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ON THE S-MATRIX OF SCHRÖDINGER OPERATOR WITH NONLOCAL δ-INTERACTION

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Abstract. Schrödinger operators with nonlocal δ-interaction are studied with the use of the Lax–Phillips scattering theory methods. The condition of applicability of the Lax–Phillips approach in terms of non-cyclic functions is established. Two formulas for the S-matrix are obtained. The first one deals with the Krein–Naimark resolvent formula and the Weyl–Titchmarsh function, whereas the second one is based on modified reflection and transmission coefficients. The S-matrix $S(z)$ is analytical in the lower half-plane $\mathbb{C}_-$ when the Schrödinger operator with nonlocal δ-interaction is positive self-adjoint. Otherwise, $S(z)$ is a meromorphic matrix-valued function in $\mathbb{C}_-$ and its properties are closely related to the properties of the corresponding Schrödinger operator. Examples of S-matrices are given.

Keywords: Lax–Phillips scattering scheme, scattering matrix, S-matrix, nonlocal δ-interaction, non-cyclic function.

Mathematics Subject Classification: 47B25, 47A40.

1. INTRODUCTION

Theory of non self-adjoint operators attracts a steady interests in various fields of mathematics and physics, see, e.g., [7] and the reference therein. This interest grew considerably due to the recent progress in theoretical physics of pseudo-Hermitian Hamiltonians [9].

In the present paper we study non-self-adjoint Schrödinger operators with *nonlocal* point interaction. Self-adjoint operators have been investigated by Nizhnik *et al.* [4–6,10]. The case of non-self-adjoint operators with nonlocal point interaction is more complicated and it requires more detailed analysis. One of the simplest models of a non-local δ-interaction is

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

where δ is the delta-function, $q \in L_2(\mathbb{R})$, and $(\cdot,\cdot)$ is the inner product (linear in the first argument) in $L_2(\mathbb{R})$. The expression (1.1) determines the following operator acting in $L_2(\mathbb{R})$:

$$H_{aq}f = -\frac{d^2 f}{dx^2} + f(0)q(x), \tag{1.2}$$

$$\mathcal{D}(H_{aq}) = \left\{ f \in W_2^2(\mathbb{R}\backslash\{0\}) \ : \ \begin{array}{l} f_s(0) = 0 \\ f_s'(0) = af_r(0) + (f,q) \end{array} \right\}, \tag{1.3}$$

where $f_s(0) = f(0+) - f(0-)$ and $f_r(0) = \dfrac{f(0+) + f(0-)}{2}$.

The operator H_{aq} is self-adjoint if and only if $a \in \mathbb{R}$ and it can be interpreted as a Hamiltonian corresponding to the non-local δ-interaction (1.1). Setting $q = 0$, we obtain an operator $H_a := H_{a0}$ generated by the ordinary δ-interaction

$$-\frac{d^2}{dx^2} + a < \delta, \cdot > \delta(x).$$

The spectral analysis of non-self-adjoint H_{aq} $(a \in \mathbb{C}\backslash\mathbb{R})$ was carried out in [21]. One of interesting features is that non-real a determines the measure of non-self-adjointness of H_{aq}, while the function q is responsible for the appearance of exceptional points and eigenvalues on continuous spectrum [21, Example 5.3 and Section 6].

In the present paper, we investigate H_{aq} by the scattering theory methods. For the case $a = 0$, the scattering matrix $S(\delta)$ of H_{0q} was constructed in [4, Section 5] with the use of modified Jost solutions. In contrast to [4] we study the general case $a \in \mathbb{C}$ with the use of an operator-theoretical interpretation of the Lax–Phillips approach in scattering theory [23] that was consistently developed in [12, 16, 18, 19]. We prefer this approach because it involves a simple algorithm for an explicit calculation of the analytic continuation[1)] of the scattering matrix into the lower half-plane $\mathbb{C}_-$.

The paper is organized as follows. We begin with presentation of necessary facts about the Lax–Phillips scattering theory. Further, in Section 3, we analyze for which operators H_{aq} one can apply the Lax–Phillips approach. For technical reasons it is convenient to work with unitary equivalent copies $\mathbf{H}_{a\mathbf{q}}$ of the operators H_{aq} acting in the Hilbert space $L_2(\mathbb{R}_+, \mathbb{C}^2)$, see (3.2), (3.3). The main result (Theorem 3.3) implies that $\mathbf{H}_{a\mathbf{q}}$ can be investigated in framework of the Lax–Phillips theory under the condition that $\mathbf{q}$ is non-cyclic with respect to the backward shift operator. For such kind of positive self-adjoint operators $\mathbf{H}_{a\mathbf{q}}$, two formulas of the analytical continuation $S(z)$ of the scattering matrix $S(\delta)$ into $\mathbb{C}_-$ are obtained in Section 4. The first one (4.8) deals with the Krein–Naimark resolvent formula (3.7) and the Weyl–Titchmarsh function (3.9), whereas the second one (4.19) is based on the modified reflection R_z^i and the transmission T_z^i coefficients that is more familiar for non-stationary scattering theory.

We mention that the relationship between scattering matrices and the extension theory subjects like Krein–Naimark formula and Weyl–Titchmarsh function was

[1)] "The most beautiful and important aspect of the Lax–Phillips approach is that certain analyticity properties of the scattering operator arise naturally" [25, p. 211].

established for various cases [2, 8, 11] and it provides additional possibilities for the study of scattering systems.

In Section 5, the formula (4.8) is used for the definition of S-matrix $S(z)$ for each operator $\mathbf{H}_{a\mathbf{q}}$ (assuming, of course, that $\mathbf{q}$ is non-cyclic). If $\mathbf{H}_{a\mathbf{q}}$ is positive self-adjoint, then the S-matrix is the direct consequence of proper arguments of the Lax–Phillips theory and it coincides with the analytical continuation of the Lax–Phillips scattering matrix into $\mathbb{C}_-$. Otherwise, $S(z)$ defined by (4.8) is a meromorphic matrix-valued function in $\mathbb{C}_-$ and it can be considered as a characteristic function of $\mathbf{H}_{a\mathbf{q}}$. Lemmas 5.1–5.5 and Corollary 5.6 justify such a point of view by showing a close relationship between properties of non-self-adjoint $\mathbf{H}_{a\mathbf{q}}$ and theirs S-matrices. Examples of S-matrices for various non-cyclic $\mathbf{q}$ are given in Section 5.1.

Throughout the paper, $\mathcal{D}(H)$, $\mathcal{R}(H)$, and $\ker H$ denote the domain, the range, and the null-space of a linear operator H, respectively, whereas $H \upharpoonright_{\mathcal{D}}$ stands for the restriction of H to the set $\mathcal{D}$ and $\bigvee_{t\in\mathbb{R}} X_t$ means the closure of linear span of sets X_t. The symbol $H^2(\mathbb{C}_+)$, where $\mathbb{C}_+ = \{z \in \mathbb{C} : Im\ z > 0\}$ is used for the Hardy space. The Sobolev space is denoted as $W_2^p(I)$ ($I \in \{\mathbb{R}, \mathbb{R}_+\}$, $p \in \{1, 2\}$).

2. ELEMENTS OF LAX–PHILLIPS SCATTERING THEORY

Here all necessary results about the Lax–Phillips scattering theory are presented. The monographs [23], [20, Chap. III] and the papers [16, 19] are recommended as complementary reading on the subject.

2.1. APPLICABILITY OF THE LAX–PHILLIPS SCATTERING APPROACH

A continuous group of unitary operators $W(t)$ acting in a Hilbert space $\mathfrak{W}$ is a subject of the Lax–Phillips scattering theory [23] if there exist so-called *incoming* D_- and *outgoing* D_+ subspaces of $\mathfrak{W}$ with properties:

(i)
$$W(t)D_+ \subset D_+, \quad W(-t)D_- \subset D_-, \quad t \geq 0,$$

(ii)
$$\bigcap_{t>0} W(t)D_+ = \bigcap_{t>0} W(-t)D_- = \{0\}.$$

Conditions (i)–(ii) allow to construct incoming and outgoing spectral representations for the restrictions of $W(t)$ onto the subspaces

$$M_- = \bigvee_{t\in\mathbb{R}} W(t)D_- \quad \text{and} \quad M_+ = \bigvee_{t\in\mathbb{R}} W(t)D_+, \tag{2.1}$$

respectively and define the corresponding Lax–Phillips scattering matrix $S(\delta)$ ($\delta \in \mathbb{R}$) whose values are contraction operators [1], [20, Chap. 3].

Furthermore, the additional condition of orthogonality

(iii)
$$D_- \perp D_+$$

guarantees that $S(\delta)$ is the boundary value of a contracting operator-valued function $S(z)$ holomorphic in the lower half-plane $\mathbb{C}_-$ [23, p. 52].

Usually, the Lax–Phillips scattering matrix is defined with the use of an operator-differential equation

$$\frac{d^2}{dt^2}u = -Hu, \tag{2.2}$$

where H is a positive[2)] self-adjoint operator in a Hilbert space $\mathfrak{H}$. Denote by $\mathfrak{H}_H$ the completion of $\mathcal{D}(H)$ with respect to the norm $\|\cdot\|_H^2 := (H\cdot, \cdot)$.

The Cauchy problem for (2.2) determines a continuous group of unitary operators $W(t)$ in the space

$$\mathfrak{W} = \mathfrak{H}_H \oplus \mathfrak{H} = \left\{ \begin{bmatrix} u \\ v \end{bmatrix} \ : \ u \in \mathfrak{H}_H, v \in \mathfrak{H} \right\}.$$

If $H = -\Delta$ and $\mathfrak{H} = L_2(\mathbb{R}^n)$, then (2.2) coincides with the wave equation $u_{tt} = \Delta u$ and the corresponding subspaces $D_\pm$ constructed in [23] possess the additional property

$$JD_- = D_+, \tag{2.3}$$

where J is a self-adjoint and unitary operator in $\mathfrak{W}$ (so-called time-reversal operator):

$$J \begin{bmatrix} u \\ v \end{bmatrix} = \begin{bmatrix} u \\ -v \end{bmatrix}. \tag{2.4}$$

Relation (2.3) is a characteristic property of dynamics governed by wave equations.

It is clear that, the existence of subspaces $D_\pm$ for $W(t)$ is determined by specific properties of H in (2.2). Before explaining which properties of H are needed, we recall that a symmetric operator B is called *simple* if its restriction on any nontrivial reducing subspace is not a self-adjoint operator. The maximality of B means that there are no symmetric extensions of B. The latter is equivalent to the fact that one of defect numbers of B is equal to zero. In what follows, without loss of generality, we assume that B has *zero defect number* in $\mathbb{C}_+$, i.e., $\dim\ker(B^* - iI) = 0$, where B^* is the adjoint of B. The latter means that

$$\ker(B^{*2} - \mu^2 I) = \ker(B^* - \mu I), \quad \mu \in \mathbb{C}_-. \tag{2.5}$$

Theorem 2.1 ([19,20])**.** *Let H be a positive self-adjoint operator in a Hilbert space $\mathfrak{H}$. The following are equivalent:*

- (i) *the group $W(t)$ of solutions of the Cauchy problem of* (2.2) *has subspaces $D_\pm$ with properties* (i)–(iii) *and* (2.3)*,*
- (ii) *there exists a simple maximal symmetric operator B acting in a subspace $\mathfrak{H}_0$ of $\mathfrak{H}$ such that H is an extension* (*with exit in the space $\mathfrak{H}$*) *of the symmetric operator B^2.*

2) i.e. $(Hf, f) > 0$ for nonzero $f \in \mathcal{D}(H)$.

