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NON-SELF-ADJOINT SCHRÖDINGER OPERATORS WITH NONLOCAL ONE-POINT INTERACTIONS

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Abstract. We generalize and study, within the framework of quantum mechanics and working with 1-dimensional, manifestly non-Hermitian Hamiltonians $H = -d^2/dx^2 + V$, the traditional class of exactly solvable models with local point interactions $V = V(x)$. We discuss the consequences of the use of nonlocal point interactions such that $(Vf)(x) = \int K(x,s)f(s)\,ds$ by means of the suitably adapted formalism of boundary triplets.

1. Introduction

An important class of Schrödinger operators is formed by operators with singular perturbations. For example, this class contains Schrödinger operators with point interactions. These operators effectively simulate short-range interactions and belong to the class of exactly solvable models. Numerous works have been devoted to the study of singularly perturbed Schrödinger operators, in which a series of approaches to the construction and investigation of such operators are developed (see, e.g., [1], [3] and references therein). These studies, in the majority of cases, deal with symmetric singular perturbations that lead to *self-adjoint* Schrödinger operators.

In the present article, we study *non-self-adjoint* Schrödinger operators with *nonlocal one-point interactions*. This new class of solvable models with point

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interactions has recently been proposed and studied (for the *self-adjoint* case) by Albeverio and Nizhnik [6] (see also [7], [2], [15]). Our interest in the non-self-adjoint case was inspired in part by an intensive development of pseudo-Hermitian ($\mathcal{PT}$-symmetric) quantum mechanics (PHQM/PTQM) in recent decades (see [8], [14], [23]).

Non-self-adjoint point-interaction solvable models (see, e.g., [4], [24], [28]) require a more detailed analysis in comparison with their self-adjoint counterparts. In contrast to the self-adjoint case, one should illustrate a typical PHQM/PTQM evolution of spectral properties which can be obtained by changing the parameters of the model: complex eigenvalues $\to$ spectral singularities; exceptional points $\to$ similarity to a self-adjoint operator. One of the simplest examples of this is the well-studied δ-interaction model $-d^2/dx^2 + a\langle\delta,\cdot\rangle\delta(x)$ with complex parameter $a \in \mathbb{C}$ (see [19], [22], or Section 6 below). However, this model seems to be sufficiently trivial due to the very simple structure of the singular potential that leads to "poor" spectral properties of the corresponding operator-realizations H_a (e.g., the H_a's have no exceptional points and bound states on the continuous spectrum).

One possible reasonable complication of the model consists in the addition of the nonlocal interaction term $\int_{-\infty}^{\infty} K(x,s)f(s)\,ds$. In an attempt to keep the solvability of the model and its intimate relationship with δ-interaction, we assume that

$$K(x,s) = q(x)\delta(s) + \delta(x)q^*(s),$$

where $q \in L_2(\mathbb{R})$ is a given piecewise continuous function. The corresponding nonlocal δ-interaction

$$-\frac{d^2}{dx^2} + a\langle\delta,\cdot\rangle\delta(x) + \langle\delta,\cdot\rangle q(x) + (q,\cdot)\delta(x), \quad a \in \mathbb{C}, \tag{1.1}$$

where $(\cdot,\cdot)$ is the inner product in $L_2(\mathbb{R})$ linear in the second argument, is studied in Section 5 with the use of the boundary triplet technique (see the Appendix). Namely, the formal expression (1.1) gives rise to the family of operators $\{H_a\}$,

$$H_a f = -\frac{d^2 f}{dx^2} + f(0)q(x), \quad a \in \mathbb{C}, q \in L_2(\mathbb{R}) \text{ is fixed}$$

with domains of definition (5.3) which are determined by the singular part of perturbation $a\langle\delta,\cdot\rangle\delta(x) + (q,\cdot)\delta(x)$ in (1.1). Our investigation of $\{H_a\}$ is based on the fact that each operator H_a is the proper extension of the symmetric operator $\widetilde{S}_{\min}$ (5.5); that is, $\widetilde{S}_{\min} \subset H_a \subset \widetilde{S}_{\max}$, where $\widetilde{S}_{\max} = \widetilde{S}_{\min}^{\dagger}$ is the adjoint of $\widetilde{S}_{\min}$ (see Section 5.1).

We show that spectral properties of H_a are completely characterized by the pair $\{a, \widetilde{W}_\lambda\}$, where $a \in \mathbb{C}$ distinguishes H_a among all proper extensions of $\widetilde{S}_{\min}$, while the Weyl–Titchmarsh function $\widetilde{W}_\lambda$ (5.10) characterizes the symmetric operator $\widetilde{S}_{\min}$ which is the "common part" of all H_a's (see Theorems 5.1, 5.4, and 5.7).

One of the interesting features of the model is the fact that $a \in \mathbb{C}$ determines the measure of non-self-adjointness of the operators H_a, while the choice of q defines the symmetric operator $\widetilde{S}_{\min}$ and, therefore, the structure of the holomorphic function $\widetilde{W}_\lambda$. Such a "separation of responsibility" of parameters of the model allows one to preserve its solvability and illustrate the possible appearance of exceptional points and eigenvalues on a continuous spectrum (see Example 5.3 and Section 6).

The proposed approach to the construction of non-self-adjoint nonlocal point interaction models is not restricted to the case of δ-interactions only, and it can be applied to the wider class of ordinary point interaction models. We illustrate this point in Sections 2–4, which are devoted to the general case of one-point interactions, including combinations of δ- and δ'-interactions.

Throughout the present article, $\mathcal{D}(H)$, $\mathcal{R}(H)$, and $\ker H$ denote the domain, range, and null-space of a linear operator H, respectively, while $H\restriction_{\mathcal{D}}$ stands for the restriction of H to the set $\mathcal{D}$. The adjoint of H with respect to the natural inner product $(\cdot,\cdot)$ (linear in the second argument) in $L_2(\mathbb{R})$ is denoted by $H^\dagger$.

2. One-point interactions

2.1. **Ordinary one-point interactions.** A 1-dimensional Schrödinger operator with interactions supported at the point $x=0$ can be defined by the formal expression

$$-\frac{d^2}{dx^2}+a\langle\delta,\cdot\rangle\delta(x)+b\langle\delta',\cdot\rangle\delta(x)+c\langle\delta,\cdot\rangle\delta'(x)+d\langle\delta',\cdot\rangle\delta'(x), \tag{2.1}$$

where δ and δ' are, respectively, the Dirac δ-function and its derivative, the parameters a,b,c,d are complex numbers, and

$$\langle\delta,f\rangle=f(0),\qquad \langle\delta',f\rangle:=-f'(0),\quad \forall f\in W_2^2(\mathbb{R}).$$

Denote

$$\mathbf{T}=\begin{bmatrix} a & b\\ c & d\end{bmatrix}.$$

Then (2.1) can be rewritten in more compact form as

$$-\frac{d^2}{dx^2}+[\delta,\delta']\mathbf{T}\begin{bmatrix}\langle\delta,\cdot\rangle\\ \langle\delta',\cdot\rangle\end{bmatrix}. \tag{2.2}$$

The expression (2.2) determines the symmetric (non-self-adjoint) operator

$$S=-\frac{d^2}{dx^2},\qquad \mathcal{D}(S)=\big\{f\in W_2^2(\mathbb{R}):f(0)=f'(0)=0\big\},$$

in $L_2(\mathbb{R})$, which does not depend on the choice of a,b,c,d. In order to take into account the impact of these parameters, we should extend the action of δ and δ' onto $W_2^2(\mathbb{R}\backslash\{0\})$. The most natural way is

$$\langle\delta,f\rangle:=f_r(0)=\frac{f(0+)+f(0-)}{2},\qquad \langle\delta',f\rangle:=f_r'(0)=-\frac{f'(0+)+f'(0-)}{2}.$$

Furthermore, we assume that the second derivative in (2.2) acts on $W_2^2(\mathbb{R}\backslash\{0\})$ in the distributional sense, that is,

$$-f''=-\big\{f''(x)\big\}_{x\neq0}-f_s(0)\delta'(x)-f_s'(0)\delta(x),\quad f\in W_2^2\big(\mathbb{R}\backslash\{0\}\big),$$

where

$$f_s(0)=f(0+)-f(0-), \qquad f'_s(0)=f'(0+)-f'(0-).$$

Then the action of (2.2) on functions $f\in W_2^2(\mathbb{R}\backslash\{0\})$ can be represented as

$$-\big\{f''(x)\big\}_{x\neq 0}+[\delta,\delta'][\mathbf{T}\Gamma_0 f-\Gamma_1 f], \tag{2.3}$$

where

$$\Gamma_0 f=\begin{bmatrix}\langle\delta,f\rangle\\ \langle\delta',f\rangle\end{bmatrix}=\begin{bmatrix}f_r(0)\\ -f'_r(0)\end{bmatrix}, \qquad \Gamma_1 f=\begin{bmatrix}f'_s(0)\\ f_s(0)\end{bmatrix}.$$

Obviously, (2.3) determines a function from $L_2(\mathbb{R})$ if and only if $\mathbf{T}\Gamma_0 f=\Gamma_1 f$. Therefore, the expression (2.1) gives rise to the operator $-d^2/dx^2$ in $L_2(\mathbb{R})$ with the domain of definition $\{f\in W_2^2(\mathbb{R}\backslash\{0\}):\mathbf{T}\Gamma_0 f-\Gamma_1 f=0\}$.

