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On Eisenbud's and Wigner's R-matrix: A general approach

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Abstract

The main objective of this paper is to give a rigorous treatment of Wigner's and Eisenbud's R-matrix method for scattering matrices of scattering systems consisting of two selfadjoint extensions of the same symmetric operator with finite deficiency indices. In the framework of boundary triplets and associated Weyl functions an abstract generalization of the R-matrix method is developed and the results are applied to Schrödinger operators on the real axis.

Keywords: Scattering; Scattering matrix; R-matrix; Symmetric and selfadjoint operators; Extension theory; Boundary triplet; Weyl function; Ordinary differential operators

1. Introduction

The R-matrix approach to scattering was originally developed by Kapur and Peierls [20] in connection with nuclear reactions. Their ideas were improved by Wigner [39,40] and Wigner and Eisenbud [41], where the notion of R-matrix first appeared. A comprehensive overview of the

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R-matrix theory in nuclear physics can be found in [7,23]. The key ideas of the R-matrix theory are rather independent from the concrete physical situation. In fact, later the R-matrix method has also found several applications in atomic and molecular physics (see e.g. [6,8]) and recently it was applied to transport problems in semiconductor nano-structures [27–32,42–44]. In [25,26] an attempt was made to make the R-matrix method rigorous for elliptic differential operators, see also [33,34] for Schrödinger operators and [35,36] for an extension to Dirac operators.

The essential idea of the R-matrix theory is to divide the whole physical system into two spatially divided subsystems which are called internal and external systems, see [39–41]. The internal system is usually related to a bounded region, while the external system is given on its complement and is, therefore, spatially infinite. The goal is to represent the scattering matrix of a certain scattering system in terms of eigenvalues and eigenfunctions of an operator corresponding to the internal system with suitable chosen selfadjoint boundary conditions at the interface between the internal and external systems. This might seem a little strange at first sight since scattering is rather related to the external system than to the internal one.

It is the main objective of the present paper to make a further step towards a rigorous foundation of the R-matrix method in the framework of abstract scattering theory [5], in particular, in the framework of scattering theory for open quantum systems developed in [3,4]. This abstract approach has the advantage that any type of operators, in particular, Schrödinger or Dirac operators can be treated. We start with the direct orthogonal sum $L := A \oplus T$ of two symmetric operators A and T with equal deficiency indices acting in the Hilbert spaces $\mathfrak{H}$ and $\mathfrak{K}$, respectively. From a physical point of view the systems $\{A, \mathfrak{H}\}$ and $\{T, \mathfrak{K}\}$ can be regarded as incomplete internal and external systems, respectively. The system $\{L, \mathfrak{L}\}$, $\mathfrak{L} := \mathfrak{H} \oplus \mathfrak{K}$, is also an incomplete quantum system which is completed or closed by choosing a selfadjoint extension of L. The operator L admits several selfadjoint extensions in $\mathfrak{L}$. In particular, there are selfadjoint extensions of the form $L_0 = A_0 \oplus T_0$, where A_0 and T_0 are selfadjoint extensions of A and T in $\mathfrak{H}$ and $\mathfrak{K}$, respectively. Of course, in this case the quantum system $\{L_0, \mathfrak{L}\}$ decomposes into the closed internal and external systems $\{A_0, \mathfrak{H}\}$ and $\{T_0, \mathfrak{K}\}$, respectively, which do not interact. There are other selfadjoint extensions of L in $\mathfrak{L}$ which are not of this structure and can be regarded as Hamiltonians of quantum systems which take into account a certain interaction of the internal and external systems $\{A, \mathfrak{H}\}$ and $\{T, \mathfrak{K}\}$. In the following we choose a special selfadjoint extension $\widetilde{L}$ of L introduced in [9] and used in [3], see also Theorem 5.1, which gives the right physical Hamiltonian in many applications.

For example, let the internal system $\{A, \mathfrak{H}\}$ and external system $\{T, \mathfrak{K}\}$ be given by the minimal second order differential operators $A = -\frac{d^2}{dx^2} + v$ and $T = -\frac{d^2}{dx^2} + V$ in $\mathfrak{H} = L^2((x_l, x_r))$ and $\mathfrak{K} = L^2(\mathbb{R} \setminus (x_l, x_r))$, where (x_l, x_r) is a finite interval and v, V are real potentials. The extension L_0 can be chosen to be the direct sum of the selfadjoint extensions of A and T corresponding to Dirichlet boundary conditions at x_l and x_r. According to [3,9] the selfadjoint extension $\widetilde{L}$ coincides in this case with the usual selfadjoint Schrödinger operator

$$\widetilde{L} = -\frac{d^2}{dx^2} + \widetilde{v}, \qquad \widetilde{v}(x) := \begin{cases} v(x), & x \in (x_l, x_r), \\ V(x), & x \in \mathbb{R} \setminus (x_l, x_r), \end{cases}$$

in $\mathfrak{L} = L^2(\mathbb{R})$, cf. Section 6.1.

Let again A and T be symmetric operators with equal deficiency indices in $\mathfrak{H}$ and $\mathfrak{K}$, respectively. It will be assumed that the deficiency indices of A and T are finite. Then the selfadjoint operator $\widetilde{L}$ is a finite rank perturbation in resolvent sense of $L_0 = A_0 \oplus T_0$ and therefore $\{\widetilde{L}, L_0\}$ is a complete scattering system, i.e., the wave operators

$$W_\pm(\widetilde{L}, L_0) := \operatorname*{s-lim}_{t\to\pm\infty} e^{it\widetilde{L}} e^{-itL_0} P^{ac}(L_0)$$

exist and map onto the absolutely continuous subspace $\mathfrak{H}^{ac}(\widetilde{L})$ of $\widetilde{L}$, where $P^{ac}(L_0)$ is the orthogonal projection onto $\mathfrak{H}^{ac}(L_0)$, cf. [2]. The scattering operator

$$S := W_+(\widetilde{L}, L_0)^* W_-(\widetilde{L}, L_0)$$

regarded as a unitary operator in the absolutely continuous subspace $\mathfrak{H}^{ac}(L_0)$ is unitarily equivalent to a multiplication operator induced by a family of unitary matrices $\{S(\lambda)\}_{\lambda\in\mathbb{R}}$ in a spectral representation of the absolutely continuous part of L_0. This multiplication operator $\{S(\lambda)\}_{\lambda\in\mathbb{R}}$ is called the scattering matrix of the scattering system $\{\widetilde{L}, L_0\}$ and is one of the most important objects in mathematical scattering theory. The case that the spectrum $\sigma(A_0)$ is discrete is of particular importance in physical applications, e.g., modeling of quantum transport in semiconductors. In this case the scattering matrix of $\{\widetilde{L}, L_0\}$ is given by

$$S(\lambda) = I - 2i\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\big(M(\lambda) + \tau(\lambda)\big)^{-1}\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)},$$

where $M(\cdot)$ and $\tau(\cdot)$ are certain "abstract" Titchmarsh–Weyl functions corresponding to the internal and external systems, respectively, see Corollary 5.2.

The R-matrix $\{R(\lambda)\}_{\lambda\in\mathbb{R}}$ of $\{\widetilde{L}, L_0\}$ is defined as the Cayley transform of the scattering matrix $\{S(\lambda)\}_{\lambda\in\mathbb{R}}$, i.e.,

$$R(\lambda) = i\big(I - S(\lambda)\big)\big(I + S(\lambda)\big)^{-1},$$

and the problem in the R-matrix theory is to represent $\{R(\lambda)\}_{\lambda\in\mathbb{R}}$ in terms of eigenvalues and eigenfunctions of a suitable chosen closed internal system $\{\widehat{A}, \mathfrak{H}\}$. By the inverse Cayley transform this immediately also yields a representation of the scattering matrix by the same quantities.

For Schrödinger operators the problem is usually solved by choosing appropriate selfadjoint boundary conditions at the interface between the internal and external systems, in particular, Neumann boundary conditions. We show that in the abstract approach to the R-matrix theory the problem can be solved within the framework of abstract boundary triplets, which allow to characterize all selfadjoint extensions of A by abstract boundary conditions, cf. [10–12,18]. It is one of our main objectives to prove that there always exists a family of closed internal systems $\{A(\lambda), \mathfrak{H}\}_{\lambda\in\mathbb{R}}$ given by abstract boundary conditions connected with the function $\tau(\cdot)$, cf. [37], such that the R-matrix $\{R(\lambda)\}_{\lambda\in\mathbb{R}}$ and the scattering matrix $\{S(\lambda)\}_{\lambda\in\mathbb{R}}$ of $\{\widetilde{L}, L_0\}$ can be expressed with the help of the eigenvalues and eigenfunctions of $A(\lambda)$ for a.e. $\lambda \in \mathbb{R}$, cf. Theorem 5.5. This representation requires in addition that the internal Hamiltonians $A(\lambda)$ satisfy $A(\lambda) \leqslant A_0$, which is always true if A_0 is the Friedrichs extension of A. Moreover, our general representation results also indicate that even for small energy ranges it is rather unusual that the R-matrix and the scattering matrix can be represented by the eigenvalues and eigenfunctions of a single λ-independent internal Hamiltonian $\widehat{A}$.

As an application again the differential operators $A = -\frac{d^2}{dx^2} + v$ and $T = -\frac{d^2}{dx^2} + V$ from above are investigated and particular attention is paid to the case where the potential V is a real constant. Then the family $\{A(\lambda)\}_{\lambda\in\mathbb{R}}$ reduces to a single selfadjoint operator, namely, to the Schrödinger operator in $L^2((x_l,x_r))$ with Neumann boundary conditions. In general, however, this is not the case. Indeed, even in the simple case where V is constant on $(-\infty,x_l)$ and (x_r,∞) but the constants are different, a λ-dependent family of internal Hamiltonians is required for a certain energy interval to obtain a representation of the R-matrix and the scattering matrix in terms of eigenfunctions, see Section 6.2.1. The condition $A(\lambda)\leqslant A_0$ is always satisfied if A_0 is chosen to be the Schrödinger operator with Dirichlet boundary conditions. Finally, we emphasize that it is not possible to represent the R-matrix and the scattering matrix in terms of eigenfunctions of the internal Hamiltonian A_0 with Dirichlet boundary conditions.

The paper is organized as follows. In Section 2 we briefly recall some basic facts on boundary triplets and associated Weyl functions corresponding to symmetric operators in Hilbert spaces. It is the aim of the simple examples from semiconductor modeling in Section 2.3 to make the reader more familiar with this efficient tool in extension and spectral theory of symmetric and selfadjoint operators. Section 3 deals with semibounded extensions and representations of Weyl functions in terms of eigenfunctions of selfadjoint extensions of a given symmetric operator. In Section 4 we prove general representation theorems for the scattering matrix and the R-matrix of a scattering system which consists of two selfadjoint extensions of the same symmetric operator. Section 5 is devoted to scattering theory in open quantum systems, and with the preparations from the previous sections we easily obtain the above-mentioned representation of the R-matrix and scattering matrix of $\{\widetilde{L},L_0\}$ in terms of the eigenfunctions of an energy dependent selfadjoint operator family. In the last section the general results are applied to scattering systems consisting of orthogonal sums of regular and singular ordinary second order differential operators.

2. Boundary triplets and Weyl functions

2.1. Boundary triplets

Let $\mathfrak{H}$ be a separable Hilbert space and let A be a densely defined closed symmetric operator with equal deficiency indices $n_\pm(A)=\dim\ker(A^*\mp i)\leqslant\infty$ in $\mathfrak{H}$. We use the concept of boundary triplets for the description of the closed extensions of A in $\mathfrak{H}$, see e.g. [10–12,18].