2.2. THE LAX–PHILLIPS SCATTERING MATRIX AND ITS ANALYTICAL CONTINUATION

By Theorem 2.1, the unitary group $W(t)$ can be investigated by the Lax–Phillips scattering methods if and only if H is an extension of a symmetric operator B^2 acting in a subspace $\mathfrak{H}_0$ of $\mathfrak{H}$. A simple maximal symmetric operator B in Theorem 2.1 turns out to be a useful technical tool allowing one to exhibit principal parts of the Lax–Phillips theory in a simple form. In particular, the subspaces $D_\pm$ coincide with the closure[3)] of the sets:

$$\left\{\begin{bmatrix} u \\ iBu \end{bmatrix} \mid \forall u \in \mathcal{D}(B^2)\right\} \quad \text{and} \quad \left\{\begin{bmatrix} u \\ -iBu \end{bmatrix} \mid \forall u \in \mathcal{D}(B^2)\right\}, \tag{2.6}$$

respectively. Moreover, for all $t \geq 0$,

$$W(t)\begin{bmatrix} u \\ iBu \end{bmatrix} = \begin{bmatrix} V(t)u \\ iBV(t)u \end{bmatrix}, \quad W(-t)\begin{bmatrix} u \\ -iBu \end{bmatrix} = \begin{bmatrix} V(t)u \\ -iBV(t)u \end{bmatrix}, \tag{2.7}$$

where $V(t) = e^{iBt}$ is a semigroup of isometric operators in $\mathfrak{H}_0$.

The formulas (2.1), (2.6), and (2.7) allow one to construct the incoming/outgoing spectral representations for the restrictions of $W(t)$ onto $M_\pm$ in an explicit form [14, Section 2.1]. The latter leads to a simple method for the calculation of the Lax–Philips scattering matrix $S(\cdot)$ [12, 18]. Actually, we need only a positive boundary triplet[4)] $(\mathcal{H}, \Gamma_0, \Gamma_1)$ of B^{*2} defined as follows: denote $\mathcal{H} = \ker(B^{*2} + I)$, then $\mathcal{D}(B^{*2}) = \mathcal{D}(B^*B) \dot{+} \mathcal{H}$ and each vector $f \in \mathcal{D}(B^{*2})$ can be decomposed:

$$f = u + h, \quad u \in \mathcal{D}(B^*B), \quad h \in \mathcal{H}. \tag{2.8}$$

The formula (2.8) allows to define the linear mappings $\Gamma_i : \mathcal{D}(B^{*2}) \to \mathcal{H}$

$$\Gamma_0 f = \Gamma_0(u + h) = h, \quad \Gamma_1 f = \Gamma_1(u + h) = P_{\mathcal{H}}(B^*B + I)u, \tag{2.9}$$

where $P_{\mathcal{H}}$ is the orthogonal projector of $\mathfrak{H}_0$ onto the subspace $\mathcal{H}$.

Theorem 2.2 ([12, 18])**.** *If conditions of Theorem 2.1 hold, then the Lax–Phillips scattering matrix $S(\cdot)$ for the unitary group $W(t)$ of Cauchy problem solutions of* (2.2) *has the following analytical continuation into $\mathbb{C}_-$:*

$$S(z) = [I - 2(1 + iz)C(z)][I - 2(1 - iz)C(z)]^{-1}, \quad z \in \mathbb{C}_-, \tag{2.10}$$

where the operators $C(z) : \mathcal{H} \to \mathcal{H}$ are determined by the relation

$$C(z)\Gamma_1 u = \Gamma_0 u, \quad u \in P_{\mathfrak{H}_0}(H - z^2 I)^{-1} \ker(B^* + \overline{z} I), \quad z \in \mathbb{C}_-. \tag{2.11}$$

An investigation of $C(z)$ carried out in [18] shows that the values of $S(z)$ are contraction operators in $\mathcal{H}$ and $S^*(z) = S(-\overline{z})$.

3) In the space $\mathfrak{W}$.

4) See [15, Chap. 3] for definition of boundary triplets and positive boundary triplets.

In what follows, the analytical continuation (2.10) of the Lax–Phillips scattering matrix will be called the *S-matrix* of the positive self-adjoint operator H in (2.2). For this reason it is natural to ask: *To what extend the S-matrix determines H?*

We recall that a self-adjoint operator H is called *minimal* if each subspace of $\mathfrak{H}\ominus\mathfrak{H}_0$ that reduces H is trivial. Minimal self-adjoint extensions H_1 and H_2 of B^2 are called *unitary equivalent* if there exists an unitary operator Z in $\mathfrak{H}$ such that $ZH_1 = H_2Z$ and $Zf = f$ for all $f \in \mathfrak{H}_0$.

It follows from [18] that the S-matrix determines a minimal positive self-adjoint extension H of B^2 up to unitary equivalence.

Remark 2.3. Various approaches in non-stationary scattering theory are based on the comparing of two evolutions: "unperturbed" and "perturbed". The subspaces $D_\pm$ characterize unperturbed evolution in the Lax–Phillips approach. Due to (2.6), the subspaces $D_\pm$ are described by the operator B. The operator B^*B is a positive self-adjoint extension of B^2 in the space $\mathfrak{H}_0$ and the group $W_0(t)$ of solutions of the Cauchy problem of (2.2) (with B^*B instead of H) determines an unperturbed evolution. The corresponding wave operators $\Omega_\pm = s - \lim_{t\to\pm\infty} W(-t)W_0(t)$ exist and are isometric in $\mathfrak{H}_0$. The scattering operator $\Omega_+^*\Omega_-$ coincides with the Lax–Phillips scattering matrix $S(\delta)$ in the spectral representation of the unperturbed evolution $W_0(t)$ [18].

3. PROPERTIES OF OPERATORS $\mathbf{H}_{a\mathbf{q}}$

3.1. PRELIMINARIES

For technical reasons it is convenient to calculate the S-matrix for unitary equivalent copy of the operator H_{aq} in the Hilbert space $L_2(\mathbb{R}_+, \mathbb{C}^2)$. To do that, for each function $f \in L_2(\mathbb{R})$, we define the operator[5)]

$$Yf = \begin{bmatrix} f(x) \\ f(-x) \end{bmatrix} = \mathbf{f}(x), \quad x > 0$$

that maps isometrically $L_2(\mathbb{R})$ onto $L_2(\mathbb{R}_+, \mathbb{C}^2)$ and maps $W_2^2(\mathbb{R}\backslash\{0\})$ onto $W_2^2(\mathbb{R}_+, \mathbb{C}^2)$. For all $\mathbf{f} = Yf$, $f \in W_2^2(\mathbb{R}\backslash\{0\})$ we denote $[\mathbf{f}]_r = f_r(0)$ and $[\mathbf{f}]_s = f_s(0)$. In other words,

$$[\mathbf{f}]_r = \frac{1}{2}\lim_{x\to+0}(f_1(x) + f_2(x)), \quad [\mathbf{f}]_s = \lim_{x\to+0}(f_1(x) - f_2(x)), \quad \mathbf{f} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}. \tag{3.1}$$

It is easy to see that $YH_{aq} = \mathbf{H}_{a\mathbf{q}}Y$, where H_{aq} is defined by (1.2), (1.3) and the operator

$$\mathbf{H}_{a\mathbf{q}}\mathbf{f} = -\frac{d^2\mathbf{f}}{dx^2} + [\mathbf{f}]_r\mathbf{q}(x), \quad \mathbf{q} = \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} = Yq \tag{3.2}$$

5) We will use the mathbf font for $\mathbb{C}^2$-valued functions of $L_2(\mathbb{R}_+, \mathbb{C}^2)$ in order to avoid confusion with functions from $L_2(\mathbb{R})$. In particular, $\mathbf{e}^{-i\mu x} \equiv \begin{bmatrix} e^{-i\mu x} \\ e^{-i\mu x} \end{bmatrix}$.

acts in $L_2(\mathbb{R}_+, \mathbb{C}^2)$ with domain of definition

$$\mathcal{D}(\mathbf{H}_{a\mathbf{q}}) = \{\mathbf{f} \in W_2^2(\mathbb{R}_+, \mathbb{C}^2) : \ [\mathbf{f}]_s = 0, \quad [\mathbf{f}']_r = a[\mathbf{f}]_r + (\mathbf{f}, \mathbf{q})_+\}, \tag{3.3}$$

where $(\mathbf{f}, \mathbf{q})_+ = (Yf, Yq)_+ = (f, q)$ is the scalar product in $L_2(\mathbb{R}_+, \mathbb{C}^2)$.

When $a \to \infty$, the formulas (3.2) and (3.3) determine a positive self-adjoint operator in $L_2(\mathbb{R}_+, \mathbb{C}^2)$

$$\mathbf{H}_\infty \equiv \mathbf{H}_{\infty\mathbf{q}} = -\frac{d^2}{dx^2}, \quad \mathcal{D}(\mathbf{H}_\infty) = \{\mathbf{f} \in W_2^2(\mathbb{R}_+, \mathbb{C}^2) : \ \mathbf{f}(0) = 0\}$$

that does not depend on the choice of $\mathbf{q}$ and can be decomposed

$$\mathbf{H}_\infty \mathbf{f} = \begin{bmatrix} H_\infty f_1 \\ H_\infty f_2 \end{bmatrix}, \quad H_\infty = -\frac{d^2}{dx^2}, \quad \mathcal{D}(H_\infty) = \{f \in W_2^2(\mathbb{R}_+) : \ f(0) = 0\}.$$

By analogy with [21, Section 5] (where the case of operators H_{aq} has been studied) we consider $\mathbf{H}_{a\mathbf{q}}$ and $\mathbf{H}_\infty$ as restrictions of the maximal operator

$$\mathbf{H}_{max}\mathbf{f} = -\frac{d^2\mathbf{f}}{dx^2} + [\mathbf{f}]_r \mathbf{q}(x), \quad \mathcal{D}(\mathbf{H}_{max}) = \{\mathbf{f} \in W_2^2(\mathbb{R}_+, \mathbb{C}^2) : \ [\mathbf{f}]_s = 0\}$$

onto the corresponding domain of definition.