2.2. **Nonlocal one-point interactions.** Let us generalize the one-point interactions potential considered in (2.1) by adding a nonlocal point interactions part

$$\langle\delta,\cdot\rangle q_1(x)+(q_1,\cdot)\delta(x)+(q_2,\cdot)\delta'(x)+\langle\delta',\cdot\rangle q_2(x),$$

where functions $q_j\in L_2(\mathbb{R})$ are assumed to be piecewise continuous and $(\cdot,\cdot)$ is the standard inner product (linear in the second argument) of $L_2(\mathbb{R})$. Then the generalization of (2.2) takes the form

$$-\frac{d^2}{dx^2}+[\delta,\delta']\left(\mathbf{T}\begin{bmatrix}\langle\delta,\cdot\rangle\\ \langle\delta',\cdot\rangle\end{bmatrix}+\begin{bmatrix}(q_1,\cdot)\\ (q_2,\cdot)\end{bmatrix}\right)+[q_1,q_2]\begin{bmatrix}\langle\delta,\cdot\rangle\\ \langle\delta',\cdot\rangle\end{bmatrix}. \tag{2.4}$$

Extending, by analogy with (2.2), the action of (2.4) onto $W_2^2(\mathbb{R}\backslash\{0\})$ we obtain

$$-\big\{f''(x)\big\}_{x\neq 0}+[\delta,\delta'][\mathbf{T}\Gamma_0 f-\Gamma_1 f]+[q_1,q_2]\Gamma_0 f, \tag{2.5}$$

where

$$\Gamma_0 f=\begin{bmatrix}\langle\delta,f\rangle\\ \langle\delta',f\rangle\end{bmatrix}=\begin{bmatrix}f_r(0)\\ -f'_r(0)\end{bmatrix}, \qquad \Gamma_1 f=\begin{bmatrix}f'_s(0)-(q_1,f)\\ f_s(0)-(q_2,f)\end{bmatrix}. \tag{2.6}$$

The expression (2.5) makes sense as a function from $L_2(\mathbb{R})$ if and only if the second term of (2.5) vanishes (i.e., if $\mathbf{T}\Gamma_0 f-\Gamma_1 f=0$). This means that the formal expression (2.4) allows one to define the operator in $L_2(\mathbb{R})$,

$$H_{\mathbf{T}}f=-\frac{d^2 f}{dx^2}+[q_1,q_2]\Gamma_0 f=-\big\{f''(x)\big\}_{x\neq 0}+f_r(0)q_1(x)-f'_r(0)q_2(x) \tag{2.7}$$

with the domain of definition

$$\mathcal{D}(H_{\mathbf{T}})=\big\{f\in W_2^2\big(\mathbb{R}\backslash\{0\}\big):(\mathbf{T}\Gamma_0-\Gamma_1)f=0\big\}, \tag{2.8}$$

where the Γ_i's are determined by (2.6) and $\mathbf{T}=\left[\begin{smallmatrix}a&b\\ c&d\end{smallmatrix}\right]$.

Each operator $H_{\mathbf{T}}$ is the restriction of the maximal operator

$$S_{\max}f=-\frac{d^2 f}{dx^2}+[q_1,q_2]\Gamma_0 f=-\big\{f''(x)\big\}_{x\neq 0}+f_r(0)q_1(x)-f'_r(0)q_2(x), \tag{2.9}$$

with $\mathcal{D}(S_{\max})=W_2^2(\mathbb{R}\backslash\{0\})$ acting in $L_2(\mathbb{R})$.

The operator $S_{\max}$ satisfies Green's identity

$$(S_{\max}f,g)-(f,S_{\max}g)=(\Gamma_1 f)\cdot\Gamma_0 g-(\Gamma_0 f)\cdot\Gamma_1 g, \tag{2.10}$$

where the dot $\cdot$ in the right-hand side means the standard inner product in $\mathbb{C}^2$. Moreover, according to [6, Lemma 1], for any vectors $h_0, h_1 \in \mathbb{C}^2$, there exists $f \in \mathcal{D}(S_{\max})$ such that $\Gamma_0 f = h_0$ and $\Gamma_1 f = h_1$.

The next operator plays an important role in what follows:

$$H_\infty = S_{\max} \restriction_{\mathcal{D}(H_\infty)}, \qquad \mathcal{D}(H_\infty) = \big\{ f \in \mathcal{D}(S_{\max}) : \Gamma_0 f = 0 \big\}. \tag{2.11}$$

In view of (2.6) and (2.9),

$$H_\infty f = -\frac{d^2 f}{dx^2}, \quad f \in \mathcal{D}(H_\infty) = \big\{ f \in W_2^2\big(\mathbb{R}\backslash\{0\}\big) : f_r(0) = f_r'(0) = 0 \big\}.$$

It is easy to check that H_∞ is a positive (since $(H_\infty f, f) = \int_{\mathbb{R}} |f'(x)|^2\, dx > 0$ for nonzero $f \in \mathcal{D}(H_\infty)$) self-adjoint operator in $L_2(\mathbb{R})$.

Taking into account [12, Corollary 2.5], the self-adjointness of H_∞, Green's identity (2.10), and the surjectivity of the mapping $(\Gamma_0, \Gamma_1) : \mathcal{D}(S_{\max}) \to \mathbb{C}^2 \oplus \mathbb{C}^2$, one is led to the conclusion that the operator $S_{\min} = S_{\max} \restriction_{\mathcal{D}(S_{\min})}$ with domain of definition $\mathcal{D}(S_{\min}) = \{ f \in \mathcal{D}(S_{\max}) : \Gamma_0 f = \Gamma_1 f = 0 \}$ is a closed symmetric operator in $L_2(\mathbb{R})$. Precisely, $S_{\min} f = -\frac{d^2 f}{dx^2}$ with the domain

$$\mathcal{D}(S_{min}) = \left\{ f \in W_2^2\big(\mathbb{R}\backslash\{0\}\big) : \begin{matrix} f_r(0) = 0 \; f_s(0) = (q_2, f) \\ f_r'(0) = 0 \; f_s'(0) = (q_1, f) \end{matrix} \right\}. \tag{2.12}$$

Moreover, the relation $S_{\min}^\dagger = S_{\max}$ holds and the collection $(\mathbb{C}^2, \Gamma_0, \Gamma_1)$ is a boundary triplet (see the Appendix) of $S_{\max}$. The latter property is especially important because the operators $H_{\mathbf{T}}$ are intermediate extensions between $S_{\min}$ and $S_{\max}$ and their domains are determined in terms of boundary operators Γ_j. Precisely, the definition (2.7) and domain of definition (2.8) of $H_{\mathbf{T}}$ can be rewritten as follows:

$$H_{\mathbf{T}} = S_{\max} \restriction_{\mathcal{D}(H_{\mathbf{T}})}, \qquad \mathcal{D}(H_{\mathbf{T}}) = \big\{ f \in \mathcal{D}(S_{\max}) : \mathbf{T}\Gamma_0 f = \Gamma_1 f \big\}. \tag{2.13}$$

Therefore, the well-developed methods of the theory of boundary triplets (see [27]) can be applied for the investigation of $H_{\mathbf{T}}$.

3. Special cases of nonlocal one-point interactions

3.1. **Self-adjoint nonlocal one-point interactions.**

Lemma 3.1. *If the entries of* $\mathbf{T}$ *satisfy the conditions* $a, d \in \mathbb{R}$, $b = c^*$, *then the corresponding operator* $H_{\mathbf{T}}$ *defined by (2.7) is self-adjoint in* $L_2(\mathbb{R})$ *for any choice of* $q_j \in L_2(\mathbb{R})$.

Proof. It follows from the theory of boundary triplets (see the Appendix) that $H_{\mathbf{T}}^\dagger = H_{\mathbf{T}^\dagger}$, where $\mathbf{T}^\dagger = (\mathbf{T}^*)^t$. Therefore, $H_{\mathbf{T}}$ is a self-adjoint operator if and only if the matrix $\mathbf{T}$ is Hermitian. The latter is equivalent to the conditions $a, d \in \mathbb{R}$, $b = c^*$. □

3.2. **$\mathcal{PT}$-symmetric nonlocal one-point interactions.** As usual (see [14]), we consider the space parity operator $\mathcal{P}f(x) = f(-x)$ and the conjugation operator $\mathcal{T}f = f^*$. An operator H acting in $L_2(\mathbb{R})$ is called *$\mathcal{PT}$-symmetric* if $\mathcal{PT}H = H\mathcal{PT}$.

Lemma 3.2. *If the entries of $\mathbf{T}$ and the functions q_j satisfy the conditions*

$$a, d \in \mathbb{R}, b, c \in i\mathbb{R}, \quad \mathcal{PT}q_1 = q_1, \qquad \mathcal{PT}q_2 = -q_2, \tag{3.1}$$

then the corresponding operator $H_{\mathbf{T}}$ defined by (2.7) is $\mathcal{PT}$-symmetric.

Proof. It is easy to check that, for any $f \in W_2^2(\mathbb{R}\backslash\{0\})$,

$$(\mathcal{P}f)_r(0) = f_r(0), \qquad (\mathcal{P}f)_s(0) = -f_s(0),$$
$$(\mathcal{P}f)'_r(0) = -f'_r(0), \qquad (\mathcal{P}f)'_s(0) = f'_s(0).$$

These relations, definition (2.6) of Γ_j, and (3.1) lead to the conclusion that

$$\Gamma_j\mathcal{PT}f = \sigma_3\mathcal{T}\Gamma_j f, \qquad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad j = 0, 1. \tag{3.2}$$

(The same symbol $\mathcal{T}$ is used for the conjugation operators in $L_2(\mathbb{R})$ and $\mathbb{C}^2$.) Therefore, if (3.1) holds, then the operator $S_{\max}$ defined by (2.9) is $\mathcal{PT}$-symmetric:

$$\mathcal{PT}S_{\max}f = -\frac{d^2}{dx^2}\mathcal{PT}f + [q_1, q_2]\sigma_3\mathcal{T}\Gamma_0 f = S_{\max}\mathcal{PT}f.$$

Since $H_{\mathbf{T}}$ is the restriction of $S_{\max}$ onto $\mathcal{D}(H_{\mathbf{T}})$, the invariance of $\mathcal{D}(H_{\mathbf{T}})$ with respect to $\mathcal{PT}$ will guarantee the $\mathcal{PT}$-symmetricity of $H_{\mathbf{T}}$.

