epsilon,\delta)$ and $C_2(\epsilon,\delta)$ denote the upper and lower parts of the curve $C(\epsilon,\delta)$, and L_1 and L_2 the lateral segments. Now, the integral over $L_1\cup L_2$ vanishes when δ and ϵ tend to zero, and therefore we find

$$(2\pi\,\mathrm{i})\rho_{21}([E_1,E_2]) = \lim_{\delta\to0}\lim_{\epsilon\to0+}\int_{C_1(\epsilon,\delta)\cup C_2(\epsilon,\delta)}\left[\theta_{21}^{-}(E-\mathrm{i}\epsilon)-\theta_{21}^{-}(E+\mathrm{i}\epsilon)\right]\mathrm{d}E \tag{65}$$

$$= \lim_{\delta\to0}\lim_{\epsilon\to0+}\int_{C(\epsilon,\delta)}\left[\theta_{21}^{-}(E-\mathrm{i}\epsilon)-\theta_{21}^{-}(E+\mathrm{i}\epsilon)\right]\mathrm{d}E, \tag{66}$$

where equation (65) is simply the definition of ρ_{21}. Therefore, we obtain

$$\rho_{21}([E_1,E_2]) = \sum_j \mathrm{Res}\left\{\theta_{21}^{-}, z_j\right\}, \tag{67}$$

where the values for z_j are given by equation (62). Now we can summarize the foregoing analysis and conclude from the Weyl–Titchmarsh–Kodaira theorem that the following asymptotic expansion is valid for $u\in L^2(-\infty,\infty)$.

Theorem 8. *Let ρ_{ij} be the spectral measure associated with the self-adjoint operator H, and let σ_1, σ_2 be a pair of fundamental solutions for the eigenvalue problem (29). We set*

$$\widetilde{u}_j(E) = \int_{-\infty}^{\infty}\sigma_j(y,E)u(y)\,\mathrm{d}y, \qquad j=1,2.$$

Then,

$$u(x) = \frac{1}{\pi}\int_{-\infty}^{\infty}[\sigma_1(x,E)\widetilde{u}_1(E)+\sigma_2(x,E)\widetilde{u}_2(E)]\chi_{(0,\infty)}(E)\,\mathrm{d}E$$
$$+\sum_{j=1}^{N}\mathrm{Res}\left\{\theta_{21}^{-}, z_j\right\}\sigma_2(z_j)\widetilde{u}_1(z_j). \tag{68}$$

4. Concluding remarks

Completeness of eigenfunctions (for instance, of the energy) is a fundamental issue in Quantum Mechanics not only because it is needed for the consistency of its theoretical construction but also because it is of practical importance. In fact, completeness plays a crucial role in scattering and perturbation theory [9, 16]. Nevertheless, it is a subtle concept when a quantum system has discrete and continuum spectra simultaneously. In this paper, completeness is understood within the framework of the general Weyl–Titchmarsh–Kodaira theorem on the eigenfunction expansion for Sturm–Liouville operators [12, 20, 21]. We apply this theory to two one-dimensional quantum mechanical problems, and we are able to explicitly obtain complete sets of generalized eigenfunctions (representing bound and scattered states). We also show how to expand arbitrary $L^2(\mathbb{R})$ functions with respect to these sets of generalized eigenfunctions.

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