The maximal operator $\mathbf{H}_{max}$ has a boundary triplet $(\mathbb{C}, \Gamma_0, \Gamma_1)$, where

$$\Gamma_0 \mathbf{f} = [\mathbf{f}]_r, \quad \Gamma_1 \mathbf{f} = 2[\mathbf{f}']_r - (\mathbf{f}, \mathbf{q})_+, \quad \mathbf{f} \in \mathcal{D}(\mathbf{H}_{max}) \tag{3.4}$$

and the formulas (3.2) and (3.3) are rewritten:

$$\mathbf{H}_{a\mathbf{q}} = \mathbf{H}_{max} \restriction_{\mathcal{D}(\mathbf{H}_{a\mathbf{q}})}, \quad \mathcal{D}(\mathbf{H}_{a\mathbf{q}}) = \{\mathbf{f} \in \mathcal{D}(\mathbf{H}_{max}) \ : \ a\Gamma_0 \mathbf{f} = \Gamma_1 \mathbf{f}\}. \tag{3.5}$$

In particular, $\mathbf{H}_\infty$ is the restriction of $\mathbf{H}_{max}$ onto $\ker \Gamma_0$ and its resolvent is

$$(\mathbf{H}_\infty - z^2 I)^{-1}\mathbf{f} = \frac{i}{2z}[\mathbf{A}_z(x)e^{-izx} + \mathbf{B}_z(x)e^{izx}], \quad \mathbf{f} \in L_2(\mathbb{R}_+, \mathbb{C}^2), \tag{3.6}$$

where $z \in \mathbb{C}_-$ and

$$\mathbf{A}_z(x) = \int_0^\infty e^{-izs}\mathbf{f}(s)ds - \int_0^x e^{izs}\mathbf{f}(s)ds, \quad \mathbf{B}_z(x) = -\int_x^\infty e^{-izs}\mathbf{f}(s)ds.$$

Lemma 3.1. *The Krein–Naimark resolvent formula*

$$(\mathbf{H}_{a\mathbf{q}} - z^2 I)^{-1}\mathbf{f} = (\mathbf{H}_\infty - z^2 I)^{-1}\mathbf{f} + \frac{(\mathbf{f}, \mathbf{u}_{-\overline{z}})_+}{a - W(z^2)}\mathbf{u}_z(x) \tag{3.7}$$

holds for $a \neq W(z^2)$. Here,

$$\mathbf{u}_\mu(x) = \mathbf{e}^{-i\mu x} - (\mathbf{H}_\infty - \mu^2 I)^{-1}\mathbf{q}, \qquad \mu \in \{z, -\overline{z}\} \subset \mathbb{C}_- \tag{3.8}$$

is an eigenfunction of $\mathbf{H}_{max}$ corresponding to the eigenvalue μ^2 and

$$W(z^2) = -2iz - 2(\mathbf{e}^{-izx}, Re\ \mathbf{q})_+ + ((\mathbf{H}_\infty - z^2 I)^{-1}\mathbf{q}, \mathbf{q})_+, \quad z \in \mathbb{C}_-. \tag{3.9}$$

Proof. It follows from [21] that the subspace $\ker(\mathbf{H}_{max} - \mu^2 I)$ is one dimensional and it is generated by the function $\mathbf{u}_\mu$ defined by (3.8). Setting $\mu = z$ and using (3.4), we conclude that $\Gamma_0 \mathbf{u}_z = 1$ and the Weyl–Titchmarsh function associated to the boundary triplet $(\mathbb{C}, \Gamma_0, \Gamma_1)$ takes the form

$$W(z^2) = \Gamma_1 \mathbf{u}_z = -2iz - 2[\mathbf{v}']_r - (\mathbf{e}^{-izx} + \mathbf{v}, \mathbf{q})_+,$$

where $\mathbf{v} = (\mathbf{H}_\infty - z^2 I)^{-1}\mathbf{q}$. In view of (3.6), $\mathbf{v}'(0) = \int_0^\infty e^{-izs}\mathbf{q}(s)ds$ and hence,

$$2[\mathbf{v}']_r + (\mathbf{e}^{-izx}, \mathbf{q})_+ = 2(\mathbf{e}^{-izx}, Re\ \mathbf{q})_+, \quad Re\ \mathbf{q} = \begin{bmatrix} Re\ q_1 \\ Re\ q_2 \end{bmatrix}.$$

Substituting this expression into the formula for $W(z^2)$ we obtain (3.9).

In terms of the boundary triplet $(\mathbb{C}, \Gamma_0, \Gamma_1)$, the Krein–Naimark resolvent formula has the form [26, Theorem 14.18, Proposition 14.14]

$$(\mathbf{H}_{a\mathbf{q}} - z^2 I)^{-1}\mathbf{f} = (\mathbf{H}_\infty - z^2 I)^{-1}\mathbf{f} + \frac{\Gamma_1 \mathbf{u}}{a - W(z^2)}\mathbf{u}_z(x),$$

where $\mathbf{u} = (\mathbf{H}_\infty - z^2 I)^{-1}\mathbf{f}$. In view of (3.6), $\mathbf{u}'(0) = \int_0^\infty e^{-izs}\mathbf{f}(s)ds$. Taking (3.1) into account,

$$2[\mathbf{u}']_r = \int_0^\infty e^{-izs}(f_1(s) + f_2(s))dx = (\mathbf{f}, \mathbf{e}^{i\overline{z}x})_+.$$

Finally, using (3.4) and (3.8) with $\mu = -\overline{z}$, we obtain

$$\Gamma_1 \mathbf{u} = (\mathbf{f}, \mathbf{e}^{i\overline{z}x})_+ - (\mathbf{u}, \mathbf{q})_+ = (\mathbf{f}, \mathbf{e}^{i\overline{z}x} - (\mathbf{H}_\infty - \overline{z}^2 I)^{-1}\mathbf{q})_+ = (\mathbf{f}, \mathbf{u}_{-\overline{z}})_+$$

that completes the proof. □

3.2. APPLICABILITY OF THE LAX–PHILLIPS APPROACH FOR $\mathbf{H}_{a\mathbf{q}}$

Denote by

$$\mathcal{B} = i\frac{d}{dx}, \quad \mathcal{D}(\mathcal{B}) = \{u \in W_2^1(\mathbb{R}_+) : u(0) = 0\} \tag{3.10}$$

the first derivative operator in $L_2(\mathbb{R}_+)$. The *same notation* will be used for its analog acting in $L_2(\mathbb{R}_+, \mathbb{C}^2)$. The both operators are simple maximal symmetric with zero defect numbers in $\mathbb{C}_+$, and theirs Cayley transforms

$$T = (\mathcal{B} - iI)(\mathcal{B} + iI)^{-1} \tag{3.11}$$

are forward shift operators in the corresponding spaces.

A function $\mathbf{q} \in L_2(\mathbb{R}_+, \mathbb{C}^2)$ is called *non-cyclic* for the backward shift operator T^* if the subspace

$$E_{\mathbf{q}} = \bigvee_{n=0}^{\infty} T^{*n}\mathbf{q}$$

does not coincide with $L_2(\mathbb{R}_+, \mathbb{C}^2)$.

Considering $L_2(\mathbb{R}_+)$ as a subspace of $L_2(\mathbb{R})$ we conclude that the Fourier transform

$$Ff(\delta) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{i\delta s} f(s) ds$$

maps isometrically $L_2(\mathbb{R}_+)$ onto the Hardy space $H^2(\mathbb{C}_+)$ and

$$F\mathcal{B}u = \delta F u, \quad FTf = \frac{\delta - i}{\delta + i} Ff, \quad u \in \mathcal{D}(\mathcal{B}), f \in L_2(\mathbb{R}_+).$$

Let $\psi \in H^\infty(\mathbb{C}_+)$ be an inner function. Then

$$\psi(\mathcal{B}) = F^{-1}\psi(\delta)F \tag{3.12}$$

is an isometric operator in $L_2(\mathbb{R}_+)$ which commutes with $\mathcal{B}$ [14, Section 5].

Lemma 3.2. *The following are equivalent:*

(i) *a function* $\mathbf{q} = \begin{bmatrix} q_1 \\ q_2 \end{bmatrix}$ *is non-cyclic for the backward shift operator* T^*,

(ii) *there exists an inner function* $\psi \in H^\infty(\mathbb{C}_+)$ *such that the subspace* $\mathfrak{H}_0 = \psi(\mathcal{B})L_2(\mathbb{R}_+)$ *of* $L_2(\mathbb{R}_+)$ *is orthogonal to at least one of the functions* q_i.

Proof. (i)⇒(ii) Since $E_{\mathbf{q}} = E_{q_1} \oplus E_{q_2}$, the function $\mathbf{q}$ is non-cyclic if and only if at least one of the functions $q_i \in L_2(\mathbb{R}_+)$ is non-cyclic for the backward shift operator T^* in $L_2(\mathbb{R}_+)$. Let $q \equiv q_i$ be non-cyclic. Then the non-zero subspace

$$\mathfrak{H}_0 = L_2(\mathbb{R}_+) \ominus E_q$$

is invariant with respect to T. This means that $F\mathfrak{H}_0$ is invariant with respect to the multiplication by $\frac{\delta - i}{\delta + i}$ in $H^2(\mathbb{C}_+)$. The Beurling theorem [22, p. 164] yields the existence of an inner function $\psi \in H^\infty(\mathbb{C}_+)$ such that $F\mathfrak{H}_0 = \psi(\delta)H_2(\mathbb{C}_+)$. Therefore

$$\mathfrak{H}_0 = F^{-1}\psi(\delta)FL_2(\mathbb{R}_+) = \psi(\mathcal{B})L_2(\mathbb{R}_+).$$

By the construction, $\mathfrak{H}_0$ is orthogonal to q (since, q belongs to E_q).

(ii)⇒(i) Let $\mathfrak{H}_0 = \psi(\mathcal{B})L_2(\mathbb{R}_+)$ be orthogonal to q. Then[6)]

$$(\psi(\mathcal{B})f, T^{*n}q)_+ = (T^n\psi(\mathcal{B})f, q)_+ = (\psi(\mathcal{B})T^n f, q)_+ = 0 \quad \text{for all} \quad f \in L_2(\mathbb{R}_+).$$

Therefore, $T^{*n}q$ is orthogonal to $\mathfrak{H}_0$. This means that E_q is orthogonal to $\mathfrak{H}_0$. Therefore, E_q is a proper subspace of $L_2(\mathbb{R}_+)$ and q is non-cyclic. □

Theorem 3.3. *If* $\mathbf{q}$ *is non-cyclic for* T^*, *then there exists a simple maximal symmetric operator* B *acting in a subspace* $\mathfrak{H}_0$ *of* $L_2(\mathbb{R}_+, \mathbb{C}^2)$ *such that the operators* $\mathbf{H}_{a\mathbf{q}}$ *are extensions of the symmetric operator* B^2 *for all* $a \in \mathbb{C}$.

[6)] Here, $(\cdot,\cdot)_+$ is the scalar product in $L_2(\mathbb{R}_+)$.

Proof. If $\mathbf{q}$ is non-cyclic, then at least one of q_i is non-cyclic. Consider firstly the case where the both of functions q_i are non-cyclic. Due to the proof of Lemma 3.2, for each q_i there exists an inner function ψ_i such that the subspace $\psi_i(\mathcal{B})L_2(\mathbb{R}_+)$ is orthogonal to q_i. Denote

$$\mathfrak{H}_0 = \begin{bmatrix} \psi_1(\mathcal{B})L_2(\mathbb{R}_+) \\ \psi_2(\mathcal{B})L_2(\mathbb{R}_+) \end{bmatrix} = \psi(\mathcal{B})L_2(\mathbb{R}_+, \mathbb{C}^2), \tag{3.13}$$

where

$$\psi(\mathcal{B}) = \begin{bmatrix} \psi_1(\mathcal{B}) & 0 \\ 0 & \psi_2(\mathcal{B}) \end{bmatrix} \tag{3.14}$$

is an isometric operator in $L_2(\mathbb{R}_+, \mathbb{C}^2)$ that commutes with $\mathcal{B}$. This allows to define a simple maximal symmetric operator in $\mathfrak{H}_0$:

$$B = \psi(\mathcal{B})\mathcal{B}\psi(\mathcal{B})^*, \quad \mathcal{D}(B) = \psi(\mathcal{B})\mathcal{D}(\mathcal{B}). \tag{3.15}$$

Since $\psi(\mathcal{B})$ commutes with $\mathcal{B}$, the formula (3.15) can be rewritten as

$$B\mathbf{u} = \mathcal{B}\mathbf{u}, \quad \mathbf{u} \in \mathcal{D}(B) = \psi(\mathcal{B})\mathcal{D}(\mathcal{B}) = \mathcal{D}(\mathcal{B}) \cap \mathfrak{H}_0. \tag{3.16}$$

(i.e., B is a part of $\mathcal{B}$ restricted on $\mathfrak{H}_0$). In view of (3.10) and (3.16)

$$B^2 = -\frac{d^2}{dx^2}, \quad \mathcal{D}(B^2) = \{\mathbf{u} \in W_2^2(\mathbb{R}_+, \mathbb{C}^2) \cap \mathfrak{H}_0 : \mathbf{u}(0) = \mathbf{u}'(0) = 0\}. \tag{3.17}$$

By Lemma 3.2 and (3.13), the subspace $\mathfrak{H}_0$ is orthogonal to $\mathbf{q}$. Hence, in view of (3.2), (3.3), and (3.17), $\mathcal{D}(\mathbf{H}_{a\mathbf{q}}) \supset \mathcal{D}(B^2)$ and

$$\mathbf{H}_{a\mathbf{q}}\mathbf{u} = -\frac{d^2\mathbf{u}}{dx^2} = B^2\mathbf{u} \quad \text{for all} \quad \mathbf{u} \in \mathcal{D}(B^2).$$

The case where only one q_i is non-cyclic is considered similarly. For example, if q_1 is non-cyclic whereas q_2 is cyclic (i.e., $E_{q_2} = L_2(\mathbb{R}_+)$), then $\mathfrak{H}_0$ and $\psi(\mathcal{B})$ are determined as above with $\psi_2 = 0$. □

Corollary 3.4. *Assume that $H = \mathbf{H}_{a\mathbf{q}}$ is a positive self-adjoint operator. If $\mathbf{q}$ is non-cyclic for T^*, then the group $W(t)$ of Cauchy problem solutions of* (2.2) *has incoming/outgoing subspaces $D_\pm$ defined by* (2.6)*, where B is from* (3.16).