Let us prove that $\mathcal{PT} : \mathcal{D}(H_{\mathbf{T}}) \to \mathcal{D}(H_{\mathbf{T}})$. To do that, we consider an arbitrary $f \in \mathcal{D}(H_{\mathbf{T}})$. Then, according to (2.8), $\mathbf{T}\Gamma_0 f = \Gamma_1 f$ and the inclusion $\mathcal{PT}f \in \mathcal{D}(H_{\mathbf{T}})$ is equivalent to the condition $\mathbf{T}\Gamma_0\mathcal{PT}f = \Gamma_1\mathcal{PT}f$. By virtue of (3.2), $\mathbf{T}\Gamma_0\mathcal{PT}f = \mathbf{T}\sigma_3\mathcal{T}\Gamma_0 f$ and

$$\Gamma_1\mathcal{PT}f = \sigma_3\mathcal{T}\Gamma_1 f = \sigma_3\mathcal{T}\mathbf{T}\Gamma_0 f = \sigma_3\mathbf{T}^*\mathcal{T}\Gamma_0 f.$$

This means that the required identity $\mathbf{T}\Gamma_0\mathcal{PT}f = \Gamma_1\mathcal{PT}f$ is true if and only if $\mathbf{T}\sigma_3 = \sigma_3\mathbf{T}^*$. The latter matrix relation holds if the entries of $\mathbf{T}$ satisfy (3.1). $\square$

3.3. **$\mathcal{P}$-self-adjoint nonlocal one-point interactions.** An operator $H_{\mathbf{T}}$ defined by (2.7) is called *$\mathcal{P}$-self-adjoint* if $\mathcal{P}H_{\mathbf{T}} = H_{\mathbf{T}}^\dagger\mathcal{P}$.

Lemma 3.3. *If the entries of $\mathbf{T}$ and the functions q_j satisfy the conditions*

$$a, d \in \mathbb{R}, b = -c^*, \quad \mathcal{P}q_1 = q_1, \qquad \mathcal{P}q_2 = -q_2, \tag{3.3}$$

then the operator $H_{\mathbf{T}}$ is $\mathcal{P}$-self-adjoint.

Proof. Similarly to the proof of Lemma 3.2, we check that $\Gamma_j\mathcal{P}f = \sigma_3\Gamma_j f$ and show that the conditions (3.3) ensure the commutation relation $S_{\max}\mathcal{P} = \mathcal{P}S_{\max}$. The operators $H_{\mathbf{T}}$ and $H_{\mathbf{T}}^\dagger$ are restrictions of $S_{\max}$. Therefore, the condition $\mathcal{P} : \mathcal{D}(H_{\mathbf{T}}) \to \mathcal{D}(H_{\mathbf{T}}^\dagger)$ means the identity $\mathcal{P}H_{\mathbf{T}} = H_{\mathbf{T}}^\dagger\mathcal{P}$.

Let us verify that $\mathcal{P} : \mathcal{D}(H_{\mathbf{T}}) \to \mathcal{D}(H_{\mathbf{T}}^\dagger)$. Since $H_{\mathbf{T}}^\dagger = H_{\mathbf{T}^{*t}}$, the domains of definition $\mathcal{D}(H_{\mathbf{T}})$ and $\mathcal{D}(H_{\mathbf{T}}^\dagger)$ are determined by (2.8) with the matrices $\mathbf{T}$

and $\mathbf{T}^{*t}$, respectively. Let $f \in \mathcal{D}(H_{\mathbf{T}})$. Then $\mathbf{T}\Gamma_0 f = \Gamma_1 f$ and the inclusion $\mathcal{P}f \in \mathcal{D}(H_{\mathbf{T}}^{\dagger})$ is equivalent to the condition $\mathbf{T}^{*t}\Gamma_0\mathcal{P}f = \Gamma_1\mathcal{P}f$.

Taking into account that $\Gamma_j\mathcal{P}f = \sigma_3\Gamma_j f$, we obtain $\mathbf{T}^{*t}\Gamma_0\mathcal{P}f = \mathbf{T}^{*t}\sigma_3\Gamma_0 f$ and $\Gamma_1\mathcal{P}f = \sigma_3\Gamma_1 f = \sigma_3\mathbf{T}\Gamma_0 f$. Hence, $\mathbf{T}^{*t}\Gamma_0\mathcal{P}f = \Gamma_1\mathcal{P}f$ holds if and only if $\mathbf{T}^{*t}\sigma_3 = \sigma_3\mathbf{T}$. This matrix relation holds if the entries a, b, c, d of $\mathbf{T}$ satisfy (3.3). □

4. Spectral analysis of $H_{\mathbf{T}}$

It follows from the definition (2.11) of the self-adjoint operator H_∞ that its spectrum $\sigma(H_\infty) = [0, \infty)$ is purely continuous. This means that $(H_\infty - \lambda I)^{-1}$ is unbounded for any $\lambda \in [0, \infty)$. Since H_∞ is an extension of the symmetric operator $S_{\min}$ with finite defect numbers, we conclude that the operator $(S_{\min} - \lambda I)^{-1}$ is also unbounded. This means that the spectrum of each $H_{\mathbf{T}}$ contains $[0, \infty)$. Furthermore, only eigenvalues of $H_{\mathbf{T}}$ may appear in $\rho(H_\infty) = \mathbb{C} \setminus [0, \infty)$. This fact follows from the definition (2.13) of $H_{\mathbf{T}}$ and the relation (A.2) describing $\sigma(H_{\mathbf{T}}) \cap \rho(H_\infty)$. (An eigenfunction of $H_{\mathbf{T}}$ should be the eigenfunction of $S_{\max}$ corresponding to the same eigenvalue (since $S_{\max}$ is an extension of $H_{\mathbf{T}}$).)

The kernel subspace $\ker(S_{\max} - \lambda I)$ has dimension 2 for any choice of $\lambda \in \mathbb{C} \setminus [0, \infty)$. Let u_λ, v_λ be a basis of $\ker(S_{\max} - \lambda I)$. Then, any $f \in \ker(S_{\max} - \lambda I)$ has the form $f = c_1 u_\lambda + c_2 v_\lambda$, and f turns out to be the eigenfunction of $H_{\mathbf{T}}$ corresponding to the eigenvalue λ if and only if f belongs to the domain $\mathcal{D}(H_{\mathbf{T}})$ determined by (2.13), that is, if c_1, c_2 are nonzero solutions of the linear system

$$c_1(\mathbf{T}\Gamma_0 - \Gamma_1)u_\lambda + c_2(\mathbf{T}\Gamma_0 - \Gamma_1)v_\lambda = 0.$$

Therefore, the eigenvalues $\lambda \in \mathbb{C} \setminus [0, \infty)$ of $H_{\mathbf{T}}$ coincide with the roots of the characteristic equation

$$\det\big[(\mathbf{T}\Gamma_0 - \Gamma_1)u_\lambda, (\mathbf{T}\Gamma_0 - \Gamma_1)v_\lambda\big] = 0. \tag{4.1}$$

Let us assume without loss of generality that the eigenfunctions u_λ, v_λ are chosen in such a way that

$$\Gamma_0 u_\lambda = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \text{and} \qquad \Gamma_0 v_\lambda = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Then the characteristic equation (4.1) for the determination of eigenvalues of $H_{\mathbf{T}}$ takes the form

$$\det(\mathbf{T} - W_\lambda) = 0, \tag{4.2}$$

where the (2×2)-matrix $W_\lambda = [\Gamma_1 u_\lambda, \Gamma_1 v_\lambda]$ is called the *Weyl–Titchmarsh function associated to the boundary triplet* $(\mathbb{C}^2, \Gamma_0, \Gamma_1)$. The Weyl–Titchmarsh function W_λ is holomorphic on $\mathbb{C} \setminus [0, \infty)$ and it satisfies the relation $(W_\lambda^*)^t = W_{\lambda^*}$ (see the Appendix).

4.1. **Eigenfunctions of $S_{\max}$.** Let us write any $\lambda \in \mathbb{C} \setminus [0, \infty)$ as $\lambda = k^2$, where $k \in \mathbb{C}_+ = \{k \in \mathbb{C} : \operatorname{Im} k > 0\}$, and consider the function

$$G(x) = \frac{i}{2k} e^{ik|x|}.$$

Obviously, $G(\cdot)$ belongs to $W_2^2(\mathbb{R}\backslash\{0\})$ and

$$-G'' - k^2 G = 0, \qquad -(G')'' - k^2 G' = 0, \quad x \neq 0.$$

Moreover,

$$\begin{aligned} G_r(0) &= \frac{i}{2k}, \qquad G_r'(0) = 0, \qquad G_r''(0) = -\frac{ik}{2}, \\ G_s(0) &= 0, \qquad G_s'(0) = -1, \qquad G_s''(0) = 0. \end{aligned}$$

The convolution

$$f = (G * q)(x) = \int_{-\infty}^{\infty} G(x - s) q(s)\, ds$$

($q \in L_2(\mathbb{R})$ is a piecewise continuous function) is the solution of the differential equation $-f'' - k^2 f = q$ in $L_2(\mathbb{R})$.

Lemma 4.1. *The functions*

$$\begin{aligned} u(x) &= -(G * q_1)(x) - 2ik\big[1 + (G * q_1)(0)\big]G(x) + \frac{2i}{k}(G' * q_1)(0)G'(x), \\ v(x) &= -(G * q_2)(x) - 2ik(G * q_2)(0)G(x) - \frac{2i}{k}\big[1 - (G' * q_2)(0)\big]G'(x) \end{aligned}$$

form the basis of the eigenfunction subspace $\ker(S_{\max} - k^2 I)$.