Definition 2.1. Let A be a densely defined closed symmetric operator in $\mathfrak{H}$. A triplet $\Pi=\{\mathcal{H},\Gamma_0,\Gamma_1\}$ is called a *boundary triplet* for the adjoint operator A^* if $\mathcal{H}$ is a Hilbert space and $\Gamma_0,\Gamma_1:\mathrm{dom}(A^*)\to\mathcal{H}$ are linear mappings such that the abstract Green's identity

$$(A^*f,g)-(f,A^*g)=(\Gamma_1 f,\Gamma_0 g)-(\Gamma_0 f,\Gamma_1 g)$$

holds for all $f,g\in\mathrm{dom}(A^*)$ and the mapping $\Gamma:=\binom{\Gamma_0}{\Gamma_1}:\mathrm{dom}(A^*)\to\mathcal{H}\oplus\mathcal{H}$ is surjective.

We refer to [11] and [12] for a detailed study of boundary triplets and recall only some important facts. First of all a boundary triplet $\Pi=\{\mathcal{H},\Gamma_0,\Gamma_1\}$ for A^* always exists since the deficiency indices $n_\pm(A)$ of A are assumed to be equal. In this case $n_\pm(A)=\dim\mathcal{H}$ holds. We also note that a boundary triplet for A^* is not unique.

In order to describe the set of closed extensions $\widehat{A}\subseteq A^*$ of A with the help of a boundary triplet $\Pi=\{\mathcal{H},\Gamma_0,\Gamma_1\}$ for A^* we introduce the set $\widetilde{\mathcal{C}}(\mathcal{H})$ of closed linear relations in $\mathcal{H}$, that is, the set of closed linear subspaces of $\mathcal{H} \oplus \mathcal{H}$. If Θ is a closed linear operator in $\mathcal{H}$, then Θ will be identified with its graph $\mathcal{G}(\Theta)$,

$$\Theta \cong \mathcal{G}(\Theta) = \left\{ \begin{pmatrix} h \\ \Theta h \end{pmatrix} : \, h \in \mathrm{dom}(\Theta) \right\}.$$

Therefore, the set of closed linear operators in $\mathcal{H}$ is a subset of $\widetilde{\mathcal{C}}(\mathcal{H})$. Note that $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$ is the graph of an operator if and only if the multivalued part $\mathrm{mul}(\Theta) := \{h' \in \mathcal{H}\colon \binom{0}{h'} \in \Theta\}$ is trivial. The resolvent set $\rho(\Theta)$ and the point, continuous and residual spectrum $\sigma_p(\Theta)$, $\sigma_c(\Theta)$ and $\sigma_r(\Theta)$ of a closed linear relation Θ are defined in a similar way as for closed linear operators, cf. [13]. Recall that the adjoint relation $\Theta^* \in \widetilde{\mathcal{C}}(\mathcal{H})$ of a linear relation Θ in $\mathcal{H}$ is defined as

$$\Theta^* := \left\{ \begin{pmatrix} k \\ k' \end{pmatrix} : \, (h', k) = (h, k') \text{ for all } \begin{pmatrix} h \\ h' \end{pmatrix} \in \Theta \right\} \tag{2.1}$$

and Θ is said to be *symmetric* (*selfadjoint*) if $\Theta \subseteq \Theta^*$ (respectively $\Theta = \Theta^*$). We note that definition (2.1) extends the usual definition of the adjoint operator. Let now Θ be a selfadjoint relation in $\mathcal{H}$ and let P_{op} be the orthogonal projection in $\mathcal{H}$ onto $\mathcal{H}_{\mathrm{op}} := (\mathrm{mul}(\Theta))^\perp = \overline{\mathrm{dom}(\Theta)}$. Then

$$\Theta_{\mathrm{op}} = \left\{ \begin{pmatrix} x \\ P_{\mathrm{op}} x' \end{pmatrix} : \, \begin{pmatrix} x \\ x' \end{pmatrix} \in \Theta \right\}$$

is a selfadjoint (possibly unbounded) operator in the Hilbert space $\mathcal{H}_{\mathrm{op}}$ and Θ can be written as the direct orthogonal sum of Θ_{op} and a "pure" relation Θ_∞ in the Hilbert space $\mathcal{H}_\infty := (1 - P_{\mathrm{op}})\mathcal{H} = \mathrm{mul}(\Theta)$,

$$\Theta = \Theta_{\mathrm{op}} \oplus \Theta_\infty, \quad \Theta_\infty := \left\{ \begin{pmatrix} 0 \\ x' \end{pmatrix} : \, x' \in \mathrm{mul}(\Theta) \right\} \in \widetilde{\mathcal{C}}(\mathcal{H}_\infty). \tag{2.2}$$

With a boundary triplet $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ for A^* one associates two selfadjoint extensions of A defined by

$$A_0 := A^* \upharpoonright \ker(\Gamma_0) \quad \text{and} \quad A_1 := A^* \upharpoonright \ker(\Gamma_1). \tag{2.3}$$

A description of all proper (symmetric, selfadjoint) extensions of A is given in the next proposition.

Proposition 2.2. *Let A be a densely defined closed symmetric operator in $\mathfrak{H}$ with equal deficiency indices and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^*. Then the mapping*

$$\Theta \mapsto A_\Theta := A^* \upharpoonright \Gamma^{(-1)}\Theta = A^* \upharpoonright \{ f \in \mathrm{dom}(A^*)\colon \, (\Gamma_0 f, \Gamma_1 f)^\top \in \Theta \} \tag{2.4}$$

establishes a bijective correspondence between the set $\widetilde{\mathcal{C}}(\mathcal{H})$ and the set of closed extensions $A_\Theta \subseteq A^*$ of A. Furthermore

$$(A_\Theta)^* = A_{\Theta^*}$$

holds for any $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$. The extension A_Θ in (2.4) *is symmetric* (*selfadjoint, dissipative, maximal dissipative*) *if and only if Θ is symmetric* (*selfadjoint, dissipative, maximal dissipative*).

It is worth to note that the selfadjoint operator $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ in (2.3) corresponds to the "pure" relation $\Theta_\infty = \{\binom{0}{h}\colon h \in \mathcal{H}\}$. Moreover, if Θ is an operator, then (2.4) can also be written in the form

$$A_\Theta = A^* \upharpoonright \ker(\Gamma_1 - \Theta\Gamma_0), \tag{2.5}$$

so that, in particular A_1 in (2.3) corresponds to $\Theta = 0 \in [\mathcal{H}]$. Here and in the following $[\mathcal{H}]$ stands for the space of bounded everywhere defined linear operators in $\mathcal{H}$. We note that if the product $\Theta\Gamma_0$ in (2.5) is interpreted in the sense of relations, then (2.5) is even true for parameters Θ with $\mathrm{mul}(\Theta) \neq \{0\}$.

Later we shall often be concerned with closed simple symmetric operators. Recall that a closed symmetric operator A is said to be *simple* if there is no nontrivial subspace which reduces A to a selfadjoint operator. By [22] this is equivalent to

$$\mathfrak{H} = \mathrm{clospan}\{\ker(A^* - \lambda)\colon \lambda \in \mathbb{C} \setminus \mathbb{R}\},$$

where $\mathrm{clospan}\{\cdot\}$ denotes the closed linear span of a set. Note that a simple symmetric operator has no eigenvalues.

2.2. *Weyl functions and resolvents of extensions*

Let again A be a densely defined closed symmetric operator in $\mathfrak{H}$ with equal deficiency indices. A point $\lambda \in \mathbb{C}$ is of *regular type* if $\ker(A-\lambda) = \{0\}$ and the range $\mathrm{ran}(A-\lambda)$ is closed. We denote the *defect subspace* of A at the points $\lambda \in \mathbb{C}$ of regular type by $\mathcal{N}_\lambda = \ker(A^* - \lambda)$. The space of bounded everywhere defined linear operators mapping a Hilbert space $\mathcal{H}$ into $\mathfrak{H}$ will be denoted by $[\mathcal{H}, \mathfrak{H}]$. The following definition was given in [10,11].

Definition 2.3. Let A be a densely defined closed symmetric operator in $\mathfrak{H}$, let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* and let $A_0 = A^* \upharpoonright \ker(\Gamma_0)$. The operator-valued functions $\gamma(\cdot): \rho(A_0) \to [\mathcal{H}, \mathfrak{H}]$ and $M(\cdot): \rho(A_0) \to [\mathcal{H}]$ defined by

$$\gamma(\lambda) := (\Gamma_0 \upharpoonright \mathcal{N}_\lambda)^{-1} \quad \text{and} \quad M(\lambda) := \Gamma_1\gamma(\lambda), \quad \lambda \in \rho(A_0), \tag{2.6}$$

are called the γ*-field* and the *Weyl function*, respectively, corresponding to the boundary triplet Π.

It follows from the identity $\mathrm{dom}(A^*) = \ker(\Gamma_0) \dot{+} \mathcal{N}_\lambda$, $\lambda \in \rho(A_0)$, where $A_0 = A^* \upharpoonright \ker(\Gamma_0)$, that the γ-field $\gamma(\cdot)$ in (2.6) is well defined. It can be shown that both $\gamma(\cdot)$ and $M(\cdot)$ are holomorphic on $\rho(A_0)$, and the relations

$$\gamma(\lambda) = \bigl(1 + (\lambda - \mu)(A_0 - \lambda)^{-1}\bigr)\gamma(\mu), \quad \lambda, \mu \in \rho(A_0),$$

and

$$M(\lambda) - M(\mu)^* = (\lambda - \bar{\mu})\gamma(\mu)^*\gamma(\lambda), \quad \lambda, \mu \in \rho(A_0), \tag{2.7}$$

are valid (see [11]). The identity (2.7) yields that $M(\cdot)$ is a *Nevanlinna function*, that is, $M(\cdot)$ is holomorphic on $\mathbb{C} \setminus \mathbb{R}$, $M(\lambda) = M(\bar{\lambda})^*$ for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and $\Im\mathrm{m}(M(\lambda))$ is a nonnegative operator for all λ in the upper half-plane $\mathbb{C}_+ = \{\lambda \in \mathbb{C}\colon \Im\mathrm{m}(\lambda) > 0\}$. Moreover, it follows from (2.7) that $0 \in \rho(\Im\mathrm{m}(M(\lambda)))$ holds for all $\lambda \in \mathbb{C} \setminus \mathbb{R}$.

The following well-known theorem shows how the spectral properties of the closed extensions A_Θ of A can be described with the help of the Weyl function, cf. [11,12].

Theorem 2.4. *Let A be a densely defined closed symmetric operator in $\mathfrak{H}$ and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* with γ-field γ and Weyl function M. Let $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ and let $A_\Theta \subseteq A^*$ be a closed extension corresponding to some $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$ via (2.4)–(2.5). Then a point $\lambda \in \rho(A_0)$ belongs to the resolvent set $\rho(A_\Theta)$ if and only if $0 \in \rho(\Theta - M(\lambda))$ and the formula*

$$(A_\Theta - \lambda)^{-1} = (A_0 - \lambda)^{-1} + \gamma(\lambda)\big(\Theta - M(\lambda)\big)^{-1}\gamma(\bar{\lambda})^* \tag{2.8}$$

holds for all $\lambda \in \rho(A_0) \cap \rho(A_\Theta)$. Moreover, $\lambda \in \rho(A_0)$ belongs to the point spectrum $\sigma_p(A_\Theta)$, to the continuous spectrum $\sigma_c(A_\Theta)$ or to the residual spectrum $\sigma_r(A_\Theta)$ of A_Θ if and only if $0 \in \sigma_i(\Theta - M(\lambda))$, $i = p, c, r$, respectively.