Proof. It follows from Theorems 2.1 and 3.3. □

4. S-MATRIX FOR POSITIVE SELF-ADJOINT OPERATOR

In this section we suppose that $\mathbf{H}_{a\mathbf{q}}$ is a positive self-adjoint operator and the function $\mathbf{q}$ is non-cyclic. By Theorem 3.3, $\mathbf{H}_{a\mathbf{q}}$ is an extension of the symmetric operator B^2 defined by (3.17) that acts in the subspace $\mathfrak{H}_0 = \psi(\mathcal{B})L_2(\mathbb{R}_+, \mathbb{C}^2)$. In view of Corollary 3.4 and Theorem 2.2, the S-matrix of $\mathbf{H}_{a\mathbf{q}}$ exists and is given by (2.10). Our goal is to modify this general formula taking into account the specific choice of B in (3.16).

4.1. PRELIMINARIES

The following technical results are needed for the calculation of S-matrix.

Lemma 4.1. *Let an isometric operator $\psi(\mathcal{B})$ be defined by* (3.12). *Then*

$$\psi(\mathcal{B})^* e^{-i\mu x} = \overline{\psi(\overline{\mu})} e^{-i\mu x}, \quad \mu \in \mathbb{C}_-.$$

Proof. It follows from (3.10) that $\mathcal{B}^* = i\frac{d}{dx}$, $\mathcal{D}(\mathcal{B}^*) = W_2^1(\mathbb{R}_+)$. Therefore,

$$\ker(\mathcal{B}^* - \mu I) = \{ce^{-i\mu x} : c \in \mathbb{C}\}.$$

This means that, for all $u \in \mathcal{D}(\mathcal{B})$,

$$((\mathcal{B} - \overline{\mu} I)u, \psi(\mathcal{B})^* e^{-i\mu x})_+ = (\psi(\mathcal{B})(\mathcal{B} - \overline{\mu} I)u, e^{-i\mu x})_+ = ((\mathcal{B} - \overline{\mu} I)\psi(\mathcal{B})u, e^{-i\mu x})_+ = 0.$$

Hence $\psi(\mathcal{B})^* e^{-i\mu x}$ belongs to $\ker(\mathcal{B}^* - \mu I)$ and

$$(\psi(\mathcal{B})^* e^{-i\mu x}, e^{-i\mu x})_+ = c(e^{-i\mu x}, e^{-i\mu x})_+ = -\frac{c}{2Im\ \mu}. \tag{4.1}$$

Using (3.12) and taking into account that $F\chi_{\mathbb{R}_+}(x)e^{-i\mu x} = \frac{i}{\sqrt{2\pi}} \cdot \frac{1}{\delta - \mu}$, we verify that the inner product

$$(\psi(\mathcal{B})^* e^{-i\mu x}, e^{-i\mu x})_+ = (e^{-i\mu x}, \psi(\mathcal{B})e^{-i\mu x})_+ = (F\chi_{\mathbb{R}_+}(x)e^{-i\mu x}, \psi(\delta)F\chi_{\mathbb{R}_+}(x)e^{-i\mu x})$$

is equal to $\frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{\overline{\psi(\delta)}}{(Re\ \mu - \delta)^2 + (Im\ \mu)^2} d\delta$. The Poisson formula [24, p.147] and (4.1) lead to the conclusion that

$$c = \frac{1}{\pi}\int_{-\infty}^{\infty} \frac{-(Im\ \mu)\overline{\psi(\delta)}}{(Re\ \mu - \delta)^2 + (Im\ \mu)^2} d\delta = \overline{\psi(Re\ \mu - iIm\ \mu)} = \overline{\psi(\overline{\mu})}$$

that completes the proof. □

Lemma 4.2. *Let B and $\psi(\mathcal{B})$ be defined by* (3.15) *and* (3.14), *respectively. Then, for any $\mu \in \mathbb{C}_-$,*

$$\ker(B^{*2} - \mu^2 I) = \ker(B^* - \mu I) = \psi(\mathcal{B}) \left\{ \mathbf{h}_\mu = \begin{bmatrix} \alpha_\mu \\ \beta_\mu \end{bmatrix} e^{-i\mu x} \ : \ \alpha_\mu, \beta_\mu \in \mathbb{C} \right\}.$$

Proof. The first identity follows from (2.5). It follows from (3.15) that

$$B^* = \psi(\mathcal{B})\mathcal{B}^*\psi(\mathcal{B})^*, \quad \mathcal{D}(B^*) = \psi(\mathcal{B})\mathcal{D}(\mathcal{B}^*) = \psi(\mathcal{B})W_2^1(\mathbb{R}_+, \mathbb{C}^2). \tag{4.2}$$

By virtue of (4.2) we conclude that $\ker(B^* - \mu I) = \psi(\mathcal{B})\ker(\mathcal{B}^* - \mu I)$. It follows from the proof of Lemma 4.1 that $\ker(\mathcal{B}^* - \mu I)$ coincides with the set of vectors $\{\mathbf{h}_\mu\}$ defined above. □

Corollary 4.3. *Let $\psi(\mathcal{B})$ be defined by* (3.14). *Then, for any $\mu \in \mathbb{C}_-$,*

$$\psi(\mathcal{B})^*\mathbf{e}^{-i\mu x} = \overline{\begin{bmatrix} \psi_1(\overline{\mu}) \\ \psi_2(\overline{\mu}) \end{bmatrix}} e^{-i\mu x}, \quad \psi(\mathcal{B})^*\mathbf{u}_\mu = \begin{bmatrix} c(\mu, q_1) \\ c_(\mu, q_2) \end{bmatrix} e^{-i\mu x}, \tag{4.3}$$

where $\mathbf{u}_\mu$ is defined by (3.8) *and*

$$c(\mu, q_j) = \overline{\psi_j(\overline{\mu})} + 2(Im\ \mu)((H_\infty - \mu^2 I)^{-1} q_j, \psi_j(\mathcal{B})e^{-i\mu x})_+. \tag{4.4}$$

Proof. The first relation in (4.3) follows from Lemma 4.1.

The function $\mathbf{u}_\mu$ in the second relation is an eigenfunction of the operator $\mathbf{H}_{max}$ (see Lemma 3.1). Since $(\mathbb{C}, \Gamma_0, \Gamma_1)$ defined by (3.4) is a boundary triplet of $\mathbf{H}_{max}$, its adjoint $\mathbf{H}_{max}^*$ coincides with the symmetric operator $\mathbf{H}_{min} = \mathbf{H}_{max} \restriction_{\ker \Gamma_0 \cap \ker \Gamma_1}$. Precisely,

$$\mathbf{H}_{min} = -\frac{d^2}{dx^2}, \quad \mathcal{D}(\mathbf{H}_{min}) = \{\mathbf{f} \in W_2^2(\mathbb{R}_+, \mathbb{C}^2) : \ [\mathbf{f}]_r = 0, \ 2[\mathbf{f}']_r = (\mathbf{f}, \mathbf{q})_+\}.$$

Comparing this formula with (3.17) leads to the conclusion that $\mathbf{H}_{min} \supset B^2$, i.e., $\mathbf{H}_{min}$ is an extension of B^2 with the exit into the space $L_2(\mathbb{R}_+, \mathbb{C}^2)$. Then, for $\mathbf{f} \in \mathcal{D}(\mathbf{H}_{max})$ and $\mathbf{u} \in \mathcal{D}(B^2)$,

$$(P_{\mathfrak{H}_0}\mathbf{H}_{max}\mathbf{f}, \mathbf{u})_+ = (\mathbf{H}_{max}\mathbf{f}, \mathbf{u})_+ = (\mathbf{f}, \mathbf{H}_{min}\mathbf{u})_+ = (P_{\mathfrak{H}_0}\mathbf{f}, B^2\mathbf{u})_+ = ({B^*}^2 P_{\mathfrak{H}_0}\mathbf{f}, \mathbf{u})_+,$$

where $P_{\mathfrak{H}_0}$ is the orthogonal projection in $L_2(\mathbb{R}_+, \mathbb{C}^2)$ on the subspace $\mathfrak{H}_0$ defined by (3.13). The obtained relation means that

$$P_{\mathfrak{H}_0}\mathbf{H}_{max}\mathbf{f} = {B^*}^2 P_{\mathfrak{H}_0}\mathbf{f}, \quad \text{for all} \quad \mathbf{f} \in \mathcal{D}(\mathbf{H}_{max}) = W_2^2(\mathbb{R}_+, \mathbb{C}^2). \tag{4.5}$$

Setting $\mathbf{f} = \mathbf{u}_\mu$ in (4.5) and taking into account that $\mathbf{H}_{max}\mathbf{u}_\mu = \mu^2\mathbf{u}_\mu$, we obtain $P_{\mathfrak{H}_0}\mathbf{H}_{max}\mathbf{u}_\mu = {B^*}^2 P_{\mathfrak{H}_0}\mathbf{u}_\mu = \mu^2 P_{\mathfrak{H}_0}\mathbf{u}_\mu$. This relation and (2.5) mean

$$P_{\mathfrak{H}_0}\mathbf{u}_\mu \in \ker({B^*}^2 - \mu^2 I) = \ker(B^* - \mu I).$$

In view of Lemma 4.2, $P_{\mathfrak{H}_0}\mathbf{u}_\mu = \psi(\mathcal{B})\mathbf{h}_\mu$ for some choice of $\mathbf{h}_\mu = \begin{bmatrix} \alpha_\mu \\ \beta_\mu \end{bmatrix} e^{-i\mu x}$ or $\psi(\mathcal{B})\psi(\mathcal{B})^*\mathbf{u}_\mu = \psi(\mathcal{B})\mathbf{h}_\mu$ since $P_{\mathfrak{H}_0} = \psi(\mathcal{B})\psi(\mathcal{B})^*$. Therefore $\psi(\mathcal{B})^*\mathbf{u}_\mu = \mathbf{h}_\mu$ that leads to the second relation in (4.3) with unspecified parameters α_μ, β_μ. Taking (3.8) into account and arguing by the analogy with the determination of c in the proof of Lemma 4.1 we arrive at the conclusion that $\alpha_\mu = c(\mu, q_1)$ and $\beta_\mu = c(\mu, q_2)$, where $c(\mu, q_i)$ are defined in (4.4). □

4.2. POSITIVE BOUNDARY TRIPLET

In view of Section 2.2, the S-matrix can not be constructed without finding the positive boundary triplet $(\mathcal{H}, \Gamma_0, \Gamma_1)$ of ${B^*}^2$. Since B is the restriction of the first derivative operator $\mathcal{B}$ on $\mathfrak{H}_0$, see (3.16), one can try to express $(\mathcal{H}, \Gamma_0, \Gamma_1)$ in terms of well-known positive boundary triplet $(\mathcal{H}', \Gamma_0', \Gamma_1')$ of $\mathcal{B}^{*2}$.