Proof. An elementary analysis shows that the functions u, v belong to $W_2^2(\mathbb{R}\backslash\{0\})$ and

$$\begin{aligned} u_r(0) &= 1, \qquad u_s(0) = -\frac{2i}{k}(G' * q_1)(0), \\ v_r(0) &= 0, \qquad v_s(0) = \frac{2i}{k}\big[1 - (G' * q_2)(0)\big], \\ u_r'(0) &= 0, \qquad u_s'(0) = 2ik\big[1 + (G * q_1)(0)\big], \\ v_r'(0) &= -1, \qquad v_s'(0) = 2ik(G * q_2)(0). \end{aligned} \tag{4.3}$$

The first column in (4.3) means that u and v are linearly independent, and

$$\Gamma_0 u = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \qquad \Gamma_0 v = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Furthermore, taking into account (2.9) and (4.3), we obtain for almost all $x \in \mathbb{R}$,

$$(S_{\max} - k^2 I)u = -u'' - k^2 u + q_1 = -q_1 + q_1 = 0.$$

Similarly, $(S_{\max} - k^2 I)v = -v'' - k^2 v + q_2 = -q_2 + q_2 = 0$. Hence, the functions u, v belong to $\ker(S_{\max} - k^2 I)$ and they form a basis of this subspace. $\square$

4.2. **The Weyl–Titchmarsh function associated to** $(\mathbb{C}^2, \Gamma_0, \Gamma_1)$**.** Since

$$\Gamma_0 u = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \qquad \text{and} \qquad \Gamma_0 v = \begin{bmatrix} 0 \\ 1 \end{bmatrix},$$

the Weyl–Titchmarsh function associated to $(\mathbb{C}^2, \Gamma_0, \Gamma_1)$ has the form $W_\lambda = [\Gamma_1 u, \Gamma_1 v]$, where, in view of (2.6) and (4.3),

$$\Gamma_1 u = \begin{bmatrix} 2ik[1 + (G * q_1)(0)] - (q_1, u) \\ -\frac{2i}{k}(G' * q_1)(0) - (q_2, u) \end{bmatrix},$$

$$\Gamma_1 v = \begin{bmatrix} 2ik(G * q_2)(0) - (q_1, v) \\ \frac{2i}{k}[1 - (G' * q_2)(0)] - (q_2, v) \end{bmatrix}.$$

Making some additional rudimentary calculations (mainly related to the calculation of scalar products (q, u), (q, v) for functions u, v from Lemma 4.1), we obtain

$$W_\lambda = \begin{bmatrix} (q_1, G * q_1) & (q_1, G * q_2) \\ (q_2, G * q_1) & (q_2, G * q_2) \end{bmatrix} + \begin{bmatrix} r_{11} & r_{12} \\ r_{21} & r_{22} \end{bmatrix}, \tag{4.4}$$

where

$$r_{11} = 2ik\big[1 + (G * q_1)(0)\big]\big[1 + (G * q_1^*)(0)\big] + \frac{2i}{k}(G' * q_1)(0)(G' * q_1^*)(0),$$
$$r_{22} = \frac{2i}{k}\big[1 - (G' * q_2)(0)\big]\big[1 - (G' * q_2^*)(0)\big] + 2ik(G * q_2)(0)(G * q_2^*)(0),$$
$$r_{12} = 2ik(G * q_2)(0)\big[1 + (G * q_1^*)(0)\big] - \frac{2i}{k}(G' * q_1^*)(0)\big[1 - (G' * q_2)(0)\big],$$
$$r_{21} = 2ik(G * q_2^*)(0)\big[1 + (G * q_1)(0)\big] - \frac{2i}{k}(G' * q_1)(0)\big[1 - (G' * q_2^*)(0)\big].$$

Denote

$$B_{q_1,q_2} = \begin{bmatrix} 1 + (G * q_1)(0) & (G * q_2)(0) \\ -(G' * q_1)(0) & 1 - (G' * q_2)(0) \end{bmatrix}.$$

Then (4.4) can be rewritten as follows:

$$W_\lambda = \begin{bmatrix} (q_1, G * q_1) & (q_1, G * q_2) \\ (q_2, G * q_1) & (q_2, G * q_2) \end{bmatrix} + B^t_{q_1^*,q_2^*} \begin{bmatrix} 2ik & 0 \\ 0 & \frac{2i}{k} \end{bmatrix} B_{q_1,q_2}. \tag{4.5}$$

Substituting (4.5) into (4.2), we obtain the characteristic equation for eigenvalues $\lambda \in \mathbb{C} \setminus [0, \infty)$ of $H_{\mathbf{T}}$. In particular, if $q_1 = q_2 = 0$, the Weyl function W_λ coincides with $\left[\begin{smallmatrix} 2ik & 0 \\ 0 & 2i/k \end{smallmatrix}\right]$ and the equation (4.2) is transformed to the polynomial

$$2dk^2 + ik(\det \mathbf{T} - 4) + 2a = 0, \tag{4.6}$$

which determines spectra of ordinary point interactions considered in Section 2.1.

5. Nonlocal δ-interaction

5.1. **Definition and description of eigenvalues.** The classical one-point δ-interaction is given by the formal expression

$$-\frac{d^2}{dx^2} + a\langle\delta,\cdot\rangle\delta(x), \quad a \in \mathbb{C}. \tag{5.1}$$

It is natural to suppose that the generalization of (5.1) to the *nonlocal* case consists in the addition of the nonlocal part $\langle\delta,\cdot\rangle q(x) + (q,\cdot)\delta(x)$ of δ-interaction. For this reason, a nonlocal one-point δ-interaction can be defined via the formal expression

$$-\frac{d^2}{dx^2} + a\langle\delta,\cdot\rangle\delta(x) + \langle\delta,\cdot\rangle q(x) + (q,\cdot)\delta(x), \quad a \in \mathbb{C}, q \in L_2(\mathbb{R}),$$

which is a particular case of (2.4) with $\mathbf{T} = \left[\begin{smallmatrix} a & 0 \\ 0 & 0 \end{smallmatrix}\right]$, $q_1 = q$, and $q_2 = 0$. This means that the corresponding operator $H_{\mathbf{T}} \equiv H_a$ defined by (2.7) and (2.8) acts as

$$H_a f = -\frac{d^2 f}{dx^2} + f_r(0)q(x), \tag{5.2}$$

on the domain of definition

$$\mathcal{D}(H_a) = \left\{ f \in W_2^2(\mathbb{R}\backslash\{0\}) : \begin{array}{c} f_s(0) = 0 \\ f'_s(0) = af_r(0) + (q,f) \end{array} \right\}. \tag{5.3}$$

In view of Lemma 3.2, the operator H_a is $\mathcal{PT}$-symmetric if $a \in \mathbb{R}$ and $\mathcal{PT}q = q$. In this case, due to Lemma 3.1, the operator H_a should be self-adjoint. Therefore, $\mathcal{PT}$-symmetric nonlocal δ-interactions are realized via self-adjoint operators. The same result is true for the case of $\mathcal{P}$-self-adjoint operators H_a (see Lemma 3.3).

Theorem 5.1. *The operator H_a defined by (5.2) has an eigenvalue $\lambda = k^2 \in \mathbb{C} \setminus [0,\infty)$ if and only if the following relation holds:*

$$a = (q, G*q) + 2ik\big[1 + (G*q)(0)\big]\big[1 + (G*q^*)(0)\big], \quad k \in \mathbb{C}_+. \tag{5.4}$$

Proof. If $q = q_1$ and $q_2 = 0$, then the Weyl–Titchmarsh function (4.5) has the form

$$W_\lambda = \begin{bmatrix} (q, G*q) + r_{11} & -\frac{2i}{k}(G'*q^*)(0) \\ -\frac{2i}{k}(G'*q)(0) & \frac{2i}{k} \end{bmatrix},$$

where $r_{11} = 2ik[1+(G*q)(0)][1+(G*q^*)(0)] + \frac{2i}{k}(G'*q)(0)(G'*q^*)(0)$. By virtue of (4.2), $\lambda \in \sigma_p(H_a)$ if and only if $\det(\mathbf{T} - W_\lambda) = 0$, where $\mathbf{T} = \left[\begin{smallmatrix} a & 0 \\ 0 & 0 \end{smallmatrix}\right]$. The direct calculation of $\det(\mathbf{T} - W_\lambda)$ in the latter equation gives (5.4). □

Each operator H_a satisfies the relation $S_{\min} \subset H_a \subset S_{\max}$ because $H_a = H_{\mathbf{T}}$ with the matrix $\mathbf{T}$ determined above. This important general relation (which holds for any $H_{\mathbf{T}}$) can be made more precise for the particular case of operators H_a. Indeed, it follows from (5.3) that the H_a's are extensions of the following operator:

$$\widetilde{S}_{\min} f = -\frac{d^2 f}{dx^2}, \qquad \mathcal{D}(\widetilde{S}_{\min}) = \left\{ f \in W_2^2(\mathbb{R}\backslash\{0\}) : \begin{array}{c} f_s(0) = f_r(0) = 0 \\ f'_s(0) = (q,f) \end{array} \right\}. \tag{5.5}$$

It is easy to see (comparing $\mathcal{D}(\widetilde{S}_{\min})$ with the domain $\mathcal{D}(S_{\min})$ determined by (2.12)) that $\widetilde{S}_{\min}$ is an extension of $S_{\min}$, that is, $S_{\min} \subset \widetilde{S}_{\min}$. Moreover, the operator $\widetilde{S}_{\min}$ is symmetric. This fact follows from Green's identity (4.2) because $\Gamma_1 f = 0$ for all $f \in \mathcal{D}(\widetilde{S}_{\min})$.