2.3. Regular and singular Sturm–Liouville operators

We are going to illustrate the notions of boundary triplets, Weyl functions and γ-fields with some well-known simple examples.

2.3.1. Finite intervals

Let us first consider a Schrödinger operator on the bounded interval $(x_l, x_r) \subset \mathbb{R}$. The minimal operator A in $\mathfrak{H} = L^2((x_l, x_r))$ is defined by

$$\begin{gathered}(Af)(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\tfrac{d}{dx}f(x) + v(x)f(x),\\ \mathrm{dom}(A) := \left\{ f \in \mathfrak{H}\colon \begin{array}{l} f, \frac{1}{m}f' \in W^{1,2}((x_l, x_r)) \\ f(x_l) = f(x_r) = 0 \\ \big(\frac{1}{m}f'\big)(x_l) = \big(\frac{1}{m}f'\big)(x_r) = 0 \end{array} \right\},\end{gathered} \tag{2.9}$$

where it is assumed that the effective mass m satisfies $m > 0$ and $m, \frac{1}{m} \in L^\infty((x_l, x_r))$, and that also $v \in L^\infty((x_l, x_r))$ is a real function. It is well known that A is a densely defined closed simple symmetric operator in $\mathfrak{H}$ with deficiency indices $n_+(A) = n_-(A) = 2$. The adjoint operator A^* is given by

$$\begin{gathered}(A^*f)(x) = -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}f(x) + v(x)f(x),\\ \mathrm{dom}(A^*) = \left\{ f \in \mathfrak{H}\colon f, \frac{1}{m}f' \in W^{1,2}((x_l, x_r)) \right\}.\end{gathered}$$

It is straightforward to verify that $\Pi_A = \{\mathbb{C}^2, \Gamma_0, \Gamma_1\}$, where

$$\Gamma_0 f := \begin{pmatrix} f(x_l) \\ f(x_r) \end{pmatrix} \quad \text{and} \quad \Gamma_1 f := \frac{1}{2}\begin{pmatrix} \big(\frac{1}{m}f'\big)(x_l) \\ -\big(\frac{1}{m}f'\big)(x_r) \end{pmatrix},$$

$f \in \mathrm{dom}(A^*)$, is a boundary triplet for A^*. Note, that $A_0 := A^* \upharpoonright \ker(\Gamma_0)$ corresponds to Dirichlet boundary conditions, that is,

$$\mathrm{dom}(A_0) = \left\{ f \in \mathfrak{H}\colon\ f, \frac{1}{m} f' \in W^{1,2}((x_l, x_r)),\ f(x_l) = f(x_r) = 0 \right\}. \tag{2.10}$$

The selfadjoint extension $A_1 := A^* \upharpoonright \ker \Gamma_1$ corresponds to Neumann boundary conditions, i.e.,

$$\mathrm{dom}(A_1) = \left\{ f \in \mathfrak{H}\colon\ f, \frac{1}{m} f' \in W^{1,2}((x_l, x_r)),\ \left(\frac{1}{m} f'\right)(x_l) = \left(\frac{1}{m} f'\right)(x_r) = 0 \right\}. \tag{2.11}$$

Let φ_λ and ψ_λ, $\lambda \in \mathbb{C}$, be the fundamental solutions of the homogeneous differential equation $-\frac{1}{2}\frac{d}{dx}\frac{1}{m}\frac{d}{dx}u + vu = \lambda u$ satisfying the boundary conditions

$$\varphi_\lambda(x_l) = 1, \quad \left(\frac{1}{2m}\varphi'_\lambda\right)(x_l) = 0 \quad \text{and} \quad \psi_\lambda(x_l) = 0, \quad \left(\frac{1}{2m}\psi'_\lambda\right)(x_l) = 1.$$

Observe that φ_λ and ψ_λ belong to $L^2((x_l, x_r))$ since (x_l, x_r) is a finite interval. A straightforward computation shows

$$\begin{aligned} \big((A_0 - \lambda)^{-1} f\big)(x) &= \varphi_\lambda(x) \int_{x_l}^{x} \psi_\lambda(t) f(t)\,dt + \psi_\lambda(x) \int_{x}^{x_r} \varphi_\lambda(t) f(t)\,dt \\ &\quad - \frac{\varphi_\lambda(x_r)}{\psi_\lambda(x_r)} \psi_\lambda(x) \int_{x_l}^{x_r} \psi_\lambda(t) f(t)\,dt \end{aligned}$$

for $x \in (x_l, x_r)$, $f \in L^2((x_l, x_r))$ and all $\lambda \in \rho(A_0)$. In order to calculate the γ-field and Weyl function corresponding to $\Pi_A = \{\mathbb{C}^2, \Gamma_0, \Gamma_1\}$ note that every element $f_\lambda \in \mathcal{N}_\lambda = \ker(A^* - \lambda)$ admits the representation

$$f_\lambda(x) = \xi_0 \varphi_\lambda(x) + \xi_1 \psi_\lambda(x), \quad x \in (x_l, x_r),\ \lambda \in \mathbb{C},\ \xi_0, \xi_1 \in \mathbb{C},$$

where the coefficients ξ_0, ξ_1 are uniquely determined. Then

$$\Gamma_0 f_\lambda = \begin{pmatrix} 1 & 0 \\ \varphi_\lambda(x_r) & \psi_\lambda(x_r) \end{pmatrix} \begin{pmatrix} \xi_0 \\ \xi_1 \end{pmatrix}$$

yields

$$\frac{1}{\psi_\lambda(x_r)} \begin{pmatrix} \psi_\lambda(x_r) & 0 \\ -\varphi_\lambda(x_r) & 1 \end{pmatrix} \Gamma_0 f_\lambda = \begin{pmatrix} \xi_0 \\ \xi_1 \end{pmatrix}$$

for $\psi_\lambda(x_r) \neq 0$ (that is $\lambda \notin \sigma(A_0)$) and it follows that the γ-field is given by

$$\gamma(\lambda):\mathbb{C}^2 \to L^2((x_l,x_r)),$$
$$\begin{pmatrix}\xi_0\\ \xi_1\end{pmatrix} \mapsto \frac{1}{\psi_\lambda(x_r)}\big(\big(\varphi_\lambda(\cdot)\psi_\lambda(x_r)-\psi_\lambda(\cdot)\varphi_\lambda(x_r)\big)\xi_0+\psi_\lambda(\cdot)\xi_1\big).$$

We remark that the adjoint operator admits the representation

$$\gamma(\lambda)^* f = \frac{1}{\overline{\psi_\lambda(x_r)}}\begin{pmatrix}\int_{x_l}^{x_r}\big(\overline{\varphi_\lambda(y)}\,\overline{\psi_\lambda(x_r)}-\overline{\psi_\lambda(y)}\,\overline{\varphi_\lambda(x_r)}\big)f(y)\,dy\\ \int_{x_l}^{x_r}\overline{\psi_\lambda(y)}\,f(y)\,dy\end{pmatrix},$$

$f\in L^2((x_l,x_r))$. The Weyl function $M(\lambda)=\Gamma_1\gamma(\lambda)$, $\lambda\in\rho(A_0)$, then becomes

$$M(\lambda)=\frac{1}{\psi_\lambda(x_r)}\begin{pmatrix}-\varphi_\lambda(x_r) & 1\\ 1 & -\big(\frac{1}{2m}\psi_\lambda'\big)(x_r)\end{pmatrix}.$$

All selfadjoint extensions of A in $L^2((x_l,x_r))$ can now be described with the help of selfadjoint relations $\Theta=\Theta^*$ in $\mathbb{C}^2$ via (2.4)–(2.5) and their resolvents can be expressed in terms of the resolvent of A_0, the Weyl function $M(\cdot)$ and the γ-field $\gamma(\cdot)$, cf. Theorem 2.4. We leave the general case to the reader and note only that if Θ is a selfadjoint matrix of the form

$$\Theta=\begin{pmatrix}\kappa_l & 0\\ 0 & \kappa_r\end{pmatrix},\quad \kappa_l,\kappa_r\in\mathbb{R},$$

then

$$\operatorname{dom}(A_\Theta)=\left\{f\in\operatorname{dom}(A^*):\ \begin{array}{l}\big(\frac{1}{2m}f'\big)(x_l)=\kappa_l f(x_l)\\ \big(\frac{1}{2m}f'\big)(x_r)=-\kappa_r f(x_r)\end{array}\right\}$$

and

$$\big(\Theta-M(\lambda)\big)^{-1} = \frac{1}{\psi_\lambda(x_r)\det(\Theta-M(\lambda))}\begin{pmatrix}\kappa_r\psi_\lambda(x_r)+\big(\frac{1}{2m}\psi_\lambda'\big)(x_r) & 1\\ 1 & \kappa_l\psi_\lambda(x_r)+\varphi_\lambda(x_r)\end{pmatrix}.$$

Obviously the case $\kappa_l=\kappa_r=0$ leads to the Neumann operator A_1.

2.3.2. Infinite intervals

Next we consider a singular problem on the infinite interval $(-\infty,x_l)$ in the Hilbert space $\mathfrak{K}_l=L^2((-\infty,x_l))$. The minimal operator is defined by

$$(T_l g_l)(x):=-\frac{1}{2}\frac{d}{dx}\frac{1}{m_l(x)}\frac{d}{dx}g_l(x)+v_l(x)g_l(x),$$

$$\operatorname{dom}(T_l):=\left\{g_l\in\mathfrak{K}_l:\ g_l,\frac{1}{m_l}g_l'\in W^{1,2}((-\infty,x_l)),\ g_l(x_l)=\left(\frac{1}{m_l}g_l'\right)(x_l)=0\right\},$$

where $m_l > 0$, $m_l, \frac{1}{m_l} \in L^\infty((-\infty, x_l))$ and $v_l \in L^\infty((-\infty, x_l))$ is real. Then T_l is a densely defined closed simple symmetric operator with deficiency indices $n_-(T_l) = n_+(T_l) = 1$, see e.g. [38] and [17] for the fact that T_l is simple. The adjoint operator T_l^* is given by

$$\big(T_l^* g_l\big)(x) = -\frac{1}{2}\frac{d}{dx}\frac{1}{m_l(x)}\frac{d}{dx} g_l(x) + v_l(x) g_l(x),$$

$$\operatorname{dom}\big(T_l^*\big) = \left\{ g_l \in \mathfrak{K}_l \colon\ g_l, \frac{1}{m_l} g_l' \in W^{1,2}((-\infty, x_l)) \right\}.$$

One easily verifies that $\Pi_{T_l} = \{\mathbb{C}, \Upsilon_0^l, \Upsilon_1^l\}$,

$$\Upsilon_0^l g_l := g_l(x_l) \quad \text{and} \quad \Upsilon_1^l g_l := -\left(\frac{1}{2m_l} g_l'\right)(x_l), \qquad g_l \in \operatorname{dom}\big(T_l^*\big),$$

is a boundary triplet for T_l^*. Let $\varphi_{\lambda,l}$ and $\psi_{\lambda,l}$ be the fundamental solutions of the equation $-\frac{1}{2}\frac{d}{dx}\frac{1}{m_l}\frac{d}{dx} u + v_l u = \lambda u$ satisfying the boundary conditions

$$\varphi_{\lambda,l}(x_l) = 1, \quad \left(\frac{1}{2m_l}\varphi_{\lambda,l}'\right)(x_l) = 0 \quad \text{and} \quad \psi_{\lambda,l}(x_l) = 0, \quad \left(\frac{1}{2m_l}\psi_{\lambda,l}'\right)(x_l) = 1.$$