Lemma 4.4. *The following relations hold:*

$$\mathcal{H} = \psi(\mathcal{B})\mathcal{H}', \quad \Gamma_0\psi(\mathcal{B}) = \psi(\mathcal{B})\Gamma_0', \quad \Gamma_1\psi(\mathcal{B}) = \psi(\mathcal{B})\Gamma_1'.$$

Proof. It follows from (4.2) that

$$B^{*2} = \psi(\mathcal{B})\mathcal{B}^{*2}\psi(\mathcal{B})^*, \quad \mathcal{D}(B^{*2}) = \psi(\mathcal{B})\mathcal{D}(\mathcal{B}^{*2}) = \psi(\mathcal{B})W_2^2(\mathbb{R}_+, \mathbb{C}^2). \tag{4.6}$$

By definition $\mathcal{H} = \ker(B^{*2} + I)$ and $\mathcal{H}' = \ker(\mathcal{B}^{*2} + I)$. Using (4.6), we obtain

$$\mathcal{H} = \ker(B^{*2} + I) = \psi(\mathcal{B}) \ker(\mathcal{B}^{*2} + I) = \psi(\mathcal{B})\mathcal{H}'.$$

It follows from (3.15) and (4.2) that

$$B^*B = \psi(\mathcal{B})\mathcal{B}^*\mathcal{B}\psi(\mathcal{B})^*, \quad \mathcal{D}(B^*B) = \psi(\mathcal{B})\mathcal{D}(\mathcal{B}^*\mathcal{B}). \tag{4.7}$$

For brevity, we denote $V = \psi(\mathcal{B})$ and consider $\mathbf{f} \in \mathcal{D}(\mathcal{B}^{*2})$. Then $\mathbf{f} = \mathbf{u} + \mathbf{h}$, where $\mathbf{u} \in \mathcal{D}(\mathcal{B}^*\mathcal{B})$ and $\mathbf{h} \in \mathcal{H}'$. By virtue of (4.6), (4.7), $V\mathbf{f} \in \mathcal{D}(B^{*2})$ and $V\mathbf{f} = V\mathbf{u} + V\mathbf{h}$, where $V\mathbf{u} \in \mathcal{D}(B^*B)$ and $V\mathbf{h} \in \mathcal{H}$. In view of (2.9), $\Gamma_0 V\mathbf{f} = V\mathbf{h} = V\Gamma_0'\mathbf{f}$.

Since $\mathcal{H} = V\mathcal{H}'$ and $\mathcal{R}(B^2 + I) = V\mathcal{R}(\mathcal{B}^2 + I)$, the orthogonal projectors $P_{\mathcal{H}}$ and $P_{\mathcal{H}'}$ are related as follows: $VP_{\mathcal{H}'} = P_{\mathcal{H}}V$. Therefore,

$$\Gamma_1 V\mathbf{f} = P_{\mathcal{H}}(B^*B + I)V\mathbf{u} = P_{\mathcal{H}}(V\mathcal{B}^*\mathcal{B}V^* + I)V\mathbf{u} = P_{\mathcal{H}}V(\mathcal{B}^*\mathcal{B} + I)\mathbf{u} = V\Gamma_1'\mathbf{f}$$

that completes the proof. □

Corollary 4.5. *The positive boundary triplet $(\mathcal{H}, \Gamma_0, \Gamma_1)$ of B^{*2} consists of the space*

$$\mathcal{H} = \psi(\mathcal{B}) \left\{ \begin{bmatrix} \alpha \\ \beta \end{bmatrix} e^{-x} \ : \ \alpha, \beta \in \mathbb{C} \right\}$$

and the mappings $\Gamma_i : \psi(\mathcal{B})W_2^2(\mathbb{R}_+, \mathbb{C}^2) \to \mathcal{H}$ that are defined as follows:

$$\Gamma_0\psi(\mathcal{B})\mathbf{f}(x) = \psi(\mathcal{B})\mathbf{f}(0)e^{-x}, \quad \Gamma_1\psi(\mathcal{B})\mathbf{f}(x) = 2\psi(\mathcal{B})[\mathbf{f}'(0) + \mathbf{f}(0)]e^{-x}.$$

Proof. It is well known (see, e.g., [12]) that the positive boundary triplet $(\mathcal{H}', \Gamma_0', \Gamma_1')$ of $\mathcal{B}^{*2}$ has the form: $\mathcal{H}' = \left\{ \begin{bmatrix} \alpha \\ \beta \end{bmatrix} e^{-x} : \alpha, \beta \in \mathbb{C} \right\}$ and

$$\Gamma_0'\mathbf{f} = \mathbf{f}(0)e^{-x}, \quad \Gamma_1\mathbf{f} = 2[\mathbf{f}'(0) + \mathbf{f}(0)]e^{-x}, \quad \mathbf{f} \in W_2^2(\mathbb{R}_+, \mathbb{C}^2).$$

Applying Lemma 4.4 we complete the proof. □

4.3. THE S-MATRIX FOR POSITIVE SELF-ADJOINT $\mathbf{H}_{a\mathbf{q}}$

Theorem 4.6. *The S-matrix for positive self-adjoint operator $\mathbf{H}_{a\mathbf{q}}$ has the form*

$$S(z) = \begin{bmatrix} \Psi_1(z) & 0 \\ 0 & \Psi_2(z) \end{bmatrix} - \frac{2zi}{a - W(z^2)} \begin{bmatrix} c(z, q_1)\overline{c(-\overline{z}, q_1)} & c(z, q_1)\overline{c(-\overline{z}, q_2)} \\ c(z, q_2)\overline{c(-\overline{z}, q_1)} & c(z, q_2)\overline{c(-\overline{z}, q_2)} \end{bmatrix}, \tag{4.8}$$

where $c(\mu, q_i)$ are determined by (4.4) and $\Psi_j(z)$ are holomorphic continuations of the functions $\psi_j(-\delta)/\psi_j(\delta)$ ($\delta \in \mathbb{R}$) into $\mathbb{C}_-$ such that $|\Psi_j(z)| < 1$ and $\overline{\Psi_j(z)} = \Psi_j(-\overline{z})$.

Proof. By Theorem 2.2, for the calculation of S-matrix, one need to find operators $C(z)$ in (2.11). To do that we analyze vectors

$$\mathbf{u}\in P_{\mathfrak{H}_0}(\mathbf{H}_{a\mathbf{q}}-z^2I)^{-1}\ker(B^*+\overline{z}I)$$

in more detail. First of all we note that $\ker(B^*+\overline{z}I)=\psi(\mathcal{B})\{\mathbf{h}_{-\overline{z}}\}$ by Lemma 4.2. Consider the equation[7)]

$$(\mathbf{H}_{a\mathbf{q}}-z^2I)\mathbf{f}=(\overline{z}^2-z^2)\psi(\mathcal{B})\mathbf{h}_{-\overline{z}},\quad z\in\mathbb{C}_-\setminus i\mathbb{R}_-. \tag{4.9}$$

Its solution $\mathbf{f}\in\mathcal{D}(\mathbf{H}_{a\mathbf{q}})$ is determined uniquely and

$$\mathbf{u}=P_{\mathfrak{H}_0}\mathbf{f}=(\overline{z}^2-z^2)P_{\mathfrak{H}_0}(\mathbf{H}_{a\mathbf{q}}-z^2I)^{-1}\psi(\mathcal{B})\mathbf{h}_{-\overline{z}} \tag{4.10}$$

belongs to $\mathcal{D}(B^{*2})$ due to (4.5). In view of (4.6), $\mathbf{u}=\psi(\mathcal{B})\mathbf{v}$, where $\mathbf{v}\in W_2^2(\mathbb{R}_+,\mathbb{C}^2)$ and $B^{*2}\psi(\mathcal{B})\mathbf{v}=\psi(\mathcal{B})\mathcal{B}^{*2}\mathbf{v}$. Moreover, since $P_{\mathfrak{H}_0}=\psi(\mathcal{B})\psi(\mathcal{B})^*$, the relation (4.10) yields

$$\mathbf{v}=(\overline{z}^2-z^2)\psi(\mathcal{B})^*(\mathbf{H}_{a\mathbf{q}}-z^2I)^{-1}\psi(\mathcal{B})\mathbf{h}_{-\overline{z}}. \tag{4.11}$$

Applying $P_{\mathfrak{H}_0}$ to the both parts of (4.9) and using (4.5) we obtain

$$(B^{*2}-z^2I)\mathbf{u}=\psi(\mathcal{B})(\mathcal{B}^{*2}-z^2I)\mathbf{v}=(\overline{z}^2-z^2)\psi(\mathcal{B})\mathbf{h}_{-\overline{z}}.$$

Therefore, $(\mathcal{B}^{*2}-z^2I)\mathbf{v}=(-\frac{d^2}{dx^2}-z^2I)\mathbf{v}=(\overline{z}^2-z^2)\mathbf{h}_{-\overline{z}}$. This means that

$$\mathbf{v}=\mathbf{h}_{-\overline{z}}+\mathbf{h}_z,\quad \mathbf{u}=\psi(\mathcal{B})\mathbf{v}=\psi(\mathcal{B})\mathbf{h}_{-\overline{z}}+\psi(\mathcal{B})\mathbf{h}_z, \tag{4.12}$$

where $\mathbf{h}_z\in\ker(B^*-zI)$ is determined uniquely by the choice of $\mathbf{h}_{-\overline{z}}$. Applying operators Γ_i from Corollary 4.5 we obtain

$$\Gamma_0\mathbf{u}=\psi(\mathcal{B})\begin{bmatrix}\alpha_{-\overline{z}}+\alpha_z\\ \beta_{-\overline{z}}+\beta_z\end{bmatrix}e^{-x},\quad \Gamma_1\mathbf{u}=2\psi(\mathcal{B})\begin{bmatrix}(1+i\overline{z})\alpha_{-\overline{z}}+(1-iz)\alpha_z\\ (1+i\overline{z})\beta_{-\overline{z}}+(1-iz)\beta_z\end{bmatrix}e^{-x}.$$

Since $\dim\mathcal{H}=2$, the function $C(z)$ in Theorem 2.2 is 2×2-matrix-valued. The substitution of $\Gamma_i\mathbf{u}$ into the characteristic relation (2.11) gives

$$2C(z)\begin{bmatrix}(1+i\overline{z})\alpha_{-\overline{z}}+(1-iz)\alpha_z\\ (1+i\overline{z})\beta_{-\overline{z}}+(1-iz)\beta_z\end{bmatrix}=\begin{bmatrix}\alpha_{-\overline{z}}+\alpha_z\\ \beta_{-\overline{z}}+\beta_z\end{bmatrix}$$

and, after elementary transformations,

$$[I-2(1-iz)C(z)]^{-1}\begin{bmatrix}\alpha_{-\overline{z}}\\ \beta_{-\overline{z}}\end{bmatrix}=\frac{1}{2iRe\ z}\begin{bmatrix}(1+i\overline{z})\alpha_{-\overline{z}}+(1-iz)\alpha_z\\ (1+i\overline{z})\beta_{-\overline{z}}+(1-iz)\beta_z\end{bmatrix}. \tag{4.13}$$

The substitution of (4.13) into (2.10) gives the S-matrix

$$S(z)\begin{bmatrix}\alpha_{-\overline{z}}\\ \beta_{-\overline{z}}\end{bmatrix}=-i\frac{Im\ z}{Re\ z}\begin{bmatrix}\alpha_{-\overline{z}}\\ \beta_{-\overline{z}}\end{bmatrix}-\frac{z}{Re\ z}\begin{bmatrix}\alpha_z\\ \beta_z\end{bmatrix},\quad z\in\mathbb{C}_-\setminus i\mathbb{R}_-. \tag{4.14}$$

7) The coefficient $(\overline{z}^2-z^2)$ is used for the simplification of formulas below.