Denote $\widetilde{S}_{\max} = \widetilde{S}^{\dagger}_{\min}$. The calculation of the adjoint operator gives

$$\widetilde{S}_{\max} f = -\frac{d^2 f}{dx^2} + f_r(0)q(x), \qquad \mathcal{D}(\widetilde{S}_{\max}) = \bigl\{f \in W_2^2\bigl(\mathbb{R}\backslash\{0\}\bigr) : f_s(0) = 0\bigr\}.$$

It is easy to check that $S_{\min} \subset \widetilde{S}_{\min} \subset H_a \subset \widetilde{S}_{\max} \subset S_{\max}$. Thus, H_a is a proper extension of the symmetric operator $\widetilde{S}_{\min}$. Furthermore, an elementary analysis shows that:

(i) the kernel subspace $\ker(\widetilde{S}_{\max} - \lambda I)$ is 1-dimensional and that it is generated by the function (cf. Lemma 4.1)

$$u_\lambda(x) = -(G * q)(x) - 2ik\bigl[1 + (G * q)(0)\bigr]G(x); \tag{5.6}$$

(ii) the triple $(\mathbb{C}, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1)$, where

$$\widetilde{\Gamma}_0 f = f_r(0), \qquad \widetilde{\Gamma}_1 f = f_s'(0) - (q, f), \quad f \in \mathcal{D}(\widetilde{S}_{\max}) \tag{5.7}$$

is the boundary triplet of $\widetilde{S}_{\max}$ and

$$\widetilde{\Gamma}_0 u_\lambda = 1, \qquad \widetilde{\Gamma}_1 u_\lambda = (q, G * q) + 2ik\bigl[1 + (G * q)(0)\bigr]\bigl[1 + (G * q^*)(0)\bigr], \tag{5.8}$$

where u_λ is determined by (5.6);

(iii) the operators H_a initially defined by (5.2) and (5.3) can be rewritten in terms of the boundary triplet $(\mathbb{C}, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1)$:

$$H_a = \widetilde{S}_{\max} \restriction_{\mathcal{D}(H_a)}, \qquad \mathcal{D}(H_a) = \bigl\{f \in \mathcal{D}(\widetilde{S}_{\max}) : a\widetilde{\Gamma}_0 f = \widetilde{\Gamma}_1 f\bigr\}; \tag{5.9}$$

(iv) the operator

$$\widetilde{H}_\infty = \widetilde{S}_{\max} \restriction_{\mathcal{D}(\widetilde{H}_\infty)}, \qquad \mathcal{D}(\widetilde{H}_\infty) = \bigl\{f \in \mathcal{D}(\widetilde{S}_{\max}) : \widetilde{\Gamma}_0 f = 0\bigr\}$$

is positive self-adjoint and its spectrum $\sigma(\widetilde{H}_\infty) = [0, \infty)$ is purely continuous.

The items (i)–(iv) allow one to simplify the investigation of H_a. First of all we note that the Weyl–Titchmarsh function $\widetilde{W}_\lambda$ associated to the boundary triplet $(\mathbb{C}, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1)$ is a holomorphic function on $\rho(\widetilde{H}_\infty) = \mathbb{C} \setminus [0, \infty)$ and that, due to (5.8), it has the form

$$\widetilde{W}_\lambda = \widetilde{\Gamma}_1 u_\lambda = (q, G * q) + 2ik\bigl[1 + (G * q)(0)\bigr]\bigl[1 + (G * q^*)(0)\bigr]. \tag{5.10}$$

The obtained formula immediately justifies (5.4) because $\lambda \in \mathbb{C} \setminus [0, \infty)$ is an eigenvalue of H_a if and only if $\det(a - \widetilde{W}_\lambda) = 0$ (or, which is equivalent, if $a = \widetilde{W}_\lambda$). The latter identity shows that at least one of the subspaces $\mathbb{C}_\pm$ belongs to $\rho(H_a)$. Indeed, if $a \in \mathbb{R}$, then $\rho(H_a) \supset \mathbb{C}_\pm$. If $a \in \mathbb{C} \setminus \mathbb{R}$, then only nonreal eigenvalues of H_a might be in $\mathbb{C}_\pm$. Let us assume that $\lambda_\pm \in \sigma_p(H_a)$ with $\operatorname{Im}\lambda_+ > 0$ and $\operatorname{Im}\lambda_- < 0$. Then, simultaneously, $\operatorname{Im} a > 0$ and $\operatorname{Im} a < 0$ (since $\widetilde{W}_{\lambda\pm} = a$

and $(\operatorname{Im}\lambda)(\operatorname{Im}\widetilde{W}_\lambda) > 0$ for $\operatorname{Im}\lambda \neq 0$; see the Appendix), which is impossible. Therefore, at least one of the $\mathbb{C}_\pm$'s does not belong to $\sigma(H_a)$. This result is not true for the general case of one-point interactions considered in Section 2. For instance, if $q_1 = q_2 = 0$ and $a = d = 0$, $bc = 4$, then the characteristic equation (4.6) vanishes and the eigenvalues of $H_{\mathbf{T}}$ fill the whole domain $\mathbb{C} \setminus [0, \infty)$.

Corollary 5.2. *The existence of a real eigenvalue of H_a means that H_a is a self-adjoint operator in $L_2(\mathbb{R})$.*

Proof. Let $u_\lambda \in L_2(\mathbb{R})$ be an eigenfunction of H_a corresponding to a real eigenvalue λ. It follows from the definition of $\widetilde{S}_{\min}$ that $\ker(\widetilde{S}_{\min} - \lambda I) = \{0\}$. Therefore, the domain of H_a can be represented as

$$\mathcal{D}(H_a) = \left\{ f = v + cu_\lambda : v \in \mathcal{D}(\widetilde{S}_{\min}), c \in \mathbb{C} \right\}$$

(since the symmetric operator $\widetilde{S}_{\min}$ has the defect index 1) and

$$H_a f = H_a(v + cu_\lambda) = \widetilde{S}_{\min} v + \lambda c u_\lambda.$$

Using the last expression we check that $\operatorname{Im}(H_a f, f) = 0$ for all $f = v + cu_\lambda$ from the domain of H_a. Therefore, H_a is a self-adjoint operator. □

In contrast to the case of ordinary one-point interactions considered in Section 2.1, the operators H_a may have real eigenvalues embedded into the continuous spectrum $[0, \infty)$ of $\widetilde{H}_\infty$. To see this, we rewrite the function u_λ in (5.6) as

$$u_\lambda(x) = \begin{cases} A_k(x) e^{ikx} + B_k(x) e^{-ikx}, & x > 0, \\ C_k(x) e^{ikx} + D_k(x) e^{-ikx}, & x < 0, \end{cases} \quad \lambda = k^2, \tag{5.11}$$

where

$$\begin{aligned}
A_k(x) &= 1 + \frac{i}{2k} \int_0^\infty e^{iks} q(s)\, ds - \frac{i}{2k} \int_0^x e^{-iks} q(s)\, ds, \\
D_k(x) &= 1 + \frac{i}{2k} \int_{-\infty}^0 e^{-iks} q(s)\, ds - \frac{i}{2k} \int_x^0 e^{iks} q(s)\, ds, \\
B_k(x) &= -\frac{i}{2k} \int_x^\infty e^{iks} q(s)\, ds, \\
C_k(x) &= -\frac{i}{2k} \int_{-\infty}^x e^{-iks} q(s)\, ds.
\end{aligned}$$

If $\lambda = k^2$ with $k \in \mathbb{C}_+$, then the function u_λ belongs to $L_2(\mathbb{R})$ and it solves the differential equation $-f''(x) + f_r(0)q(x) = \lambda f(x)$ for $x \neq 0$. According to (5.8) and (5.10), u_λ belongs to the domain of definition (5.3) of the operator H_a with $a = \widetilde{W}_\lambda$. In other words, u_λ is the eigenfunction of H_a.

If $\lambda = k^2$ with $k \in \mathbb{R} \setminus \{0\}$, then the function u_λ defined by (5.11) turns out to be a *generalized eigenfunction* of H_a. This means that u_λ preserves all the above properties except the property of being in $L_2(\mathbb{R})$. It should be noted that u_λ may belong to $L_2(\mathbb{R})$. In this case, the generalized eigenfunction coincides with the ordinary eigenfunction and the corresponding operator H_a will have a positive eigenvalue $\lambda = k^2$. In view of Corollary 5.2, this phenomenon is possible only for self-adjoint operators H_a.

Example 5.3. We have the case of an even function with finite support. Let q be an even function with support in $[-\rho, \rho]$. The elementary calculation in (5.11) gives that, for all $|x| > \rho$,

$$u_\lambda(x) = \beta_k e^{ik|x|}, \qquad \beta_k = 1 - \frac{1}{k}\int_0^\rho \sin ks\; q(s)\, ds.$$

It is easy to see that u_λ will be in $L_2(\mathbb{R})$ if and only if $\beta_k = 0$. If $k \in \mathbb{R} \setminus \{0\}$ is a solution of the last equation, then u_λ turns out to be an eigenfunction of the self-adjoint operator H_a, where $a = \widetilde{W}_\lambda$ and $\widetilde{W}_\lambda$ is formally defined by (5.10) with $\lambda = k^2 \in (0, \infty)$. It should be noted that the case of odd functions with finite support is completely different. Indeed, if q is odd with the support in $[-\rho, \rho]$, then

$$u_\lambda(x) = \begin{cases} (1 - \frac{1}{k}\int_0^\rho \sin ksq(s)\, ds)e^{ikx}, & x > \rho, \\ (1 + \frac{1}{k}\int_0^\rho \sin ksq(s)\, ds)e^{-ikx}, & x < -\rho. \end{cases}$$

Obviously, such a function u_λ does not belong to $L_2(\mathbb{R})$ and it cannot be an eigenfunction of H_a. Therefore, in the case of an odd function q with finite support, the corresponding operators H_a $(a \in \mathbb{C})$ have no positive eigenvalues.

Let us consider the simplest example of an even function

$$q(x) = Z\chi_{[-\rho,\rho]}(x) = \begin{cases} Z, & x \in [-\rho, \rho], \\ 0, & x \in \mathbb{R} \setminus [-\rho, \rho], \end{cases} \qquad Z \in \mathbb{R}, \rho > 0. \tag{5.12}$$

The characteristic equation $\beta_k = 0$ takes the form $Z(1 - \cos k\rho) = k^2$. Let $k_0 \in \mathbb{R} \setminus \{0\}$ be the solution of this equation. Then the function

$$u_\lambda(x) = \frac{Z(1 - \cos k_0(\rho - |x|))}{k_0^2}\chi_{[-\rho,\rho]}(x), \quad \lambda = k_0^2,$$

belongs to the domain of definition

$$\mathcal{D}(H_a) = \left\{ f \in W_2^2\big(\mathbb{R}\backslash\{0\}\big) : \begin{array}{l} f(0-) = f(0+) \equiv f(0) \\ f'(0+) - f'(0-) = af(0) + Z\int_{-\rho}^{\rho} f(x)\, dx \end{array} \right\}$$

of the self-adjoint operator $H_a f = -\frac{d^2 f}{dx^2} + Zf(0)\chi_{[-\rho,\rho]}(x)$, where

$$a = [u_\lambda']_s(0) - Z\int_{-\rho}^{\rho} u_\lambda(x)\, dx = \frac{Z^2}{k_0^2}\Big(\frac{\sin 2k_0\rho}{k_0} - 2\rho\Big).$$

The function u_λ is an eigenfunction of H_a corresponding to the positive eigenvalue $\lambda = k_0^2$.