Then there exists a scalar function $\mathfrak{m}_l$ such that for each $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the function

$$x \mapsto g_{\lambda,l}(x) := \varphi_{\lambda,l}(x) - \mathfrak{m}_l(\lambda)\psi_{\lambda,l}(x)$$

belongs to $L^2((-\infty, x_l))$, cf. [38]. The function $\mathfrak{m}_l$ is usually called the Titchmarsh–Weyl function or Titchmarsh–Weyl coefficient and in our setting $\mathfrak{m}_l$ coincides with the Weyl function of the boundary triplet $\Pi_{T_l} = \{\mathbb{C}, \Upsilon_0^l, \Upsilon_1^l\}$, since

$$\Upsilon_1^l g_{\lambda,l} = \mathfrak{m}_l(\lambda)\Upsilon_0^l g_{\lambda,l}, \qquad g_{\lambda,l} \in \mathcal{N}_{\lambda,l} := \ker\big(T_l^* - \lambda\big),\ \lambda \in \mathbb{C} \setminus \mathbb{R}.$$

An analogous example is the Schrödinger operator on the infinite interval (x_r, ∞) in the Hilbert space $\mathfrak{K}_r = L^2((x_r, \infty))$ defined by

$$(T_r g_r)(x) := -\frac{1}{2}\frac{d}{dx}\frac{1}{m_r(x)}\frac{d}{dx} g_r(x) + v_r(x) g_r(x),$$

$$\operatorname{dom}(T_r) := \left\{ g_r \in \mathfrak{K}_r \colon\ \begin{matrix} g_r, \frac{1}{m_r} g_r' \in W^{1,2}((x_r, \infty)) \\ g_r(x_r) = \big(\frac{1}{m_r} g_r'\big)(x_r) = 0 \end{matrix} \right\},$$

where $m_r > 0$, $m_r, \frac{1}{m_r} \in L^\infty((x_r, \infty))$ and $v_r \in L^\infty((x_r, \infty))$ is real. The adjoint operator T_r^* is

$$\big(T_r^* g_r\big)(x) = -\frac{1}{2}\frac{d}{dx}\frac{1}{m_r(x)}\frac{d}{dx} g_r(x) + v_r(x) g_r(x),$$

$$\operatorname{dom}\big(T_r^*\big) = \left\{ g_r \in \mathfrak{K}_r \colon\ g_r, \frac{1}{m_r} g_r' \in W^{1,2}((x_r, \infty)) \right\}$$

and $\Pi_{T_r} = \{\mathbb{C}, \Upsilon_0^r, \Upsilon_1^r\}$,

$$\Upsilon_0^r g_r := g_r(x_r) \quad \text{and} \quad \Upsilon_1^r g_r := \left(\frac{1}{2m_r} g_r'\right)(x_r), \quad g_r \in \operatorname{dom}\bigl(T_r^*\bigr),$$

is a boundary triplet for T_r^*. Let $\varphi_{\lambda,r}$ and $\psi_{\lambda,r}$ be the fundamental solutions of the equation $-\frac{1}{2}\frac{d}{dx}\frac{1}{m_r}\frac{d}{dx}u + v_r u = \lambda u$ satisfying the boundary conditions

$$\varphi_{\lambda,r}(x_r) = 1, \quad \left(\frac{1}{2m_r}\varphi_{\lambda,r}'\right)(x_r) = 0 \quad \text{and} \quad \psi_{\lambda,r}(x_r) = 0, \quad \left(\frac{1}{2m_r}\psi_{\lambda,r}'\right)(x_r) = 1.$$

Then there exists a scalar function $\mathfrak{m}_r$ such that for each $\lambda \in \mathbb{C} \setminus \mathbb{R}$ the function

$$x \mapsto g_{\lambda,r}(x) := \varphi_{\lambda,r}(x) + \mathfrak{m}_r(\lambda)\psi_{\lambda,r}(x)$$

belongs to $L^2((x_r,\infty))$. As above $\mathfrak{m}_r$ coincides with the Weyl function of the boundary triplet $\Pi_{T_r} := \{\mathbb{C}, \Upsilon_0^r, \Upsilon_1^r\}$.

For our purposes it is useful to consider the direct sum of the two operators T_l and T_r. To this end we introduce the Hilbert space

$$\mathfrak{K} := L^2\bigl((-\infty, x_l) \cup (x_r,\infty)\bigr) \cong \mathfrak{K}_l \oplus \mathfrak{K}_r.$$

An element $g \in \mathfrak{K}$ will be written in the form $g = g_l \oplus g_r$, where $g_l \in L^2((-\infty, x_l))$ and $g_r \in L^2((x_r,\infty))$. The operator $T = T_l \oplus T_r$ in $\mathfrak{K}$ is given by

$$(Tg)(x) = \begin{pmatrix} -\frac{1}{2}\frac{d}{dx}\frac{1}{m_l(x)}\frac{d}{dx}g_l(x) + v_l g_l(x) & 0 \\ 0 & -\frac{1}{2}\frac{d}{dx}\frac{1}{m_r(x)}\frac{d}{dx}g_r(x) + v_r g_r(x) \end{pmatrix},$$

$$\operatorname{dom}(T) = \operatorname{dom}(T_l) \oplus \operatorname{dom}(T_r),$$

and T is a densely defined closed simple symmetric operator in $\mathfrak{K}$ with deficiency indices $n_+(T) = n_-(T) = 2$. The adjoint operator T^* is given by

$$(T^*g)(x) = \begin{pmatrix} -\frac{1}{2}\frac{d}{dx}\frac{1}{m_l(x)}\frac{d}{dx}g_l(x) + v_l g_l(x) & 0 \\ 0 & -\frac{1}{2}\frac{d}{dx}\frac{1}{m_r(x)}\frac{d}{dx}g_r(x) + v_r g_r(x) \end{pmatrix},$$

$$\operatorname{dom}(T^*) = \operatorname{dom}\bigl(T_l^*\bigr) \oplus \operatorname{dom}\bigl(T_r^*\bigr).$$

One easily checks that $\Pi_T = \{\mathbb{C}^2, \Upsilon_0, \Upsilon_1\}$, $\Upsilon_0 := (\Upsilon_0^l, \Upsilon_0^r)^\top$, $\Upsilon_1 := (\Upsilon_1^l, \Upsilon_1^r)^\top$, that is,

$$\Upsilon_0 g = \begin{pmatrix} g_l(x_l) \\ g_r(x_r) \end{pmatrix} \quad \text{and} \quad \Upsilon_1 g = \frac{1}{2}\begin{pmatrix} -\bigl(\frac{1}{m_l}g_l'\bigr)(x_l) \\ \bigl(\frac{1}{m_r}g_r'\bigr)(x_r) \end{pmatrix},$$

$g \in \operatorname{dom}(T^*)$, is a boundary triplet for T^*. Note that $T_0 = T^* \restriction \ker(\Upsilon_0)$ is the restriction of T^* to the domain

$$\operatorname{dom}(T_0) = \bigl\{g \in \operatorname{dom}(T^*)\colon\ g_l(x_l) = g_r(x_r) = 0\bigr\},$$

that is, T_0 corresponds to Dirichlet boundary conditions at x_l and x_r. The Weyl function $\tau(\cdot)$ corresponding to the boundary triplet $\Pi_T = \{\mathbb{C}^2, \Upsilon_0, \Upsilon_1\}$ is given by

$$\lambda \mapsto \tau(\lambda) = \begin{pmatrix} \mathfrak{m}_l(\lambda) & 0 \\ 0 & \mathfrak{m}_r(\lambda) \end{pmatrix}, \quad \lambda \in \rho(T_0).$$

3. Semibounded extensions and expansions in eigenfunctions

Let A be a densely defined closed symmetric operator in the separable Hilbert space $\mathfrak{H}$ and let $\{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* with γ-field $\gamma(\cdot)$ and Weyl function $M(\cdot)$. Fix some $\Theta = \Theta^* \in \widetilde{\mathcal{C}}(\mathcal{H})$ and let $A_\Theta \subseteq A^*$ be the corresponding selfadjoint extension via (2.4).

In the next proposition it will be assumed that $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ and A_Θ (and hence also the symmetric operator A) are semibounded from below. Observe that if A has finite defect it is sufficient for semiboundedness of A_0 and A_Θ to assume that A is semibounded, cf. Corollary 3.2.

Proposition 3.1. *Let A be a densely defined closed symmetric operator in $\mathfrak{H}$ and let $\{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* with γ-field $\gamma(\cdot)$ and Weyl function $M(\cdot)$. Let A_Θ be a selfadjoint extension of A corresponding to $\Theta = \Theta^* \in \widetilde{\mathcal{C}}(\mathcal{H})$ and assume that $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ and A_Θ are semibounded from below. Then $A_\Theta \leqslant A_0$ holds if and only if*

$$\operatorname{ran}\big(\gamma(\lambda)\big(\Theta - M(\lambda)\big)^{-1}\big) \subseteq \operatorname{dom}\big(\sqrt{A_\Theta - \lambda}\big) \tag{3.1}$$

is satisfied for all $\lambda < \min\{\sigma(A_0), \sigma(A_\Theta)\}$.

Proof. Let $A_\Theta \leqslant A_0$. From (2.8) we get

$$(A_\Theta - \lambda)^{-1} - (A_0 - \lambda)^{-1} = \gamma(\lambda)\big(\Theta - M(\lambda)\big)^{-1}\gamma(\lambda)^* \geqslant 0$$

for $\lambda < \min\{\sigma(A_0), \sigma(A_\Theta)\}$ which yields

$$\big(\Theta - M(\lambda)\big)^{-1} \geqslant 0.$$

By [15, Corollary 7-2] there is a contraction Y acting from $\mathfrak{H}$ into $\mathcal{H}$ such that

$$\big(\Theta - M(\lambda)\big)^{-1/2}\gamma(\lambda)^* = Y(A_\Theta - \lambda)^{-1/2}.$$

Since $\lambda \in \mathbb{R}$, $\Theta = \Theta^*$ and M is holomorphic on $(-\infty, \min\sigma(A_0))$ the adjoint has the form

$$\gamma(\lambda)\big(\Theta - M(\lambda)\big)^{-1/2} = (A_\Theta - \lambda)^{-1/2}Y^*,$$

so that

$$\operatorname{ran}\big(\gamma(\lambda)\big(\Theta - M(\lambda)\big)^{-1/2}\big) \subseteq \operatorname{dom}\big(\sqrt{A_\Theta - \lambda}\big).$$

Therefore

$$\operatorname{ran}\big(\gamma(\lambda)\big(\Theta - M(\lambda)\big)^{-1}\big) \subseteq \operatorname{ran}\big(\gamma(\lambda)\big(\Theta - M(\lambda)\big)^{-1/2}\big) \subseteq \operatorname{dom}\big(\sqrt{A_\Theta - \lambda}\big)$$

and (3.1) is proved.

Conversely, let us assume that condition (3.1) is satisfied. Then for each $\lambda < \min\{\sigma(A_0), \sigma(A_\Theta)\}$ the operator

$$F_\Theta^*(\lambda) := \sqrt{A_\Theta - \lambda}\,\gamma(\lambda)\big(\Theta - M(\lambda)\big)^{-1} \tag{3.2}$$

is well defined on $\mathcal{H}$ and closed, and hence bounded. Besides $F_\Theta^*(\lambda)$ we introduce the densely defined operator

$$\begin{aligned} F_\Theta(\lambda) &= \Gamma_0(A_\Theta - \lambda)^{-1/2}, \\ \operatorname{dom}\big(F_\Theta(\lambda)\big) &= \big\{f \in \mathfrak{H}\colon (A_\Theta - \lambda)^{-1/2} f \in \operatorname{dom}(A^*)\big\} \end{aligned} \tag{3.3}$$

for $\lambda < \min \sigma(A_\Theta)$.