Here α_z, β_z are functions of parameters $\alpha_{-\overline{z}}, \beta_{-\overline{z}} \in \mathbb{C}$. Indeed, in view of (4.11) and (4.12) $\mathbf{h}_z = -\mathbf{h}_{-\overline{z}} + (\overline{z}^2 - z^2)\psi(\mathcal{B})^*(\mathbf{H}_{a\mathbf{q}} - z^2 I)^{-1}\psi(\mathcal{B})\mathbf{h}_{-\overline{z}}$ and hence,

$$\begin{bmatrix} \alpha_z \\ \beta_z \end{bmatrix} e^{-izx} = (-I + (\overline{z}^2 - z^2)\psi(\mathcal{B})^*(\mathbf{H}_{a\mathbf{q}} - z^2 I)^{-1}\psi(\mathcal{B})) \begin{bmatrix} \alpha_{-\overline{z}} \\ \beta_{-\overline{z}} \end{bmatrix} e^{i\overline{z}x}. \quad (4.15)$$

The S-matrix $S(z)$ depends on the choice of $\mathbf{H}_{a\mathbf{q}}$. If $\mathbf{H}_{a\mathbf{q}} = \mathbf{H}_\infty$, then this operator is a positive self-adjoint extension of the symmetric operators $\mathcal{B}^2$ and B^2. By Theorem 2.1 one can construct two pairs of subspaces $D_\pm$ that are determined by $\mathcal{B}$ and B, respectively. Therefore, one can define two S-matrices $S_1(\cdot)$ and $S(\cdot)$ for $\mathbf{H}_\infty$ corresponding to the cases where $\mathbf{H}_\infty$ is considered as an extension of $\mathcal{B}^2$ or an extension of B^2. The both of S-matrices are defined by (2.10) but, in the first case, $C(z) = 0$ and, therefore $S_1(z) = \sigma_0$. In view of [14, Proposition 3.1],

$$S(z) = \begin{bmatrix} \Psi_1(z) & 0 \\ 0 & \Psi_2(z) \end{bmatrix} S_1(z) = \begin{bmatrix} \Psi_1(z) & 0 \\ 0 & \Psi_2(z) \end{bmatrix}, \quad (4.16)$$

where $\Psi_j(z)$ are holomorphic functions in $\mathbb{C}_-$ such that $|\Psi_j(z)| < 1$ and $\overline{\Psi_j(z)} = \Psi_j(-\overline{z})$. Moreover, the boundary values of $\Psi_j(z)$ on $\mathbb{R}$ coincide with $\psi_j(-\delta)/\psi_j(\delta)$.

Due to (4.15), the coefficients α_z, β_z in (4.14) depend on the choice of $\mathbf{H}_{a\mathbf{q}}$. The resolvent formula (3.7) and (4.15) allow one to present $\alpha_z = \alpha_z(\mathbf{H}_{a\mathbf{q}})$, $\beta_z = \beta_z(\mathbf{H}_{a\mathbf{q}})$ as the sum of $\alpha_z(\mathbf{H}_\infty), \beta_z(\mathbf{H}_\infty)$ and a function that is determined by the difference between $(\mathbf{H}_{a\mathbf{q}} - z^2 I)^{-1}$ and $(\mathbf{H}_\infty - z^2 I)^{-1}$ (see the second part in (3.7)). Such decomposition and (4.16) allows one to rewrite (4.14):

$$S(z)\begin{bmatrix} \alpha_{-\overline{z}} \\ \beta_{-\overline{z}} \end{bmatrix} = \begin{bmatrix} \Psi_1(z)\alpha_{-\overline{z}} \\ \Psi_2(z)\beta_{-\overline{z}} \end{bmatrix} - \frac{ze^{izx}}{Re\ z}(\overline{z}^2 - z^2)\frac{(\mathbf{h}_{-\overline{z}}, \psi(\mathcal{B})^*\mathbf{u}_{-\overline{z}})_+}{a - W(z^2)}\psi(\mathcal{B})^*\mathbf{u}_z. \quad (4.17)$$

In view of (4.3) with $\mu = -\overline{z}$

$$\frac{(\overline{z}^2 - z^2)(\mathbf{h}_{-\overline{z}}, \psi(\mathcal{B})^*\mathbf{u}_{-\overline{z}})_+}{Re\ z} = 2i\left\langle \begin{bmatrix} \alpha_{-\overline{z}} \\ \beta_{-\overline{z}} \end{bmatrix}, \begin{bmatrix} c(-\overline{z}, q_1) \\ c(-\overline{z}, q_2) \end{bmatrix} \right\rangle,$$

where $\langle \cdot, \cdot \rangle$ is the inner product in $\mathbb{C}^2$. Substituting this expression into (4.17) and using (4.3) with $\mu = z$, we obtain

$$S(z)\begin{bmatrix} \alpha_{-\overline{z}} \\ \beta_{-\overline{z}} \end{bmatrix} = \begin{bmatrix} \Psi_1(z)\alpha_{-\overline{z}} \\ \Psi_2(z)\beta_{-\overline{z}} \end{bmatrix} - \frac{2zi}{a - W(z^2)}\left\langle \begin{bmatrix} \alpha_{-\overline{z}} \\ \beta_{-\overline{z}} \end{bmatrix}, \begin{bmatrix} c(-\overline{z}, q_1) \\ c(-\overline{z}, q_2) \end{bmatrix} \right\rangle \begin{bmatrix} c(z, q_1) \\ c(z, q_2) \end{bmatrix}.$$

A rudimentary linear algebra exercise leads to the conclusion this formula for $S(z)$ can be rewritten as (4.8) for $z \in \mathbb{C}_- \setminus i\mathbb{R}_-$. Since the S-matrix is holomorphic in the lower half-plain, the formula (4.8) remains true for $\mathbb{C}_-$. □

The expression (4.8) is based on the Krein–Naimark resolvent formula (3.7) and it allows one to establish various useful relationships between S-matrix and the operator $\mathbf{H}_{a\mathbf{q}}$. An alternative formula for S-matrix in terms of reflection and transmission coefficients is presented below.

By virtue of Lemma 4.1,

$$P_{\mathfrak{H}_0}\begin{bmatrix} e^{i\overline{z}x} \\ 0 \end{bmatrix} = \psi(\mathcal{B})\psi(\mathcal{B})^*\begin{bmatrix} e^{i\overline{z}x} \\ 0 \end{bmatrix} = \psi(\mathcal{B})\begin{bmatrix} \overline{\psi_1(-z)} \\ 0 \end{bmatrix} e^{i\overline{z}x} \tag{4.18}$$

and, similarly, $P_{\mathfrak{H}_0}\begin{bmatrix} \alpha_z \\ \beta_z \end{bmatrix} e^{-izx} = \psi(\mathcal{B})\begin{bmatrix} \alpha_z\overline{\psi_1(\overline{z})} \\ \beta_z\overline{\psi_2(\overline{z})} \end{bmatrix} e^{-izx}$.

Setting $\mathbf{h}_{-\overline{z}} = \begin{bmatrix} \overline{\psi_1(-z)} \\ 0 \end{bmatrix} e^{i\overline{z}x}$ in (4.9) and using (4.18) we obtain

$$(\mathbf{H}_{a\mathbf{q}} - z^2 I)\mathbf{f} = (\overline{z}^2 - z^2)\psi(\mathcal{B})\mathbf{h}_{-\overline{z}} = (\overline{z}^2 - z^2)P_{\mathfrak{H}_0}\begin{bmatrix} e^{i\overline{z}x} \\ 0 \end{bmatrix}, \quad z \in \mathbb{C}_- \setminus i\mathbb{R}_-$$

and, in view of (4.10), (4.12), its solution $\mathbf{f}$ satisfies the relation

$$P_{\mathfrak{H}_0}\mathbf{f} = \psi(\mathcal{B})\begin{bmatrix} \overline{\psi_1(-z)} \\ 0 \end{bmatrix} e^{i\overline{z}x} + \psi(\mathcal{B})\begin{bmatrix} \alpha_z \\ \beta_z \end{bmatrix} e^{-izx} = P_{\mathfrak{H}_0}\begin{bmatrix} e^{i\overline{z}x} + R_z^1 e^{-izx} \\ T_z^1 e^{-izx} \end{bmatrix},$$

where

$$R_z^1 = \frac{\alpha_z}{\overline{\psi_1(\overline{z})}}, \quad T_z^1 = \frac{\beta_z}{\overline{\psi_2(\overline{z})}}$$

are called *the reflection* and *the transmission* coefficients, respectively.

Similarly, assuming $\mathbf{h}_{-\overline{z}} = \begin{bmatrix} 0 \\ \overline{\psi_2(-z)} \end{bmatrix} e^{i\overline{z}x}$ and considering the solution $\mathbf{f}$ of

$$(\mathbf{H}_{a\mathbf{q}} - z^2 I)\mathbf{f} = (\overline{z}^2 - z^2)P_{\mathfrak{H}_0}\begin{bmatrix} 0 \\ e^{i\overline{z}x} \end{bmatrix},$$

we obtain

$$P_{\mathfrak{H}_0}\mathbf{f} = P_{\mathfrak{H}_0}\begin{bmatrix} T_z^2 e^{-izx} \\ e^{i\overline{z}x} + R_z^2 e^{-izx} \end{bmatrix}, \quad R_z^2 = \frac{\beta_z}{\overline{\psi_2(\overline{z})}}, \quad T_z^2 = \frac{\alpha_z}{\overline{\psi_1(\overline{z})}}.$$

The reflection R_z^j and the transmission T_z^j coefficients described above allow one to obtain an alternative formula for S-matrix.