5.2. **Exceptional points.** The geometric multiplicity of any $\lambda \in \sigma_p(H_a)$ is 1 due to (i) and the fact that $\ker(\widetilde{S}_{\min} - \lambda I) = \{0\}$. The algebraic multiplicity can be calculated with the use of [10, Corollary 4.4].

An eigenvalue of H_a is called an *exceptional point* if its geometrical multiplicity does not coincide with the algebraic multiplicity. The presence of an exceptional point means that H_a cannot be self-adjoint for any choice of inner product in $L_2(\mathbb{R})$. By virtue of Corollary 5.2, the operators H_a may only have nonreal exceptional points.

Theorem 5.4. *A nonreal eigenvalue λ_0 of H_a is an exceptional point if and only if $\widetilde{W}'_{\lambda_0} = 0$, where $\widetilde{W}'_\lambda = \frac{d}{d\lambda}\widetilde{W}_\lambda$.*

Proof. The resolvent $(\widetilde{H}_\infty - \lambda I)^{-1}$ of a self-adjoint operator $\widetilde{H}_\infty$ is a holomorphic operator-valued function on $\rho(\widetilde{H}_\infty) = \mathbb{C} \setminus [0, \infty)$. On the other hand, the resolvent $(H_a - \lambda I)^{-1}$ may be a meromorphic function on $\mathbb{C} \setminus [0, \infty)$ with its poles being eigenvalues of H_a.

Let $\lambda_0 \in \mathbb{C} \setminus \mathbb{R}$ be a pole of $(H_a - \lambda I)^{-1}$. Then its order coincides with the maximal length of Jordan vectors associated with λ_0 (see, e.g., [9, Chapter 2]). Therefore, the existence of an exceptional point λ_0 of H_a is equivalent to the existence of a pole λ_0 of order greater than 1 for the meromorphic operator-valued function

$$\Xi(\lambda) = (H_a - \lambda I)^{-1} - (\widetilde{H}_\infty - \lambda I)^{-1}. \tag{5.13}$$

In other words, λ_0 turns out to be an exceptional point of H_a if and only if there exists $v \in L_2(\mathbb{R})$ such that

$$\lim_{\lambda \to \lambda_0} \|(\lambda - \lambda_0)\Xi(\lambda)v\| = \infty. \tag{5.14}$$

It is sufficient to suppose in (5.14) that $v = u_{\lambda^*} \in \ker(\widetilde{S}_{\max} - \lambda^* I)$ (since H_a and $\widetilde{H}_\infty$ are extensions of $\widetilde{S}_{\min}$ and, hence, $\Xi(\lambda) \restriction_{\mathcal{R}(\widetilde{S}_{\min} - \lambda I)} = 0$).

It follows from the Krein–Naimark resolvent formula (A.4) that

$$\|(\lambda - \lambda_0)\Xi(\lambda)u_{\lambda^*}\| = \left|\frac{\lambda - \lambda_0}{a - \widetilde{W}_\lambda}\right| \|\gamma(\lambda)\gamma(\lambda^*)^\dagger u_{\lambda^*}\|. \tag{5.15}$$

Let us evaluate the part $\|\gamma(\lambda)\gamma(\lambda^*)^\dagger u_{\lambda^*}\|$ in (5.15). In view of (A.3),

$$\gamma(\lambda^*)^\dagger u_{\lambda^*} = \widetilde{\Gamma}_1(\widetilde{H}_\infty - \lambda I)^{-1} u_{\lambda^*}.$$

The operator $\widetilde{H}_\infty$ is defined in (iv) and it acts as $\widetilde{H}_\infty f = -\frac{d^2 f}{dx^2}$ for all functions $f \in \mathcal{D}(\widetilde{H}_\infty) = \{f \in W_2^2(\mathbb{R} \setminus \{0\}) : f(0-) = f(0+) = 0\}$. The resolvent of $\widetilde{H}_\infty$ is well known and it takes an especially simple form for $f = u_{\lambda^*}$:

$$(\widetilde{H}_\infty - \lambda I)^{-1} u_{\lambda^*} = \frac{1}{2i(\operatorname{Im}\lambda)}(u_\lambda - u_{\lambda^*}).$$

The definition of the Weyl–Titchmarsh function $\widetilde{W}_\lambda$ associated to the boundary triplet $(\mathbb{C}, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1)$ and the relation $\widetilde{\Gamma}_0 u_\lambda = 1$ in (5.8) imply that $\widetilde{\Gamma}_1 u_\lambda = \widetilde{W}_\lambda$ for all $\lambda \in \mathbb{C} \setminus [0, \infty)$. Therefore,

$$\gamma(\lambda^*)^\dagger u_{\lambda^*} = \widetilde{\Gamma}_1(\widetilde{H}_\infty - \lambda I)^{-1} u_{\lambda^*} = \frac{\widetilde{\Gamma}_1(u_\lambda - u_{\lambda^*})}{2i(\operatorname{Im}\lambda)} = \frac{\widetilde{W}_\lambda - \widetilde{W}_{\lambda^*}}{2i(\operatorname{Im}\lambda)} = \frac{\operatorname{Im}\widetilde{W}_\lambda}{\operatorname{Im}\lambda}.$$

Furthermore, it follows from the definition of γ-field $\gamma(\cdot)$ associated with $(\mathbb{C}, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1)$ (see the Appendix) and (5.8) that $\gamma(\lambda)c = cu_\lambda$ for all $c \in \mathbb{C}$. Hence, $\gamma(\lambda)\gamma(\lambda^*)^\dagger u_{\lambda^*} = \frac{\operatorname{Im}\widetilde{W}_\lambda}{\operatorname{Im}\lambda} u_\lambda$. Setting $f_\lambda = u_\lambda$ in (A.1), we decide that

$$\|u_\lambda\|^2 = \frac{\operatorname{Im}\widetilde{W}_\lambda}{\operatorname{Im}\lambda}, \quad \lambda \in \mathbb{C} \setminus \mathbb{R}. \tag{5.16}$$

Therefore,

$$\alpha(\lambda) = \left\|\gamma(\lambda)\gamma(\lambda^*)^\dagger u_{\lambda^*}\right\| = \left(\frac{\operatorname{Im}\widetilde{W}_\lambda}{\operatorname{Im}\lambda}\right)^{3/2}.$$

The function $\alpha(\lambda)$ is continuous in a neighborhood of the nonreal point λ_0 and $\alpha(\lambda_0) \neq 0$. Therefore, taking (5.15) into account, we decide that (5.14) is equivalent to the condition

$$\lim_{\lambda \to \lambda_0} \frac{a - \widetilde{W}_\lambda}{\lambda - \lambda_0} = 0.$$

Remembering that $a = \widetilde{W}_{\lambda_0}$ (since λ_0 is an eigenvalue of H_a), we complete the proof. □

Remark 5.5. A result of similar type (but in a different context) was published recently in [13, Lemma 2.4].

Corollary 5.6. *If H_a has an exceptional point λ_0, then λ_0^* is an exceptional point for H_{a^*}*

The proof follows from Theorem 5.4 and the relation $\widetilde{W}_\lambda^* = \widetilde{W}_{\lambda^*}$.

5.3. **Spectral singularities.** Let H_a be *a non-self-adjoint* operator with real spectrum. The operator H_a cannot have real eigenvalues due to Corollary 5.2. Therefore, the spectrum of H_a is continuous and it coincides with $[0, \infty)$.

If H_a turns out to be self-adjoint with respect to an appropriative choice of inner product of $L_2(\mathbb{R})$ (i.e., if H_a is similar to a self-adjoint operator in $L_2(\mathbb{R})$), then its resolvent $(H_a - \lambda I)^{-1}$ should satisfy the standard evaluation

$$\left\|(H_a - \lambda I)^{-1} f\right\| \leq \frac{C}{|\operatorname{Im}\lambda|}\|f\|, \tag{5.17}$$

where $C > 0$ does not depend on $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and $f \in L_2(\mathbb{R})$.

The case where H_a is not similar to a self-adjoint operator in $L_2(\mathbb{R})$ deals with the existence of special spectral points of H_a which are impossible for the spectra of self-adjoint operators. Traditionally, these spectral points are called *spectral singularities* if they are located on the continuous spectrum of H_a. This particular role pertaining to spectral singularities was discovered for the first time by Naimark [26]. Recently, various aspects of spectral singularities, including their physical meaning and possible practical applications, have been analyzed with a wealth of technical tools (see, e.g., [20], [25]).