It follows from (2.8), $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ and $\Gamma_0\gamma(\lambda) = I_{\mathcal{H}}$ that

$$\Gamma_0(A_\Theta - \lambda)^{-1} = \big(\Theta - M(\lambda)\big)^{-1}\gamma(\bar\lambda)^* \tag{3.4}$$

holds for all $\lambda \in \rho(A_0) \cap \rho(A_\Theta)$. Thus for $\lambda < \min\{\sigma(A_0), \sigma(A_\Theta)\}$ (3.2) becomes

$$F_\Theta^*(\lambda) = \sqrt{A_\Theta - \lambda}\big(\Gamma_0(A_\Theta - \lambda)^{-1}\big)^*$$

and together with (3.3) we conclude

$$F_\Theta(\lambda) = \Gamma_0(A_\Theta - \lambda)^{-1/2} \subseteq \big(\sqrt{A_\Theta - \lambda}\big(\Gamma_0(A_\Theta - \lambda)^{-1}\big)^*\big)^* = \big(F_\Theta^*(\lambda)\big)^*.$$

This implies that $F_\Theta(\lambda)$ admits a bounded everywhere defined extension $\overline{F}_\Theta(\lambda)$ for every $\lambda < \min\{\sigma(A_0), \sigma(A_\Theta)\}$ such that $F_\Theta(\lambda)^* = \overline{F}_\Theta(\lambda)^* = F_\Theta^*(\lambda)$. From (3.4) and $M(\bar\lambda) = M(\lambda)^*$ we find

$$\Gamma_0\big(\Gamma_0(A_\Theta - \bar\lambda)^{-1}\big)^* = \big(\Theta - M(\lambda)\big)^{-1}, \quad \lambda \in \rho(A_0) \cap \rho(A_\Theta),$$

so that for $\lambda < \min\{\sigma(A_0), \sigma(A_\Theta)\}$

$$\begin{aligned} \big(\Theta - M(\lambda)\big)^{-1} &= \Gamma_0(A_\Theta - \lambda)^{-1/2}\sqrt{A_\Theta - \lambda}\big(\Gamma_0(A_\Theta - \lambda)^{-1}\big)^* \\ &= \overline{F}_\Theta(\lambda)\overline{F}_\Theta(\lambda)^* \geqslant 0. \end{aligned} \tag{3.5}$$

Using (2.8) we find

$$(A_\Theta - \lambda)^{-1} \geqslant (A_0 - \lambda)^{-1}$$

for $\lambda < \min\{\sigma(A_0), \sigma(A_\Theta)\}$ which yields $A_\Theta \leqslant A_0$. $\square$

Corollary 3.2. *Let A be a densely defined closed symmetric operator in $\mathfrak{H}$ and let $\{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* with γ-field $\gamma(\cdot)$ and Weyl function $M(\cdot)$. Assume that A has finite* *defect and that $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ is the Friedrichs extension. Then every selfadjoint extension A_Θ of A in $\mathfrak{H}$ is semibounded from below and*

$$\operatorname{ran}\bigl(\gamma(\lambda)\bigl(\Theta - M(\lambda)\bigr)^{-1}\bigr) \subseteq \operatorname{dom}\bigl(\sqrt{A_\Theta - \lambda}\bigr)$$

is satisfied for all $\lambda < \min \sigma(A_\Theta)$.

In the next proposition we obtain a representation of the function $\lambda \mapsto (\Theta - M(\lambda))^{-1}$ in terms of eigenvalues and eigenfunctions of A_Θ. This representation will play an important role in Section 5.

Proposition 3.3. *Let A be a densely defined closed symmetric operator in $\mathfrak{H}$ and let $\{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* with Weyl function $M(\cdot)$. Let A_Θ be a selfadjoint extension of A corresponding to $\Theta = \Theta^* \in \widetilde{\mathcal{C}}(\mathcal{H})$ and assume that $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ and A_Θ are semibounded from below, $A_\Theta \leqslant A_0$, and that the spectrum of A_Θ is discrete. Then the $[\mathcal{H}]$-valued function $\lambda \mapsto (\Theta - M(\lambda))^{-1}$ admits the representation*

$$\bigl(\Theta - M(\lambda)\bigr)^{-1} = \sum_{k=1}^{\infty} (\lambda_k - \lambda)^{-1} (\cdot, \Gamma_0 \psi_k) \Gamma_0 \psi_k, \quad \lambda \in \rho(A_0) \cap \rho(A_\Theta), \tag{3.6}$$

where $\{\lambda_k\}$, $k = 1, 2, \ldots,$ are the eigenvalues of A_Θ in increasing order (counting multiplicities) and $\{\psi_k\}$ are the corresponding eigenfunctions. The convergence in (3.6) is understood in the strong sense.

Proof. Let $\lambda_0 < \min\{\inf \sigma(A_0), \inf \sigma(A_\Theta)\}$ and let E_m, $m \in \mathbb{N}$, be the orthogonal projection in $\mathfrak{H}$ onto the subspace spanned by the eigenfunctions $\{\psi_k\}$, $k = 1, \ldots, m < \infty$, of A_Θ. Considerations similar as in the proof of Proposition 3.1 show

$$\begin{aligned}\Gamma_0 E_m \gamma(\lambda_0)\bigl(\Theta - M(\lambda_0)\bigr)^{-1} &= \Gamma_0 (A_\Theta - \lambda_0)^{-1/2} E_m \sqrt{A_\Theta - \lambda_0}\, \gamma(\lambda_0)\bigl(\Theta - M(\lambda_0)\bigr)^{-1} \\ &= \overline{F}_\Theta(\lambda_0) E_m \overline{F}_\Theta(\lambda_0)^*,\end{aligned}$$

where $F_\Theta(\lambda_0)$ is defined as in (3.3) and $\overline{F}_\Theta(\lambda_0) \in [\mathfrak{H}, \mathcal{H}]$ denotes the closure. Hence we have

$$\lim_{m\to\infty} \Gamma_0 E_m \gamma(\lambda_0)\bigl(\Theta - M(\lambda_0)\bigr)^{-1} = \overline{F}_\Theta(\lambda_0)\overline{F}_\Theta(\lambda_0)^* = \bigl(\Theta - M(\lambda_0)\bigr)^{-1}$$

in the strong topology, cf. (3.5). For $\lambda \in \rho(A_0) \cap \rho(A_\Theta)$ we conclude from the representations

$$\bigl(\Theta - M(\lambda)\bigr)^{-1} = \Gamma_0\bigl(\Gamma_0(A_\Theta - \bar{\lambda})^{-1}\bigr)^* = \overline{F}_\Theta(\lambda_0)(A_\Theta - \lambda_0)(A_\Theta - \lambda)^{-1}\overline{F}_\Theta(\lambda_0)^*$$

and

$$\Gamma_0 E_m \gamma(\lambda)\bigl(\Theta - M(\lambda)\bigr)^{-1} = \overline{F}_\Theta(\lambda_0)(A_\Theta - \lambda_0)(A_\Theta - \lambda)^{-1} E_m \overline{F}_\Theta(\lambda_0)^*$$

that

$$\lim_{m\to\infty} \Gamma_0 E_m \gamma(\lambda)\bigl(\Theta - M(\lambda)\bigr)^{-1} = \bigl(\Theta - M(\lambda)\bigr)^{-1}$$

in the strong sense for all $\lambda \in \rho(A_0) \cap \rho(A_\Theta)$.

Furthermore, since the resolvent of A_Θ admits the representation

$$(A_\Theta - \lambda)^{-1} = \sum_{k=1}^{\infty} (\lambda_k - \lambda)^{-1} (\cdot, \psi_k)\psi_k, \quad \lambda \in \rho(A_\Theta),$$

where the convergence is in the strong sense, we find

$$\Gamma_0 (A_\Theta - \lambda)^{-1} E_m = \sum_{k=1}^{m} (\lambda_k - \lambda)^{-1} (\cdot, \psi_k) \Gamma_0 \psi_k.$$

For $\lambda \in \rho(A_0) \cap \rho(A_\Theta)$ the adjoint operator is given by

$$\begin{aligned} E_m \big(\Gamma_0 (A_\Theta - \lambda)^{-1}\big)^* &= E_m \big(\big(\Theta - M(\lambda)\big)^{-1} \gamma(\bar\lambda)^*\big)^* = E_m \gamma(\bar\lambda)\big(\Theta - M(\bar\lambda)\big)^{-1} \\ &= \sum_{k=1}^{m} (\lambda_k - \bar\lambda)^{-1} (\cdot, \Gamma_0 \psi_k)\psi_k. \end{aligned}$$

Here we have again used (2.8), $A_0 = A^* \restriction \ker(\Gamma_0)$ and $\Gamma_0 \gamma(\lambda) = I_{\mathcal{H}}$. Replacing λ by $\bar\lambda$ and applying Γ_0 we obtain from the above formula the representation

$$\Gamma_0 E_m \gamma(\lambda)\big(\Theta - M(\lambda)\big)^{-1} = \sum_{k=1}^{m} (\lambda_k - \lambda)^{-1} (\cdot, \Gamma_0 \psi_k)\Gamma_0 \psi_k$$

for all $\lambda \in \rho(A_0) \cap \rho(A_\Theta)$. By the above arguments the left-hand side converges in the strong sense to $(\Theta - M(\lambda))^{-1}$. Therefore we obtain (3.6). □

The special case $\Theta = 0 \in [\mathcal{H}]$ will be of particular interest in our further investigations. In this situation Proposition 3.3 reads as follows.

Corollary 3.4. *Let A be a densely defined closed symmetric operator in $\mathfrak{H}$ and let $\{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* with Weyl function $M(\cdot)$. Assume that $A_0 = A^* \restriction \ker(\Gamma_0)$ and $A_1 = A^* \restriction \ker(\Gamma_1)$ are semibounded from below, $A_1 \leqslant A_0$, and that $\sigma(A_1)$ is discrete. Then the $[\mathcal{H}]$-valued function $\lambda \mapsto M(\lambda)^{-1}$ admits the representation*

$$M(\lambda)^{-1} = \sum_{k=1}^{\infty} (\lambda - \lambda_k)^{-1} (\cdot, \Gamma_0 \psi_k)\Gamma_0 \psi_k, \quad \lambda \in \rho(A_0) \cap \rho(A_1), \tag{3.7}$$

where $\{\lambda_k\}$, $k = 1, 2, \ldots,$ are the eigenvalues of A_1 in increasing order (counting multiplicities), $\{\psi_k\}$ are the corresponding eigenfunctions, and the convergence in (3.7) is understood in the strong sense.

Proposition 3.3 and Corollary 3.4 might suggest that the Weyl function M can be represented as a convergent series involving the eigenvalues and eigenfunctions of the selfadjoint operator A_0. The following proposition shows that this is not possible if A_0 is chosen to be the Friedrichs extension.

Proposition 3.5. *Let A be a densely defined closed symmetric operator in $\mathfrak{H}$ with finite or infinite deficiency indices and let $\{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^*. Assume that the operator $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ and $A_1 = A^* \upharpoonright \ker(\Gamma_1)$ are semibounded, that A_0 coincides with the Friedrichs extension of A and that $\sigma(A_0)$ is discrete. Then the limit*

$$\lim_{m\to\infty} \sum_{k=1}^{m} (\lambda - \mu_k)^{-1} (\cdot, \Gamma_1\phi_k)\Gamma_1\phi_k, \quad \lambda \in \rho(A_0),$$

where $\{\mu_k\}$, $k = 1, 2, \ldots,$ are the eigenvalues of A_0 in increasing order (counting multiplicities) and $\{\phi_k\}$ are the corresponding eigenfunctions, does not exist.