Theorem 4.7. *The S-matrix of a positive self-adjoint operator $\mathbf{H}_{a\mathbf{q}}$ has the form*

$$S(z) = \frac{-z}{Re\ z}\begin{bmatrix} \theta_{11}(z)R_z^1 + i\frac{Im\ z}{z} & \theta_{12}(z)T_z^2 \\ \theta_{21}(z)T_z^1 & \theta_{22}(z)R_z^2 + i\frac{Im\ z}{z} \end{bmatrix}, \quad \theta_{nm}(z) = \frac{\overline{\psi_n(\overline{z})}}{\overline{\psi_m(-z)}}. \tag{4.19}$$

Proof. Setting in (4.14)

$$\alpha_{-\overline{z}} = \overline{\psi_1(-z)}, \quad \beta_{-\overline{z}} = 0, \quad \alpha_z = \overline{\psi_1(\overline{z})}R_z^1, \quad \beta_z = \overline{\psi_2(\overline{z})}T_z^1$$

and

$$\alpha_{-\overline{z}} = 0, \quad \beta_{-\overline{z}} = \overline{\psi_2(-z)}, \quad \alpha_z = \overline{\psi_1(\overline{z})}T_z^2, \quad \beta_z = \overline{\psi_2(\overline{z})}R_z^2$$

we obtain a system of four linear equations with respect to unknowns coefficients of the S-matrix $S(z) = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix}$. Its solution gives rise to (4.19) for all $z \in \mathbb{C}_- \setminus i\mathbb{R}_-$. Since $S(z)$ is holomorphic in $\mathbb{C}_-$, the formula (4.19) holds for all $z \in \mathbb{C}_-$. □

4.3.1. Example of ordinary δ-interaction

In view of (3.2), the ordinary δ-interaction corresponds to $\mathbf{q} = 0$. The operators $\mathbf{H}_a = \mathbf{H}_{a0} = -\frac{d^2}{dx^2}$ have the domains:

$$\mathcal{D}(\mathbf{H}_{a\mathbf{q}}) = \{\mathbf{f} \in W_2^2(\mathbb{R}_+, \mathbb{C}^2) : \ [\mathbf{f}]_s = 0, \quad [\mathbf{f}']_r = a[\mathbf{f}]_r\}.$$

The function $\mathbf{q} = 0$ is non-cyclic and one can set $\psi_1 = \psi_2 = 1$. Then $P_{\mathfrak{H}_0} = I$ and the reflection and the transmission coefficients are determined as follows:

$$R_z^1 = R_z^2 = \frac{-a + i(\overline{z} - z)}{a + 2iz}, \quad T_z^1 = T_z^2 = \frac{2iRe\ z}{a + 2iz}.$$

Substituting the obtained expressions in (4.19) and taking into account that $\theta_{nm}(z) = 1$, we obtain a matrix-valued S-function

$$S(z) = \frac{1}{a + 2iz} \begin{bmatrix} a & -2iz \\ -2iz & a \end{bmatrix}, \tag{4.20}$$

which is holomorphic on $\mathbb{C}_-$ for positive self-adjoint operators $\mathbf{H}_a$ (the positivity of $\mathbf{H}_a$ is distinguished by the condition $a \geq 0$).

The same formula (4.20) can be deduced from (4.8) if one take into account that $\Psi_j = 1$ since $\psi_j = 1$ and $W(z^2) = -2iz$, $c(z, q_j) = 1$ by virtue of (3.9) and (4.4), respectively.

5. OPERATORS $\mathbf{H}_{a\mathbf{q}}$ AND THEIR S-MATRICES

The example above leads to a natural assumption that the formulas (4.8), (4.19) allow to construct a function $S(z)$ for each operator $\mathbf{H}_{a\mathbf{q}}$ (assuming, of course, that $\mathbf{q}$ is non-cyclic). We will call it *the S-matrix* of $\mathbf{H}_{a\mathbf{q}}$. If $\mathbf{H}_{a\mathbf{q}}$ is positive self-adjoint, then the S-matrix is the consequence of proper arguments of the Lax–Phillips theory and it coincides with the analytical continuation of the Lax–Phillips scattering matrix into $\mathbb{C}_-$. Otherwise, $S(z)$ is defined directly by (4.8), (4.19) and it can be considered as a characteristic function of $\mathbf{H}_{a\mathbf{q}}$. In this section, we describe properties of $\mathbf{H}_{a\mathbf{q}}$ in terms of the corresponding S-matrix.

It follows from (4.8) that a S-matrix of $\mathbf{H}_{a\mathbf{q}}$ is a meromorphic matrix-valued function on $\mathbb{C}_-$. Its poles describe the point spectrum of $\mathbf{H}_{a\mathbf{q}}$ in $\mathbb{C} \setminus [0, \infty)$.

Lemma 5.1. *If $z \in \mathbb{C}_-$ is a pole of $S(z)$, then z^2 belongs to the point spectrum of $\mathbf{H}_{a\mathbf{q}}$.*

Proof. By virtue of (4.8), if $z \in \mathbb{C}_-$ is a pole for $S(z)$ then $a = W(z^2)$. This identity means that $z^2 \in \sigma_p(\mathbf{H}_{a\mathbf{q}})$ because $\mathbf{H}_{a\mathbf{q}}$ is defined by (3.5) and $W(z^2)$ is the Weyl–Titchmarsh function associated to the boundary triplet $(\mathbb{C}, \Gamma_0, \Gamma_1)$ (see Section 3.1 and [26, Proposition 14.17]). □

Remark 5.2. It may happen that the S-matrix 'does not hear' an eigenvalue z^2. This is the case where the corresponding eigenfunction $\mathbf{u}_z$ is orthogonal to $\psi(\mathcal{B})L_2(\mathbb{R}_+, \mathbb{C}^2)$ and, as a result, the coefficients $c(z, q_i)$ vanish, see Section 5.1.1.

Divide the half-plane $\mathbb{C}_-$ into three parts

$$\mathbb{C}_-^- = \{z : Re\ z < 0\}, \quad \mathbb{C}_-^0 = \{z : Re\ z = 0\}, \quad \mathbb{C}_-^+ = \{z : Re\ z > 0\}.$$

Lemma 5.3. *If $S(z)$ has a pole in $\mathbb{C}_-^\mp$, then $S(z)$ has to be analytical on the opposite part $\mathbb{C}_-^\pm$. If $S(z)$ has a pole on the middle part $\mathbb{C}_-^0$, then $S(z)$ is analytical on $\mathbb{C}_-^- \cup \mathbb{C}_-^+$ and $\mathbf{H}_{a\mathbf{q}}$ is a self-adjoint operator.*

Proof. Let $z \in \mathbb{C}_-^-$ be a pole for $S(z)$. By virtue of (4.8), $a = W(z^2)$, where $Im\ z^2 > 0$ and $Im\ a > 0$ since $Im\ W(z^2)/Im\ z^2 > 0$ [26, Section 14.5]. Similar arguments for a pole $z \in \mathbb{C}_-^+$ lead to the conclusion that $Im\ a < 0$. The obtained contradiction means that the existence of a pole in $\mathbb{C}_-^+$ ($\mathbb{C}_-^-$) implies the absence of poles in $\mathbb{C}_-^-$ ($\mathbb{C}_-^+$).

If $z \in \mathbb{C}_-^0$ is a pole, then $\mathbf{H}_{a\mathbf{q}}$ has a negative eigenvalue and $\mathbf{H}_{a\mathbf{q}}$ has to be self-adjoint due to [21, Corollary 5.2]. □

An eigenvalue $z^2 \in \mathbb{C} \setminus [0, \infty)$ of $\mathbf{H}_{a\mathbf{q}}$ is called *an exceptional point* if its geometrical multiplicity does not coincide with the algebraic one. The presence of an exceptional point means that $\mathbf{H}_{a\mathbf{q}}$ cannot be self-adjoint for any choice of inner product. It follows from Lemma 5.3 that an exceptional point z^2 is necessarily non-real and $z \in \mathbb{C}_-^- \cup \mathbb{C}_-^+$.

Lemma 5.4. *A non-simple pole*[8)] *z of $S(z)$ corresponds to an exceptional point z^2 of $\mathbf{H}_{a\mathbf{q}}$.*

Proof. A non-simple pole z of $S(z)$ means that the function $(a - W(\lambda))^{-1}$ has a non-simple pole for $\lambda = z^2$. This yields that $W'(z^2) = 0$, where $W'(\lambda) = dW/d\lambda$. In view of [21, Theorem 5.4], an eigenvalue z^2 of $\mathbf{H}_{a\mathbf{q}}$ is an exceptional point if and only if $W'(z^2) = 0$. □

Lemma 5.5. *Let $S_{\mathbf{H}_{a\mathbf{q}}}(z)$ be a S-matrix of $\mathbf{H}_{a\mathbf{q}}$. Then*

$$S^*_{\mathbf{H}_{a\mathbf{q}}}(z) = S_{\mathbf{H}_{\overline{a}\mathbf{q}}}(-\overline{z}) = S_{\mathbf{H}^*_{a\mathbf{q}}}(-\overline{z}).$$

Proof. Using (4.8) for the calculation of the adjoint, we get

$$S^*_{\mathbf{H}_{a\mathbf{q}}}(z) = \begin{bmatrix} \overline{\Psi_1(z)} & 0 \\ 0 & \overline{\Psi_2(z)} \end{bmatrix} + \frac{2\overline{z}i}{\overline{a} - \overline{W(z^2)}} \begin{bmatrix} c(-\overline{z}, q_1)\overline{c(z, q_1)} & c(-\overline{z}, q_1)\overline{c(z, q_2)} \\ c(-\overline{z}, q_2)\overline{c(z, q_1)} & c(-\overline{z}, q_2)\overline{c(z, q_2)} \end{bmatrix}.$$

In view of Theorem 4.6 $\overline{\Psi_j(z)} = \Psi_j(-\overline{z})$. Moreover, $\overline{W(z^2)} = W((-\overline{z})^2)$. This well-known property of the Weyl–Titchmarsh functions [26, Chap. 14] can easily be derived from (3.9). Taking these facts into account and using (4.8) for the calculation of $S_{\mathbf{H}_{\overline{a}\mathbf{q}}}(-\overline{z})$, we arrive at the conclusion that $S^*_{\mathbf{H}_{a\mathbf{q}}}(z) = S_{\mathbf{H}_{\overline{a}\mathbf{q}}}(-\overline{z})$. Now, to complete the proof it suffices to remark that $\mathbf{H}^*_{a\mathbf{q}} = \mathbf{H}_{\overline{a}\mathbf{q}}$ due to (3.5) and [26, Lemma 14.6]. □

Corollary 5.6. *Let $S(z)$ be a S-matrix of $\mathbf{H}_{a\mathbf{q}}$. Then $\mathbf{H}_{a\mathbf{q}}$ is self-adjoint if and only if $S^*(z) = S(-\overline{z})$.*

Proof. If $\mathbf{H}_{a\mathbf{q}}$ is self-adjoint, then $a \in \mathbb{R}$ and $S^*(z) = S(-\overline{z})$ due to Lemma 5.5. Conversely, as follows from the proof above, the relation $S^*(z) = S(-\overline{z})$ is possible only in the case of real a. This implies the self-adjointness of $\mathbf{H}_{a\mathbf{q}}$. □

[8)] A pole of order greater then one.

5.1. EXAMPLES

5.1.1. Even function q with finite support

We consider the simplest example of even function with finite support

$$q(x) = M\chi_{[-\rho,\rho]}(x), \quad M \in \mathbb{C}, \quad \rho > 0.$$

In this case, $Yq = \mathbf{q} = M \begin{bmatrix} \chi_{[0,\rho]}(x) \\ \chi_{[0,\rho]}(x) \end{bmatrix}$.