It is natural to suppose that a spectral singularity $\lambda_0 \in (0, \infty)$ of H_a is characterized by atypical behavior of the resolvent $(H_a - \lambda I)^{-1}$ in a neighborhood of λ_0. This assumption leads to the following definition: *a positive number λ_0 is called a* spectral singularity *of H_a if there exists $f \in L_2(\mathbb{R})$ such that the evaluation (5.17) does not hold when a nonreal λ tends to λ_0.*

Theorem 5.7. *Let $\lambda_0 \in (0, \infty)$, and let there exist a sequence of nonreal λ_n's such that $\lambda_n \to \lambda_0$ and $\lim_{n\to\infty} \widetilde{W}_{\lambda_n} = a \in \mathbb{C} \setminus \mathbb{R}$. Then λ_0 is a spectral singularity of the non-self-adjoint operators H_a and H_{a^*}.*

Proof. The inequality (5.17) is equivalent to the inequality

$$\big\|\Xi(\lambda) f\big\| \leq \frac{C}{|\operatorname{Im} \lambda|} \|f\|, \tag{5.18}$$

where $\Xi(\lambda)$ is defined by (5.13). Moreover, it follows from the proof of Theorem 5.4 that it is sufficient to verify (5.18) for $f = u_{\lambda^*}$ only. By virtue of (5.15) and the proof of Theorem 5.4,

$$\big\|\Xi(\lambda) u_{\lambda^*}\big\| = \frac{\|\gamma(\lambda)\gamma(\lambda^*)^\dagger u_{\lambda^*}\|}{|a - \widetilde{W}_\lambda|} = \frac{\operatorname{Im} \widetilde{W}_\lambda}{\operatorname{Im} \lambda} \frac{\|u_\lambda\|}{|a - \widetilde{W}_\lambda|}. \tag{5.19}$$

It follows from (5.16) that $\|u_\lambda\| = \|u_{\lambda^*}\|$. Replacing $\|u_\lambda\|$ by $\|u_{\lambda^*}\|$ in (5.19), we rewrite (5.18) in the following equivalent form:

$$\frac{|\operatorname{Im} \widetilde{W}_\lambda|}{|a - \widetilde{W}_\lambda|} \leq C, \quad \lambda \in \mathbb{C} \setminus \mathbb{R}. \tag{5.20}$$

If the condition of Theorem 5.7 is satisfied, then the inequality (5.20) cannot be true in a neighborhood of λ_0. Therefore, λ_0 should be a spectral singularity of H_a. The same result holds for H_{a^*} if we consider the sequences $\lambda_n^* \to \lambda_0$, $W_{\lambda_n^*} = W_{\lambda_n}^* \to a^*$ and take into account that $H_a^\dagger = H_{a^*}$. $\square$

If $\lambda = k^2$ with $k \in \mathbb{R} \setminus \{0\}$, then the formula (5.11) allows one to define two functions $u_\lambda^\pm$ corresponding to positive/negative values of k, respectively. In this case, the formula

$$\widetilde{W}_\lambda^\pm = [u_\lambda^{\pm\prime}]_s(0) - (q, u_\lambda^\pm) = 2ik\Big(1 + \frac{i}{k}\int_0^\infty e^{iks} q^{\mathrm{ev}}(s)\, ds\Big) - (q, u_\lambda^\pm)$$

(q^{ev} is the even part of q) gives two values of the Weyl–Titchmarsh function $\widetilde{W}_\lambda$ on $(0, \infty)$.

Let q be chosen such that the $\widetilde{W}_\lambda^\pm$'s are well posed (i.e., $\widetilde{W}_\lambda^\pm \neq \infty$). Then, the functions $\widetilde{W}_\lambda^\pm$ can be interpreted as limits on $(0, \infty)$ of the holomorphic functions $\widetilde{W}_\lambda$ considered on $\mathbb{C}_\pm$, respectively. Taking the relation $\widetilde{W}_\lambda^* = \widetilde{W}_{\lambda^*}$, $\lambda \in \mathbb{C} \setminus [0, \infty)$ into account, we deduce that $(\widetilde{W}_\lambda^+)^* = \widetilde{W}_\lambda^-$ for $\lambda > 0$. This relation and the definition of $\widetilde{W}_\lambda^\pm$ imply that u_λ^+ and u_λ^- are generalized eigenfunctions of the operators H_a and H_{a^*}, respectively, with $a = \widetilde{W}_\lambda^+$.

If $a = \widetilde{W}_\lambda^+$ is nonreal, then, due to Theorem 5.7, λ is a spectral singularity of the non-self-adjoint operators H_a and H_{a^*}. The corresponding generalized eigenfunctions coincide with u_λ^+ and u_λ^-. If $a = \widetilde{W}_\lambda^+$ is real, then the evaluation (5.17) holds (since H_a is self-adjoint) and λ cannot be a spectral singularity of H_a.

6. Examples

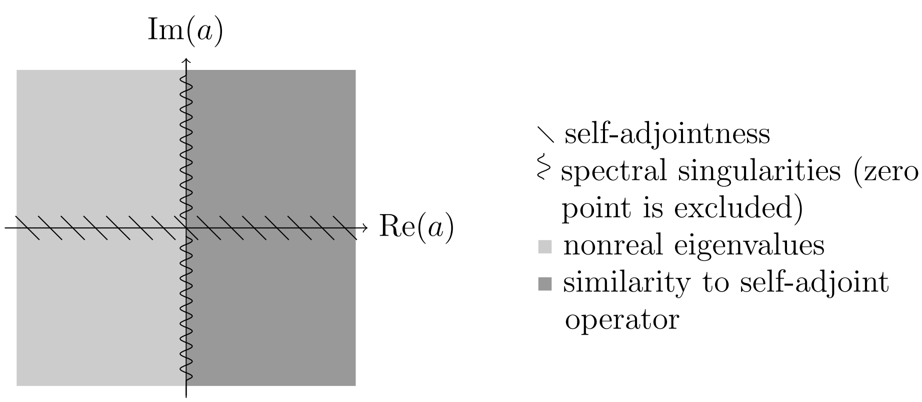
6.1. **Ordinary δ-interaction.** This simplest case corresponds to $q = 0$. The operators $H_a = -\frac{d^2}{dx^2}$ have the domains

$$\mathcal{D}(H_a) = \left\{ f \in W_2^2\big(\mathbb{R}\backslash\{0\}\big) : \begin{array}{l} f(0-) = f(0+) \equiv f(0) \\ f'(0+) - f'(0-) = af(0) \end{array} \right\}.$$

The Weyl–Titchmarsh function has the form $\widetilde{W}_\lambda = 2ik = 2i\sqrt{\lambda}$. There are no exceptional points for operators H_a because $\widetilde{W}'_\lambda = i/\sqrt{\lambda}$ does not vanish on $\mathbb{C} \setminus [0, \infty)$.

The limit functions $\widetilde{W}_\lambda^\pm = 2ik$, $k > 0/k < 0$ take nonreal values. Hence, the operators $H_{\widetilde{W}_\lambda^+}$ and $H_{\widetilde{W}_\lambda^-}$ have the spectral singularity $\lambda = k^2$.

The ordinary δ-interactions have been well studied (see [19], [22]), and the evolution of spectral properties of H_a when a runs $\mathbb{C}$ can be illustrated as follows:



6.2. **The case of an odd function.** Let q be an odd function. Then the Weyl–Titchmarsh function $\widetilde{W}_\lambda$ takes the especially simple form

$$\widetilde{W}_\lambda = 2ik - (q, u_\lambda) = 2ik + (q, G * q), \quad \lambda = k^2, k \in \mathbb{C}_+. \tag{6.1}$$

The last equality in (6.1) follows from (5.10) since $(G * q)(0) = (G * q^*)(0) = 0$ for odd functions q, while the first one is the consequence of (5.7) and the fact that $[u'_\lambda]_s(0) = 2ik[1 + (G * q)(0)] = 2ik$.

Let us consider, for simplicity, the odd function

$$q(x) = Z\,\mathsf{sign}(x)\chi_{[-\rho,\rho]}(x) = \begin{cases} Z, & 0 \le x \le \rho, \\ -Z, & -\rho \le x < 0, \\ 0, & x \in \mathbb{R} \setminus [-\rho, \rho], \end{cases} \qquad Z \in \mathbb{C}, \rho > 0.$$

The corresponding operators $H_a f = -\frac{d^2 f}{dx^2} + f(0)Z\mathsf{sign}(x)\chi_{[-\rho,\rho]}(x)$ with domains of definition

$$\mathcal{D}(H_a) = \left\{ f \in W_2^2\big(\mathbb{R}\backslash\{0\}\big) : \begin{array}{l} f(0-) = f(0+) \equiv f(0) \\ f'(0+) - f'(0-) = af(0) + Z^* \int_{-\rho}^{\rho} \mathsf{sign}(x) f(x)\, dx \end{array} \right\}$$

have no positive eigenvalues (see Example 5.3). After the substitution of q into (6.1) and elementary calculations with the use of (5.11), we obtain the explicit expression of the Weyl–Titchmarsh function

$$\widetilde{W}_\lambda = 2ik - \frac{|Z|^2}{ik^3}\big[(e^{ik\rho} - 2)^2 + 2ik\rho - 1\big], \quad \lambda = k^2, k \in \mathbb{C}_+. \tag{6.2}$$

The limit functions $\widetilde{W}_\lambda^\pm$ are determined by (6.2) for $k > 0$ and $k < 0$, respectively. It is easy to check that the imaginary part of $\widetilde{W}_\lambda^\pm$,

$$\mathsf{Im}\, \widetilde{W}_\lambda^\pm = 2k + \frac{|Z|^2}{k^3}(2\cos^2 k\rho - 4\cos k\rho + 2),$$

does not vanish when k runs $\mathbb{R} \setminus \{0\}$. Hence, any positive λ turns out to be a spectral singularity for some operators H_a. Namely, the operators H_a and H_{a^*} with $a = \widetilde{W}_\lambda^+$ will have the spectral singularity λ.

6.3. **The case of an even function** $q = ce^{-\mu|x|}$ **(**$\mu > 0$**).** The corresponding operators $H_a f = -\frac{d^2 f}{dx^2} + f(0)ce^{-\mu|x|}$ have the domains

$$\mathcal{D}(H_a) = \left\{ f \in W_2^2\big(\mathbb{R}\backslash\{0\}\big) : \begin{array}{l} f(0-) = f(0+) \equiv f(0) \\ f'(0+) - f'(0-) = af(0) + c^* \int_{\mathbb{R}} e^{-\mu|x|} f(x)\, dx \end{array} \right\}.$$

The eigenfunctions u_λ (see (5.11)) are given by the expression

$$u_\lambda = \Big(1 - \frac{c}{\mu^2 + \lambda}\Big)e^{ik|x|} + \frac{q(x)}{\mu^2 + \lambda}, \quad \lambda = k^2. \tag{6.3}$$

The Weyl–Titchmarsh function

$$\widetilde{W}_\lambda = 2ik - (q, u_\lambda) = 2ik - \frac{4\,\mathsf{Re}\, c}{\mu - ik} + \frac{\|q\|^2}{(\mu - ik)^2} \tag{6.4}$$

is defined on $\mathbb{C} \setminus [0, \infty)$ and its limit functions $\widetilde{W}_\lambda^\pm$ are determined by (6.4) with $k > 0$ and $k < 0$, respectively. Each $\lambda \in \mathbb{C} \setminus [0, \infty)$ is an eigenvalue of the operator H_a with $a = \widetilde{W}_\lambda$, and the corresponding eigenfunction is given by (6.3).