Proof. We set

$$Q(\lambda) := \Gamma_1(A_0 - \lambda)^{-1}, \quad \lambda \in \rho(A_0), \tag{3.8}$$

and

$$G(\lambda) := \Gamma_1 Q(\bar{\lambda})^* = \Gamma_1\bigl(\Gamma_1(A_0 - \bar{\lambda})^{-1}\bigr)^*, \quad \lambda \in \rho(A_0).$$

Taking into account the relation

$$(A_1 - \lambda)^{-1} = (A_0 - \lambda)^{-1} - \gamma(\lambda)M(\lambda)^{-1}\gamma(\bar{\lambda})^*, \quad \lambda \in \rho(A_0) \cap \rho(A_1),$$

and (2.6) we find

$$Q(\lambda) = \gamma(\bar{\lambda})^* \quad \text{and} \quad G(\lambda) = M(\lambda), \quad \lambda \in \rho(A_0) \cap \rho(A_1).$$

Let $m \in \mathbb{N}$, let E_m be the projection onto the subspace spanned by the eigenfunctions $\{\phi_k\}$, $k = 1, \ldots, m$, and define

$$Q_m(\lambda) := Q(\lambda)E_m \quad \text{and} \quad G_m(\lambda) := \Gamma_1 E_m Q(\bar{\lambda})^*, \quad \lambda \in \rho(A_0).$$

With the help of

$$(A_0 - \bar{\lambda})^{-1} = \sum_{k=1}^{\infty} (\mu_k - \bar{\lambda})^{-1}(\cdot, \phi_k)\phi_k$$

and (3.8) we find the representation

$$G_m(\lambda) = \sum_{k=1}^{m} (\mu_k - \lambda)^{-1}\,(\cdot, \Gamma_1\phi_k)\,\Gamma_1\phi_k, \quad \lambda \in \rho(A_0) \cap \rho(A_1),$$

and, on the other hand,

$$G_m(\lambda) = Q_m(\lambda)(A_0 - \lambda)E_m Q(\bar{\lambda})^* = \gamma(\bar{\lambda})^*(A_0 - \lambda)E_m\gamma(\lambda)$$

for $\lambda \in \rho(A_0) \cap \rho(A_1)$.

Let $\lambda \in \mathbb{R}$, $\lambda < \min\{\sigma(A_0), \sigma(A_1)\}$, and assume that there is an element $\eta \in \mathcal{H}$ such that the limit

$$\lim_{m\to\infty} G_m(\lambda)\eta = \lim_{m\to\infty} \sum_{k=1}^{m} (\mu_k - \lambda)^{-1} (\eta, \Gamma_1\phi_k)\, \Gamma_1\phi_k \tag{3.9}$$

exists. Since for $h := \gamma(\lambda)\eta \in \mathcal{N}_\lambda = \ker(A^* - \lambda)$

$$\big(G_m(\lambda)\eta, \eta\big) = \big((A_0 - \lambda)E_m\gamma(\lambda)\eta, \gamma(\lambda)\eta\big) = \big\|\sqrt{A_0 - \lambda}E_m h\big\|^2$$

we obtain from (3.9) that the limit $\lim_{m\to\infty} \|\sqrt{A_0 - \lambda}E_m h\|$ exists and is finite. Therefore there is a subsequence $\{m_n\}$, $n \in \mathbb{N}$, such that

$$g := \operatorname*{w-lim}_{n\to\infty} \sqrt{A_0 - \lambda}E_{m_n} h \quad \text{and} \quad \lim_{n\to\infty} E_{m_n} h = h.$$

Hence we conclude $h \in \operatorname{dom}(\sqrt{A_0 - \lambda})$ and $g = \sqrt{A_0 - \lambda}\, h$. But according to [1, Lemma 2.1] we have $\operatorname{dom}(\sqrt{A_0 - \lambda}) \cap \mathcal{N}_\lambda = \{0\}$, so that $h = 0$ and therefore $\eta = 0$. □

4. Scattering theory and representation of *S* and *R*-matrices

Let A be a densely defined closed simple symmetric operator in the separable Hilbert space $\mathfrak{H}$ and assume that the deficiency indices of A coincide and are finite, $n_+(A) = n_-(A) < \infty$. Let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^*, $A_0 = A^* \upharpoonright \ker(\Gamma_0)$, and let A_Θ be a selfadjoint extension of A which corresponds to a selfadjoint relation $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$. Note that $\dim \mathcal{H} = n_\pm(A)$ is finite. Let $P_{\rm op}$ be the orthogonal projection in $\mathcal{H}$ onto the subspace $\mathcal{H}_{\rm op} := \operatorname{dom}(\Theta)$ and decompose Θ as in (2.2), $\Theta = \Theta_{\rm op} \oplus \Theta_\infty$ with respect to $\mathcal{H} = \mathcal{H}_{\rm op} \oplus \mathcal{H}_\infty$. The Weyl function $M(\cdot)$ corresponding to $\mathcal{H} = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ is a matrix-valued Nevanlinna function and the same holds for

$$N_\Theta(\lambda) := \big(\Theta - M(\lambda)\big)^{-1} = \big(\Theta_{\rm op} - M_{\rm op}(\lambda)\big)^{-1} P_{\rm op}, \quad \lambda \in \mathbb{C} \setminus \mathbb{R}, \tag{4.1}$$

where $M_{\rm op}(\lambda) = P_{\rm op} M(\lambda) P_{\rm op}$, cf. [24, p. 137]. We will in general not distinguish between the orthogonal projection onto $\mathcal{H}_{\rm op}$ and the canonical embedding of $\mathcal{H}_{\rm op}$ into $\mathcal{H}$. By Fatou's theorem (see [14,16]) the limits

$$M(\lambda + i0) := \lim_{\epsilon\to+0} M(\lambda + i\epsilon)$$

and

$$N_\Theta(\lambda + i0) := \lim_{\epsilon\to+0} \big(\Theta - M(\lambda + i\epsilon)\big)^{-1}$$

from the upper half-plane exist for a.e. $\lambda \in \mathbb{R}$. We denote the set of real points where the limits exist by Σ^M and Σ^{N_Θ}, respectively, and we agree to use a similar notation for arbitrary scalar and matrix-valued Nevanlinna functions. It is not difficult to see that

$$N_\Theta(\lambda + i0) = \big(\Theta - M(\lambda + i0)\big)^{-1} = \big(\Theta_{\rm op} - M_{\rm op}(\lambda + i0)\big)^{-1} P_{\rm op}$$

holds for all $\lambda \in \Sigma^M \cap \Sigma^{N_\Theta}$ and that $\mathbb{R} \setminus (\Sigma^M \cap \Sigma^{N_\Theta})$ has Lebesgue measure zero, cf. [3, §2.3].

Since $\dim\mathcal{H}$ is finite by (2.8)

$$\dim\bigl(\operatorname{ran}\bigl((A_\Theta-\lambda)^{-1}-(A_0-\lambda)^{-1}\bigr)\bigr)<\infty,\quad \lambda\in\rho(A_\Theta)\cap\rho(A_0),$$

and therefore the pair $\{A_\Theta, A_0\}$ performs a so-called *complete scattering system*, that is, the *wave operators*

$$W_\pm(A_\Theta,A_0):=\operatorname*{s-lim}_{t\to\pm\infty} e^{itA_\Theta}e^{-itA_0}P^{ac}(A_0)$$

exist and their ranges coincide with the absolutely continuous subspace $\mathfrak{H}^{ac}(A_\Theta)$ of A_Θ, cf. [2, 21,38,45]. $P^{ac}(A_0)$ denotes the orthogonal projection onto the absolutely continuous subspace $\mathfrak{H}^{ac}(A_0)$ of A_0. The *scattering operator* S_Θ of the *scattering system* $\{A_\Theta, A_0\}$ is then defined by

$$S_\Theta:=W_+(A_\Theta,A_0)^*W_-(A_\Theta,A_0).$$

If we regard the scattering operator as an operator in $\mathfrak{H}^{ac}(A_0)$, then S_Θ is unitary, commutes with the absolutely continuous part

$$A_0^{ac}:=A_0\upharpoonright \operatorname{dom}(A_0)\cap\mathfrak{H}^{ac}(A_0)$$

of A_0 and it follows that S_Θ is unitarily equivalent to a multiplication operator induced by a family $\{S_\Theta(\lambda)\}$ of unitary operators in a spectral representation of A_0^{ac}, see e.g. [2, Proposition 9.57]. This family or multiplication operator is called the *scattering matrix* of the scattering system $\{A_\Theta, A_0\}$.

In [4] a representation theorem for the scattering matrix $\{S_\Theta(\lambda)\}$ in terms of the Weyl function $M(\cdot)$ was proved, which is of similar type as Theorem 4.1 below. We will make use of the notation

$$\mathcal{H}_{M(\lambda)}:=\operatorname{ran}\bigl(\Im\mathrm{m}\bigl(M(\lambda)\bigr)\bigr),\quad \lambda\in\Sigma^M, \tag{4.2}$$

and we will usually regard $\mathcal{H}_{M(\lambda)}$ as a subspace of $\mathcal{H}$. The orthogonal projection onto $\mathcal{H}_{M(\lambda)}$ will be denoted by $P_{M(\lambda)}$. Note that for $\lambda\in\rho(A_0)\cap\mathbb{R}$ the Hilbert space $\mathcal{H}_{M(\lambda)}$ is trivial by (2.7). The family $\{P_{M(\lambda)}\}_{\lambda\in\Sigma^M}$ of orthogonal projections in $\mathcal{H}$ onto $\mathcal{H}_{M(\lambda)}$, $\lambda\in\Sigma^M$, is measurable and defines an orthogonal projection in the Hilbert space $L^2(\mathbb{R}, d\lambda, \mathcal{H})$. The range of this projection is denoted by $L^2(\mathbb{R}, d\lambda, \mathcal{H}_{M(\lambda)})$. Let P_{op} and $M_{\mathrm{op}}(\lambda)=P_{\mathrm{op}}M(\lambda)P_{\mathrm{op}}$, $\lambda\in\Sigma^M$, be as above. For each $\lambda\in\Sigma^M$ the space $\mathcal{H}_{M(\lambda)}$ will also be written as the orthogonal sum of

$$\mathcal{H}_{M_{\mathrm{op}}(\lambda)}=\operatorname{ran}\bigl(\Im\mathrm{m}\bigl(M_{\mathrm{op}}(\lambda)\bigr)\bigr)$$

and

$$\mathcal{H}^\perp_{M_{\mathrm{op}}(\lambda)}:=\mathcal{H}_{M(\lambda)}\ominus\mathcal{H}_{M_{\mathrm{op}}(\lambda)}=\ker\bigl(\Im\mathrm{m}\bigl(M_{\mathrm{op}}(\lambda)\bigr)\bigr).$$

The following theorem is a variant of [4, Theorem 3.8]. The essential advantage here is, that the particular form of the scattering matrix $\{S_\Theta(\lambda)\}$ immediately shows that the multivalued part of the selfadjoint parameter Θ has no influence on the scattering matrix.