Denote $\psi(\delta) = e^{i\delta\rho}$. The function ψ belongs to $H^\infty(\mathbb{C}_+)$ and the operator $\psi(\mathcal{B})$ in (3.12) acts in $L_2(\mathbb{R}_+)$ as follows:

$$\psi(\mathcal{B})f = \begin{cases} f(x-\rho) & \text{for } x \geq \rho, \\ 0 & \text{for } x < \rho. \end{cases} \tag{5.1}$$

Further, we extend the action of $\psi(\mathcal{B})$ onto $L_2(\mathbb{R}_+, \mathbb{C}^2)$ assuming in (3.14) that $\psi_1(\mathcal{B}) = \psi_2(\mathcal{B}) = \psi(\mathcal{B})$. It follows from (5.1) that $\psi(\mathcal{B})^*\mathbf{f} = \mathbf{f}(x+\rho)$. Hence,

$$P_{\mathfrak{H}_0}\mathbf{f} = \psi(\mathcal{B})\psi(\mathcal{B})^*\mathbf{f} = \begin{cases} \mathbf{f}(x) & \text{for } x \geq \rho, \\ 0 & \text{for } x < \rho. \end{cases} \tag{5.2}$$

The formula (5.2) and Lemma 3.2 imply that $\mathbf{q}$ is non-cyclic. Therefore, for $\mathbf{H}_{a\mathbf{q}}$ there exists a S-matrix defined by (4.8). Let us specify the counterparts of (4.8). First of all we note that $\Psi_1(z) = \Psi_2(z) = e^{-2iz\rho}$ as the holomorphic continuation of $e^{-2i\delta\rho} = \frac{\psi(-\delta)}{\psi(\delta)}$ into $\mathbb{C}_-$. Further, in view of (3.6),

$$(\mathbf{H}_\infty - \mu^2 I)^{-1}\mathbf{q} = -\frac{M}{2\mu^2}[(e^{-i\mu\rho} + e^{i\mu m(x)} - 2)\mathbf{e}^{-i\mu x} + (e^{-i\mu m(x)} - e^{-i\mu\rho})\mathbf{e}^{i\mu x}],$$

where $m(x) = \min\{x, \rho\}$ and $\mu \in \mathbb{C}_-$. This formula and (4.4) lead to the conclusion that

$$c(\mu, q_1) = c(\mu, q_2) = e^{-i\mu\rho}\left(1 - \kappa_\mu \frac{M}{\mu^2}\right), \quad \kappa_\mu = 1 - \cos\mu\rho.$$

Our next step is the calculation of $W(z^2)$ using formula (3.9) and the expression for $(\mathbf{H}_\infty - \mu^2 I)^{-1}$, that gives

$$W(z^2) = -2iz - \frac{4Re\ M}{iz}(1 - e^{-iz\rho}) + \frac{|M|^2}{iz^3}\left[(e^{-iz\rho} - 2)^2 - 2iz\rho - 1\right].$$

Substituting the expressions obtained above into (4.8) we find the S-matrix for $\mathbf{H}_{a\mathbf{q}}$

$$S(z) = e^{-2iz\rho}\left(\sigma_0 - \frac{2i(z^2 - \kappa_z M)(z^2 - \kappa_z \overline{M})}{z^3(a - W(z^2))}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\right).$$

Let us assume that $z_0 \in \mathbb{C}_-$ satisfies the relation $z_0^2 - \kappa_{z_0}M = 0$ and $W'(z_0^2) \neq 0$. Set $a = W(z_0^2)$. Then the operator $\mathbf{H}_{a\mathbf{q}}$ has the eigenvalue z_0^2 with eigenfunction $\mathbf{u}_{z_0}$. It follows from (3.8) and the explicit expression for $(\mathbf{H}_\infty - \mu^2 I)^{-1}$ that

$$\mathbf{u}_{z_0} = \frac{1 - \cos z_0(\rho - x)}{z_0^2}\mathbf{q}.$$

In view of (5.2), the eigenfunction $\mathbf{u}_{z_0}$ is orthogonal to $\mathfrak{H}_0$ and it has no impact on the S-matrix $S(z)$ (no pole for $z = z_0$).

5.1.2. Odd function q with finite support

Similarly to the previous case, we consider the odd function

$$q(x) = M\text{sign}(x)\chi_{[-\rho,\rho]}(x), \quad M \in \mathbb{C}, \quad \rho > 0.$$

In this case, $\mathbf{q} = M \begin{bmatrix} \chi_{[0,\rho]}(x) \\ -\chi_{[0,\rho]}(x) \end{bmatrix}$ is non-cyclic and it is orthogonal to the same subspace $\mathfrak{H}_0 = \psi(\mathcal{B})L_2(\mathbb{R}_+, \mathbb{C}^2)$ as above. Further,

$$c(\mu, q_1) = e^{-i\mu\rho}\left(1 - \kappa_\mu \frac{M}{\mu^2}\right), \quad c(\mu, q_2) = e^{-i\mu\rho}\left(1 + \kappa_\mu \frac{M}{\mu^2}\right)$$

and $W(z^2) = -2iz + \frac{|M|^2}{iz^3}\left[(e^{-iz\rho} - 2)^2 - 2iz\rho - 1\right]$. Then (4.8) takes the form

$$S(z) = e^{-2iz\rho}\left(\sigma_0 - \frac{2zi}{a - W(z^2)}\begin{bmatrix} 1 - \kappa_z \frac{2\text{Re}M}{z^2} + \kappa_z^2 \frac{|M|^2}{z^4} & 1 - \kappa_z \frac{2\text{Im}M}{z^2} - \kappa_z^2 \frac{|M|^2}{z^4} \\ 1 + \kappa_z \frac{2\text{Im}M}{z^2} - \kappa_z^2 \frac{|M|^2}{z^4} & 1 + \kappa_z \frac{2\text{Re}M}{z^2} + \kappa_z^2 \frac{|M|^2}{z^4} \end{bmatrix}\right).$$

It is easy to see that the entries of the last matrix can not vanish simultaneously. This means that $z \in \mathbb{C}_-$ is a pole of $S(z)$ if and only if $a = W(z^2)$. Therefore, in contrast to Section 5.1.1, the poles of $S(z)$ completely determine the point spectrum of $\mathbf{H}_{a\mathbf{q}}$ in $\mathbb{C} \setminus \mathbb{R}_+$.

5.1.3. Functions q with infinite support

The range of applicability of our results is not limited to operators $\mathbf{H}_{a\mathbf{q}}$, where $\mathbf{q} = Yq$ has finite support. Due to Lemma 3.2 and Theorem 3.3, the S-matrix (4.8) can be constructed for an operator $\mathbf{H}_{a\mathbf{q}}$ when $\mathbf{q}$ is non-cyclic with respect to the backward shift operator T^* in $L_2(\mathbb{R}_+, \mathbb{C}^2)$. Various examples of non-cyclic functions can be found in [13, 17]. Consider, for instance, the function $q(x) = P_m(x)e^{-|x|}$, where P_m is a polynomial of order m. Then

$$\mathbf{q} = \begin{bmatrix} P_m(x) \\ P_m(-x) \end{bmatrix} e^{-x}, \quad x \geq 0.$$

Decompose the functions $P_m(\pm x)e^{-x} \in L_2(\mathbb{R}_+)$:

$$e^{-x}P_m(x) = \sum_{n=0}^{m} c_n q_n(2x), \quad e^{-x}P_m(-x) = \sum_{n=0}^{m} d_n q_n(2x), \tag{5.3}$$

with respect to the orthonormal basis of the Laguerre functions

$$q_n(x) = \frac{e^{x/2}}{n!}\frac{d^n}{dx^n}(x^n e^{-x}), \quad n = 0, 1 \ldots$$

Using the relation $Tq_n(2x) = q_{n+1}(2x)$ [3, p. 363], where T is defined by (3.11) and taking (5.3) into account we arrive at the conclusion that $\mathbf{q}$ is orthogonal to the subspace $T^{m+1}L_2(\mathbb{R}_+) = \psi(\mathcal{B})L_2(\mathbb{R}_+)$, where $\psi(\delta) = \left(\frac{\delta-i}{\delta+i}\right)^{m+1}$ belongs to $H^\infty(\mathbb{C}_+)$. Hence, $\mathbf{q}$ is a non-cyclic function and for operators $\mathbf{H}_{a\mathbf{q}}$ there exist S-matrices defined by (4.8).

Let us calculate the S-matrix for the function $q(x) = Me^{-|x|}$. In this case, one can set $m = 0$, $\psi(\delta) = \frac{\delta-i}{\delta+i}$, and $\Psi_1(z) = \Psi_2(z) = \left(\frac{z+i}{z-i}\right)^2$ as the holomorphic continuation of $\frac{\psi(-\delta)}{\psi(\delta)} = \left(\frac{\delta+i}{\delta-i}\right)^2$ into $\mathbb{C}_-$. Further,

$$(\mathbf{H}_\infty - z^2 I)^{-1}\mathbf{e}^{-x} = \frac{\mathbf{e}^{-izx} - \mathbf{e}^{-x}}{1+z^2}, \quad W(z^2) = -2iz - \frac{4Re\ M}{1+iz} + \frac{|M|^2}{(1+iz)^2}.$$

It follows from (4.4) and the Poisson formula [24, p.147] that

$$c(\mu, q_i) = \frac{\mu+i}{\mu-i} - \frac{M}{(\mu-i)^2} = \frac{\mu^2+1-M}{(\mu-i)^2}.$$

After substitution of the expressions above into (4.8) and elementary transformations we find

$$S(z) = \left(\frac{z+i}{z-i}\right)^2 \left(\sigma_0 - \frac{2iz(1-\frac{M}{z^2+1})(1-\frac{\overline{M}}{z^2+1})}{a-W(z^2)}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\right).$$

Let us assume for the simplicity that $M \in i\mathbb{R}$. Then

$$S(z) = \left(\frac{z+i}{z-i}\right)^2 \left(\sigma_0 - \frac{2iz(1+\frac{|M|^2}{(z^2+1)^2})}{a-W(z^2)}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\right) \tag{5.4}$$

and $W(\lambda) = -2i\sqrt{\lambda} + \frac{|M|^2}{(1+i\sqrt{\lambda})^2}$, where $\lambda = z^2$ and $\sqrt{\lambda} = z$.

Since the first derivative of $W(\lambda)$ is

$$W'(\lambda) = -\frac{i}{\sqrt{\lambda}}\left(1 + \frac{|M|^2}{(1+i\sqrt{\lambda})^3}\right),$$

the equation $W'(\lambda) = 0$ have the following roots $\lambda_j = z_j^2$, $j \in \{1,2,3\}$, where

$$z_1 = -\frac{\sqrt{3}}{2}|M|^{\frac{2}{3}} + i(1 - \frac{1}{2}|M|^{\frac{2}{3}}), \quad z_2 = -\overline{z_1}, \quad z_3 = i(|M|^{\frac{2}{3}}+1).$$

Assume that $|M|^2 > 8$. Then $z_1, z_2 \in \mathbb{C}_-$. Denote $a = W(z_1^2)$. Then the S-matrix (5.4) has a non-simple pole for $z = z_1$ and, by Lemma 5.4, the operator $\mathbf{H}_{a\mathbf{q}}$ has an exceptional point z_1^2. (The choice of $z_2 = -\overline{z}_1$ instead of z_1 leads to the conclusion that the point $\overline{z}_1^2$ is exceptional for the adjoint operator $\mathbf{H}^*_{a\mathbf{q}} = \mathbf{H}_{\overline{a}\mathbf{q}}$.)

The obtained result shows that the existence of exceptional points for some operators of the set $\{\mathbf{H}_{a\mathbf{q}}\}_{a\in\mathbb{C}}$, where $\mathbf{q}(x) = M\mathbf{e}^{-x}$, $M \in i\mathbb{R}$ depends on the absolute value of the imaginary M. If $|M|^2 > 8$, then there exist two operators $\mathbf{H}_{a\mathbf{q}}$ and $\mathbf{H}_{\overline{a}\mathbf{q}}$ with the exceptional points z_1^2 and $\overline{z}_1^2$, respectively. On the other hand, if $|M|$ is sufficiently small ($|M|^2 \leq 8$), then the collection of operators $\{\mathbf{H}_{a\mathbf{q}}\}_{a\in\mathbb{C}}$ has no exceptional points.

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