It follows from (6.3) that a positive eigenvalue λ exists for some operator H_a *if and only if* $c \geq \mu^2$. In this case, $\lambda = c - \mu^2$, the corresponding eigenfunction u_λ coincides with $\frac{q(x)}{\mu^2 + \lambda} = e^{-\mu|x|}$, and u_λ is an eigenfunction of a self-adjoint operator H_a with $a = \widetilde{W}_\lambda^\pm = -3\mu - \frac{\lambda}{\mu}$.

Let us assume for the simplicity that $c \in i\mathbb{R}$ and $\|q\|^2 = \frac{|c|^2}{\mu} = 1$. Then

$$\widetilde{W}_\lambda = 2ik + \frac{1}{(\mu - ik)^2} = 2i\sqrt{\lambda} + \frac{1}{(\mu - i\sqrt{\lambda})^2}. \tag{6.5}$$

If k is real in (6.5), then the imaginary part of $\widetilde{W}_\lambda^{\pm}$,

$$\mathsf{Im}\,\widetilde{W}_\lambda^{\pm} = 2k + \frac{2k\mu}{|\mu - ik|^2},$$

does not vanish when $\lambda = k^2 \in (0, \infty)$. Hence, any positive λ is a spectral singularity of operators H_a and H_{a^*} with $a = \widetilde{W}_\lambda^{+}$.

It follows from (6.5) that

$$\widetilde{W}'_\lambda = \frac{i}{k}\Big[1 + \frac{1}{(\mu - ik)^3}\Big] = \frac{i}{\sqrt{\lambda}}\Big[1 + \frac{1}{(\mu - i\sqrt{\lambda})^3}\Big].$$

Therefore, $\widetilde{W}'_\lambda = 0$ for certain $\lambda \in \mathbb{C} \setminus [0, \infty)$ if and only if $(\mu - ik)^3 = -1$ for $k \in \mathbb{C}_+$. The latter equation has two required solutions,

$$k_0 = \frac{\sqrt{3}}{2} + i\Big(\frac{1}{2} - \mu\Big), \qquad k_1 = -k_0^*,$$

when $0 < \mu < \frac{1}{2}$. By virtue of Theorem 5.4, $\lambda_0 = k_0^2$ is an exceptional point of the operator H_a with

$$a = \widetilde{W}_{\lambda_1} = 2ik_0 + \frac{1}{(\mu - ik_0)^2} = 2ik_0 + \frac{\mu - ik_0}{(\mu - ik_0)^3} = 3ik_0 - \mu,$$

while $\lambda_1 = k_1^2 = \lambda_0^*$ will be an exceptional point of its adjoint $H_{a^*} = H_a^\dagger$ (see Corollary 5.6).

The obtained result shows that the existence of exceptional points for some operators from the collection $\{H_a\}_{a\in\mathbb{C}}$ depends on the behavior of the function $q(x) = ce^{-\mu|x|}$. If $q(x)$ decreases (relatively) slowly on ∞ (the case $0 < \mu < \frac{1}{2}$), then there exist two operators H_a and $H_a^\dagger$ with exceptional points λ_0 and λ_0^*, respectively.

Appendix: Boundary triplets

Let $S_{\min}$ be a closed symmetric (densely defined) operator in a Hilbert space $\mathfrak{H}$ with inner product $(\cdot,\cdot)$. Denote $S_{\max} = S_{\min}^\dagger$. Obviously, $S_{\min} \subset S_{\max}$.

A triplet $(\mathcal{H}, \Gamma_0, \Gamma_1)$, where $\mathcal{H}$ is an auxiliary Hilbert space and Γ_0, Γ_1 are linear mappings of $\mathcal{D}(S_{\max})$ into $\mathcal{H}$, is called a *boundary triplet* of $S_{\max}$ if Green's identity

$$(S_{\max}f, g) - (f, S_{\max}g) = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{H}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{H}}, \quad f, g \in \mathcal{D}(S_{\max})$$

is satisfied and the map $(\Gamma_0, \Gamma_1) : \mathcal{D}(S_{\max}) \to \mathcal{H} \oplus \mathcal{H}$ is surjective.

The symmetric operator $S_{\min}$ is the restriction of $S_{\max}$ onto $\mathcal{D}(S_{\min}) = \{f \in \mathcal{D}(S_{\max}) : \Gamma_0 f = \Gamma_1 f = 0\}$. The defect indices of $S_{\min}$ coincide with the dimension of $\mathcal{H}$. Boundary triplets of $S_{\max}$ are not determined uniquely and they exist only in the case where the symmetric operator $S_{\min}$ has self-adjoint extensions (see [5], [11], [17], [21] for various generalizations of boundary triplets).

Let $(\mathcal{H}, \Gamma_0, \Gamma_1)$ be a boundary triplet of $S_{\max}$. Then the operator

$$H_\infty = S_{\max} \restriction_{\mathcal{D}(H_\infty)}, \qquad \mathcal{D}(H_\infty) = \big\{f \in \mathcal{D}(S_{\max}) : \Gamma_0 f = 0\big\}$$

is a self-adjoint extension of $S_{\min}$. The Weyl–Titchmarsh function W_λ associated to the boundary triplet $(\mathcal{H}, \Gamma_0, \Gamma_1)$ is defined for all $\lambda \in \rho(H_\infty)$ (see [16]):

$$W_\lambda \Gamma_0 f_\lambda = \Gamma_1 f_\lambda, \quad \forall f_\lambda \in \ker(S_{\max} - \lambda I).$$

The operator-valued function W_λ is holomorphic on $\rho(H_\infty)$ and the adjoint of the operator W_λ in $\mathcal{H}$ coincides with W_{λ^*}.

Let $f_\lambda \in \ker(S_{\max} - \lambda I)$. It follows from Green's identity that

$$(\operatorname{Im} \lambda)\|f_\lambda\|^2 = \big(\Gamma_0 f_\lambda, (\operatorname{Im} W_\lambda)\Gamma_0 f_\lambda\big), \quad \text{where } \operatorname{Im} W_\lambda = \frac{W_\lambda - W_\lambda^\dagger}{2i}. \tag{A.1}$$

Therefore, $(\operatorname{Im} \lambda)(\operatorname{Im} W_\lambda) > 0$ for nonreal λ. The latter means that W_λ is a Herglotz–Nevanlinna function (see [18]).

Let $\mathbf{T}$ be a bounded operator in the auxiliary Hilbert space $\mathcal{H}$. The operator

$$H_{\mathbf{T}} = S_{\max} \restriction_{\mathcal{D}(H_{\mathbf{T}})}, \qquad \mathcal{D}(H_{\mathbf{T}}) = \big\{ f \in \mathcal{D}(S_{\max}) : \mathbf{T}\Gamma_0 f = \Gamma_1 f \big\}$$

is a proper extension of $S_{\min}$ (i.e., $S_{\min} \subset H_{\mathbf{T}} \subset S_{\max}$). Moreover, the adjoint operator $H_{\mathbf{T}}^\dagger$ is also a proper extension and $H_{\mathbf{T}}^\dagger = H_{\mathbf{T}^\dagger}$, where $\mathbf{T}^\dagger$ is the adjoint operator of $\mathbf{T}$ in the auxiliary space $\mathcal{H}$. Hence, the self-adjointness of the unbounded operator $H_{\mathbf{T}}$ in $\mathfrak{H}$ is equivalent to the self-adjointness of the bounded operator $\mathbf{T}$ in the auxiliary space $\mathcal{H}$.

The spectrum of $H_{\mathbf{T}}$ is described in terms of $\mathbf{T}$ and W_λ. Namely (see [16]), $\lambda \in \rho(H_\infty)$ belongs to the point $\sigma_p(H_{\mathbf{T}})$, to the residual $\sigma_r(H_{\mathbf{T}})$, and to the continuous $\sigma_c(H_{\mathbf{T}})$ parts of the spectrum of $H_{\mathbf{T}}$ if and only if 0 belongs to the same parts of the spectrum of $\mathbf{T} - W_\lambda$; that is,

$$\lambda \in \rho(H_\infty) \cap \sigma_\alpha(H_{\mathbf{T}}) \quad \iff \quad 0 \in \sigma_\alpha(\mathbf{T} - W_\lambda), \quad \alpha \in \{p, r, c\}. \tag{A.2}$$

For each $\lambda \in \rho(H_\infty)$, the operator Γ_0 is a bijective mapping of the subspace $\ker(S_{\max} - \lambda I)$ onto $\mathcal{H}$. Its bounded inverse

$$\gamma(\lambda) = (\Gamma_0 \restriction_{\ker(S_{\max} - \lambda I)})^{-1} : \mathcal{H} \to \ker(S_{\max} - \lambda I)$$

is called the *γ-field associated with* $(\mathcal{H}, \Gamma_0, \Gamma_1)$.

The γ-field $\gamma(\cdot)$ is a holomorphic operator-valued function on $\rho(H_\infty)$ and (see [27, Propositions 14.14, 14.15])

$$\gamma(\lambda^*)^\dagger = \Gamma_1 (H_\infty - \lambda I)^{-1}, \qquad \frac{d}{d\lambda} W_\lambda = \gamma(\lambda^*)^\dagger \gamma(\lambda), \tag{A.3}$$

where the adjoint operator $\gamma(\lambda^*)^\dagger$ maps $\ker(S_{\max} - \lambda^* I)$ into $\mathcal{H}$. For any $\lambda \in \rho(H_\infty) \cap \rho(H_{\mathbf{T}})$, the Krein–Naimark resolvent formula

$$(H_{\mathbf{T}} - \lambda I)^{-1} - (H_\infty - \lambda I)^{-1} = \gamma(\lambda)(\mathbf{T} - W_\lambda)^{-1} \gamma(\lambda^*)^\dagger \tag{A.4}$$

holds (see [27, Theorem 14.18]).

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