Theorem 4.1. *Let A be a densely defined closed simple symmetric operator with equal finite deficiency indices in the separable Hilbert space $\mathfrak{H}$ and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* with corresponding Weyl function $M(\cdot)$. Furthermore, let $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ and let A_Θ be a selfadjoint extension of A which corresponds to the selfadjoint relation $\Theta = \Theta_{\mathrm{op}} \oplus \Theta_\infty \in \widetilde{\mathcal{C}}(\mathcal{H})$ via* (2.4)*. Then the following holds*:

(i) *The absolutely continuous part A_0^{ac} of A_0 is unitarily equivalent to the multiplication operator with the free variable in $L^2(\mathbb{R}, d\lambda, \mathcal{H}_{M(\lambda)})$.*
(ii) *With respect to the decomposition $\mathcal{H}_{M(\lambda)} = \mathcal{H}_{M_{\mathrm{op}}(\lambda)} \oplus \mathcal{H}^\perp_{M_{\mathrm{op}}(\lambda)}$ the scattering matrix $\{S_\Theta(\lambda)\}$ of the complete scattering system $\{A_\Theta, A_0\}$ in $L^2(\mathbb{R}, d\lambda, \mathcal{H}_{M(\lambda)})$ is given by*

$$S_\Theta(\lambda) = \begin{pmatrix} S_{\Theta_{\mathrm{op}}}(\lambda) & 0 \\ 0 & I_{\mathcal{H}^\perp_{M_{\mathrm{op}}(\lambda)}} \end{pmatrix} \in \big[\mathcal{H}_{M_{\mathrm{op}}(\lambda)} \oplus \mathcal{H}^\perp_{M_{\mathrm{op}}(\lambda)}\big],$$

where

$$S_{\Theta_{\mathrm{op}}}(\lambda) = I_{\mathcal{H}_{M_{\mathrm{op}}(\lambda)}} + 2i\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)}\big(\Theta_{\mathrm{op}} - M_{\mathrm{op}}(\lambda)\big)^{-1}\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)}$$

and $\lambda \in \Sigma^M \cap \Sigma^{N_\Theta}$, $M_{\mathrm{op}}(\lambda) := M_{\mathrm{op}}(\lambda + i0)$.

Proof. Assertion (i) was proved in [4, Theorem 3.8] and moreover it was shown that the scattering matrix $\{\widetilde{S}_\Theta(\lambda)\}$ of the complete scattering system $\{A_\Theta, A_0\}$ in $L^2(\mathbb{R}, d\lambda, \mathcal{H}_{M(\lambda)})$ has the form

$$\widetilde{S}_\Theta(\lambda) = I_{\mathcal{H}_{M(\lambda)}} + 2i\sqrt{\Im\mathrm{m}\big(M(\lambda)\big)}\big(\Theta - M(\lambda)\big)^{-1}\sqrt{\Im\mathrm{m}\big(M(\lambda)\big)} \in [\mathcal{H}_{M(\lambda)}]$$

for all $\lambda \in \Sigma^M \cap \Sigma^{N_\Theta}$. With the help of (4.1) this becomes

$$\widetilde{S}_\Theta(\lambda) = I_{\mathcal{H}_{M(\lambda)}} + 2i\sqrt{\Im\mathrm{m}\big(M(\lambda)\big)}P_{\mathrm{op}}\big(\Theta_{\mathrm{op}} - M_{\mathrm{op}}(\lambda)\big)^{-1}P_{\mathrm{op}}\sqrt{\Im\mathrm{m}\big(M(\lambda)\big)}.$$

From the polar decomposition of $\sqrt{\Im\mathrm{m}(M(\lambda))}P_{\mathrm{op}}$, $\lambda \in \Sigma^M$, we obtain a family of isometric mappings $V(\lambda)$, $\lambda \in \Sigma^M$, from $\mathcal{H}_{M_{\mathrm{op}}(\lambda)}$ onto $\mathrm{ran}(\sqrt{\Im\mathrm{m}(M(\lambda))}P_{\mathrm{op}})$ defined by

$$V(\lambda)\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)}x := \sqrt{\Im\mathrm{m}\big(M(\lambda)\big)}P_{\mathrm{op}}x$$

and we extend $V(\lambda)$ to a family $\widetilde{V}(\lambda)$ of unitary mappings in $\mathcal{H}_{M(\lambda)}$. Note that $\widetilde{V}(\lambda)$ maps $\ker(\sqrt{\Im\mathrm{m}(M_{\mathrm{op}}(\lambda))})$ isometrically onto $\ker(P_{\mathrm{op}}\sqrt{\Im\mathrm{m}(M(\lambda))})$. It is not difficult to see that the scattering matrix

$$S_\Theta(\lambda) := \widetilde{V}(\lambda)^*\widetilde{S}_\Theta(\lambda)\widetilde{V}(\lambda), \quad \lambda \in \Sigma^M \cap \Sigma^{N_\Theta},$$

with respect to the decomposition $\mathcal{H}_{M(\lambda)} = \mathcal{H}_{M_{\mathrm{op}}(\lambda)} \oplus \mathcal{H}^\perp_{M_{\mathrm{op}}(\lambda)}$ is of the form as in assertion (ii). $\square$

We point out that the scattering matrix $\{S_\Theta(\lambda)\}$ of the complete scattering system $\{A_\Theta, A_0\}$ is defined for a.e. $\lambda \in \mathbb{R}$ and that in Theorem 4.1(ii) a special representative of the corresponding equivalence class was chosen. We also note that the operator $\sqrt{\Im\mathrm{m}(M_{\mathrm{op}}(\lambda))}$ is regarded as an operator in $\mathcal{H}_{M_{\mathrm{op}}(\lambda)}$.

Next we introduce the *R-matrix* $\{R_\Theta(\lambda)\}$ of the scattering system $\{A_\Theta, A_0\}$ in accordance with Blatt and Weisskopf [5],

$$R_\Theta(\lambda) := i\big(I_{\mathcal{H}_{M(\lambda)}} - S_\Theta(\lambda)\big)\big(I_{\mathcal{H}_{M(\lambda)}} + S_\Theta(\lambda)\big)^{-1} \tag{4.3}$$

for all $\lambda \in \Sigma^M \cap \Sigma^{N_\Theta}$ satisfying $-1 \in \rho(S_\Theta(\lambda))$. Since $S_\Theta(\lambda)$ is unitary it follows that $R_\Theta(\lambda)$ is a selfadjoint matrix. Note also that

$$S_\Theta(\lambda) = \big(iI_{\mathcal{H}_{M(\lambda)}} - R_\Theta(\lambda)\big)\big(iI_{\mathcal{H}_{M(\lambda)}} + R_\Theta(\lambda)\big)^{-1} \tag{4.4}$$

holds for all real λ where $R_\Theta(\lambda)$ is defined.

The next theorem is of similar flavor as Theorem 4.1. We express the R-matrix of the scattering system $\{A_\Theta, A_0\}$ in terms of the Weyl function $M(\cdot)$ and the selfadjoint parameter $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$. Again we make use of the special space decomposition which shows that the "pure" relation part Θ_∞ has no influence on the R-matrix.

Theorem 4.2. *Let A be a densely defined closed simple symmetric operator with equal finite deficiency indices in the separable Hilbert space $\mathfrak{H}$ and let $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* with corresponding Weyl function $M(\cdot)$. Furthermore, let $A_0 = A^* \restriction \ker(\Gamma_0)$ and let A_Θ be a selfadjoint extension of A which corresponds to the selfadjoint relation $\Theta = \Theta_{\mathrm{op}} \oplus \Theta_\infty \in \widetilde{\mathcal{C}}(\mathcal{H})$. Then for all $\lambda \in \Sigma^M \cap \Sigma^{N_\Theta}$ with*

$$\ker\big(\Theta_{\mathrm{op}} - \Re\mathrm{e}\big(M_{\mathrm{op}}(\lambda)\big)\big) = \{0\}$$

the R-matrix of $\{A_\Theta, A_0\}$ is given by

$$R_\Theta(\lambda) = \begin{pmatrix} \sqrt{\Im\mathrm{m}(M_{\mathrm{op}}(\lambda))}(\Theta_{\mathrm{op}} - \Re\mathrm{e}(M_{\mathrm{op}}(\lambda)))^{-1}\sqrt{\Im\mathrm{m}(M_{\mathrm{op}}(\lambda))} & 0 \\ 0 & 0 \end{pmatrix},$$

with respect to $\mathcal{H}_{M(\lambda)} = \mathcal{H}_{M_{\mathrm{op}}(\lambda)} \oplus \mathcal{H}^\perp_{M_{\mathrm{op}}(\lambda)}$, where $M_{\mathrm{op}}(\lambda) = M_{\mathrm{op}}(\lambda + i0)$.

Proof. It follows immediately from the definition (4.3) and the representation of the scattering matrix in Theorem 4.1(ii), that the R-matrix of $\{A_\Theta, A_0\}$ is a diagonal block matrix with respect to the space decomposition $\mathcal{H}_{M(\lambda)} = \mathcal{H}_{M_{\mathrm{op}}(\lambda)} \oplus \mathcal{H}^\perp_{M_{\mathrm{op}}(\lambda)}$ and that the restriction of $R_\Theta(\lambda)$ to $\mathcal{H}^\perp_{M_{\mathrm{op}}(\lambda)}$ is identically equal to zero.

Moreover, for every $\lambda \in \Sigma^M \cap \Sigma^{N_\Theta}$ it follows from the representation of the scattering matrix that

$$\begin{aligned}
&\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)}\big(I_{\mathcal{H}_{M_{\mathrm{op}}(\lambda)}} + S_{\Theta_{\mathrm{op}}}(\lambda)\big) \\
&\quad = 2\big\{I_{\mathcal{H}_{M_{\mathrm{op}}(\lambda)}} + i\,\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)\big(\Theta_{\mathrm{op}} - M_{\mathrm{op}}(\lambda)\big)^{-1}\big\}\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)} \\
&\quad = 2\big(\Theta_{\mathrm{op}} - \Re\mathrm{e}\big(M_{\mathrm{op}}(\lambda)\big)\big)\big(\Theta_{\mathrm{op}} - M_{\mathrm{op}}(\lambda)\big)^{-1}\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)}
\end{aligned}$$

holds. If $\lambda \in \Sigma^M \cap \Sigma^{N_\Theta}$ is such that $\Theta_{\mathrm{op}} - \Re\mathrm{e}(M_{\mathrm{op}}(\lambda))$ is invertible, then we obtain

$$\begin{aligned}
&\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)}\big(I_{\mathcal{H}_{M_{\mathrm{op}}(\lambda)}} + S_{\Theta_{\mathrm{op}}}(\lambda)\big)^{-1} \\
&\quad = \frac{1}{2}\big(\Theta_{\mathrm{op}} - M_{\mathrm{op}}(\lambda)\big)\big(\Theta_{\mathrm{op}} - \Re\mathrm{e}\big(M_{\mathrm{op}}(\lambda)\big)\big)^{-1}\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)},
\end{aligned}$$

so that

$$\begin{aligned}
&2i\big(\Theta_{\mathrm{op}} - M_{\mathrm{op}}(\lambda)\big)^{-1}\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)}\big(I_{\mathcal{H}_{M_{\mathrm{op}}(\lambda)}} + S_{\Theta_{\mathrm{op}}}(\lambda)\big)^{-1} \\
&\quad = i\big(\Theta_{\mathrm{op}} - \Re\mathrm{e}\big(M_{\mathrm{op}}(\lambda)\big)\big)^{-1}\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)}.
\end{aligned}$$

Finally multiplication by $-\sqrt{\Im\mathrm{m}(M_{\mathrm{op}}(\lambda))}$ from the left gives

$$\begin{aligned}
&\big(I_{\mathcal{H}_{M_{\mathrm{op}}(\lambda)}} - S_{\Theta_{\mathrm{op}}}(\lambda)\big)\big(I_{\mathcal{H}_{M_{\mathrm{op}}(\lambda)}} + S_{\Theta_{\mathrm{op}}}(\lambda)\big)^{-1} \\
&\quad = -i\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)}\big(\Theta_{\mathrm{op}} - \Re\mathrm{e}\big(M_{\mathrm{op}}(\lambda)\big)\big)^{-1}\sqrt{\Im\mathrm{m}\big(M_{\mathrm{op}}(\lambda)\big)}
\end{aligned}$$

so that assertion (i) follows immediately from the definition of the R-matrix in (4.3). □

5. Scattering in coupled systems

Let $\mathfrak{H}$ and $\mathfrak{K}$ be separable Hilbert spaces and let A and T be densely defined closed simple symmetric operators in $\mathfrak{H}$ and $\mathfrak{K}$, respectively. We assume that the deficiency indices of A and T coincide and are finite,

$$n := n_+(A) = n_-(A) = n_+(T) = n_-(T) < \infty.$$

Then there exist boundary triplets $\Pi_A = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ and $\Pi_T = \{\mathcal{H}, \Upsilon_0, \Upsilon_1\}$ for the adjoint operators A^* and T^*, respectively, with fixed selfadjoint extensions

$$A_0 := A^* \restriction \ker(\Gamma_0) \quad \text{and} \quad T_0 := T^* \restriction \ker(\Upsilon_0) \tag{5.1}$$

in $\mathfrak{H}$ and $\mathfrak{K}$, respectively, and $\dim \mathcal{H} = n$. The Weyl functions of $\Pi_A = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ and $\Pi_T = \{\mathcal{H}, \Upsilon_0, \Upsilon_1\}$ will be denoted by $M(\cdot)$ and $\tau(\cdot)$, respectively. Besides the spaces $\mathcal{H}_{M(\lambda)}$, $\lambda \in \Sigma^M$ (see (4.2)), we will make use of the finite dimensional spaces

$$\mathcal{H}_{\tau(\lambda)} = \mathrm{ran}\big(\Im\mathrm{m}\big(\tau(\lambda + i0)\big)\big), \quad \lambda \in \Sigma^\tau,$$

and

$$\mathcal{H}_{(M+\tau)(\lambda)} = \mathrm{ran}\big(\Im\mathrm{m}\big((M+\tau)(\lambda + i0)\big)\big), \quad \lambda \in \Sigma^{M+\tau} \supset \big(\Sigma^M \cap \Sigma^\tau\big).$$

In the following theorem we calculate the S and R-matrix of a special scattering system $\{\widetilde{L}, L_0\}$ in $\mathfrak{H} \oplus \mathfrak{K}$ in terms of the Weyl functions M and τ. Theorem 5.1 is in principle a consequence of Theorems 4.1 and 4.2, cf. [3, Theorem 4.5]. We note that the coupling procedure in the first part of the theorem is similar to the one in [9].

Theorem 5.1. *Let A, $\Pi_A = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$, $M(\cdot)$ and T, $\Pi_T = \{\mathcal{H}, \Upsilon_0, \Upsilon_1\}$, $\tau(\cdot)$ be as above. Then the following holds*:

(i) *The pair $\{\widetilde{L}, L_0\}$, where $L_0 := A_0 \oplus T_0$ and*

$$\widetilde{L} = A^* \oplus T^* \upharpoonright \left\{ f \oplus g \in \mathrm{dom}(A^* \oplus T^*)\colon \begin{array}{l} \Gamma_0 f - \Upsilon_0 g = 0 \\ \Gamma_1 f + \Upsilon_1 g = 0 \end{array} \right\}, \tag{5.2}$$

forms a complete scattering system in the Hilbert space $\mathfrak{H} \oplus \mathfrak{K}$ and L_0^{ac} is unitarily equivalent to the multiplication operator with the free variable in $L^2(\mathbb{R}, d\lambda, \mathcal{H}_{M(\lambda)} \oplus \mathcal{H}_{\tau(\lambda)})$.

(ii) *With respect to the decomposition*

$$\mathcal{H}_{(M+\tau)(\lambda)} \oplus \mathcal{H}_{(M+\tau)(\lambda)}^{\perp} \tag{5.3}$$

of $\mathcal{H}_{M(\lambda)} \oplus \mathcal{H}_{\tau(\lambda)}$ the scattering matrix $\{\widetilde{S}(\lambda)\}$ of $\{\widetilde{L}, L_0\}$ is given by

$$\widetilde{S}(\lambda) = \begin{pmatrix} S(\lambda) & 0 \\ 0 & I_{\mathcal{H}_{(M+\tau)(\lambda)}^{\perp}} \end{pmatrix} \in \left[\mathcal{H}_{(M+\tau)(\lambda)} \oplus \mathcal{H}_{(M+\tau)(\lambda)}^{\perp}\right],$$

where

$$S(\lambda) = I_{\mathcal{H}_{(M+\tau)(\lambda)}} - 2i\sqrt{\Im\mathrm{m}\big(M(\lambda) + \tau(\lambda)\big)}\big(M(\lambda) + \tau(\lambda)\big)^{-1}\sqrt{\Im\mathrm{m}\big(M(\lambda) + \tau(\lambda)\big)}$$

and $\lambda \in \Sigma^M \cap \Sigma^\tau \cap \Sigma^{(M+\tau)^{-1}}$, $M(\lambda) := M(\lambda + i0)$, $\tau(\lambda) = \tau(\lambda + i0)$.

(iii) *For all $\lambda \in \Sigma^M \cap \Sigma^\tau \cap \Sigma^{(M+\tau)^{-1}}$ with $\ker(\Re\mathrm{e}(M(\lambda) + \tau(\lambda))) = \{0\}$ the R-matrix of $\{\widetilde{L}, L_0\}$ is given by*

$$R(\lambda) = \begin{pmatrix} -\sqrt{\Im\mathrm{m}(M(\lambda) + \tau(\lambda))}(\Re\mathrm{e}(M(\lambda) + \tau(\lambda)))^{-1}\sqrt{\Im\mathrm{m}(M(\lambda) + \tau(\lambda))} & 0 \\ 0 & 0 \end{pmatrix},$$

with respect to the decomposition (5.3).

Proof. (i) Let $L := A \oplus T$, so that L is a densely defined closed simple symmetric operator in the Hilbert space $\mathfrak{H} \oplus \mathfrak{K}$. Clearly, L has deficiency indices $n_\pm(L) = 2n$, and it is easy to see that $\Pi_L = \{\widetilde{\mathcal{H}}, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$, where

$$\widetilde{\Gamma}_0(f \oplus g) := \begin{pmatrix} \Gamma_0 f \\ \Upsilon_0 g \end{pmatrix}, \quad \widetilde{\Gamma}_1(f \oplus g) := \begin{pmatrix} \Gamma_1 f \\ \Upsilon_1 g \end{pmatrix} \quad \text{and} \quad \widetilde{\mathcal{H}} := \mathcal{H} \oplus \mathcal{H},$$

$f \in \mathrm{dom}(A^*)$, $g \in \mathrm{dom}(T^*)$, is a boundary triplet for the adjoint operator $L^* = A^* \oplus T^*$ in $\mathfrak{H} \oplus \mathfrak{K}$. Together with the selfadjoint operators A_0 and T_0 from (5.1) we obviously have

$$L_0 := L^* \upharpoonright \ker(\widetilde{\Gamma}_0) = A_0 \oplus T_0.$$

It is not difficult to verify that

$$\widetilde{\Theta} := \left\{ \begin{pmatrix} (x, x)^\top \\ (y, -y)^\top \end{pmatrix}\colon x, y \in \mathcal{H} \right\} \in \widetilde{\mathcal{C}}(\mathcal{H} \oplus \mathcal{H}) \tag{5.4}$$

is a selfadjoint relation in $\widetilde{\mathcal{H}}$ and that the corresponding selfadjoint extension $L^* \upharpoonright \widetilde{\Gamma}^{(-1)}\widetilde{\Theta}$ in $\mathfrak{H} \oplus \mathfrak{K}$ via (2.4) coincides with the operator $\widetilde{L}$ in (5.2), cf. [3]. Since L has finite deficiency indices, $\widetilde{L}$ is finite rank perturbation of L_0 in resolvent sense (cf. Theorem 2.4 and Section 4), and hence $\{\widetilde{L}, L_0\}$ is a complete scattering system in $\mathfrak{H} \oplus \mathfrak{K}$. Moreover, as the Weyl function $\widetilde{M}(\cdot)$ of $\{\widetilde{\mathcal{H}}, \widetilde{\Gamma}_0, \widetilde{\Gamma}_1\}$ is given by

$$\widetilde{M}(\lambda) = \begin{pmatrix} M(\lambda) & 0 \\ 0 & \tau(\lambda) \end{pmatrix}, \quad \lambda \in \rho(L_0), \tag{5.5}$$

it follows from Theorem 4.1(i) that the absolutely continuous part L_0^{ac} of L_0 is unitarily equivalent to the multiplication operator with the free variable in the Hilbert space $L^2(\mathbb{R}, d\lambda, \mathcal{H}_{\widetilde{M}(\lambda)}) = L^2(\mathbb{R}, d\lambda, \mathcal{H}_{M(\lambda)} \oplus \mathcal{H}_{\tau(\lambda)})$.

(ii)–(iii) Note that the operator part $\widetilde{\Theta}_{\mathrm{op}}$ of the selfadjoint relation $\widetilde{\Theta}$ in (5.4) is defined on

$$\widetilde{\mathcal{H}}_{\mathrm{op}} := \operatorname{dom}(\widetilde{\Theta}) = \{(x, x)^\top : x \in \mathcal{H}\}$$

and that $\widetilde{\Theta}_{\mathrm{op}} = 0 \in [\widetilde{\mathcal{H}}_{\mathrm{op}}]$, cf. (2.2). Next we will calculate the $[\widetilde{\mathcal{H}}_{\mathrm{op}}]$-valued function $\widetilde{M}_{\mathrm{op}}(\cdot)$, and in order to avoid possible confusion we will distinguish between embeddings and projections here. The canonical embedding of $\widetilde{\mathcal{H}}_{\mathrm{op}}$ into $\mathcal{H} \oplus \mathcal{H}$ is given by

$$\tilde{\iota}_{\mathrm{op}} : \widetilde{\mathcal{H}}_{\mathrm{op}} \to \mathcal{H} \oplus \mathcal{H}, \qquad y \mapsto \frac{1}{\sqrt{2}} \begin{pmatrix} y \\ y \end{pmatrix},$$

and the adjoint $\tilde{\iota}_{\mathrm{op}}^* \in [\mathcal{H} \oplus \mathcal{H}, \widetilde{\mathcal{H}}_{\mathrm{op}}]$ is the orthogonal projection $\widetilde{P}_{\mathrm{op}}$ from $\mathcal{H} \oplus \mathcal{H}$ onto $\widetilde{\mathcal{H}}_{\mathrm{op}}$, $\widetilde{P}_{\mathrm{op}}(u \oplus v) = \frac{1}{\sqrt{2}}(u + v)$. Then we obtain

$$\widetilde{M}_{\mathrm{op}}(\lambda) = \widetilde{P}_{\mathrm{op}} \widetilde{M}(\lambda) \tilde{\iota}_{\mathrm{op}} = \frac{1}{2}\big(M(\lambda) + \tau(\lambda)\big), \quad \lambda \in \rho(L_0),$$

from (5.5). Now the assertions (ii) and (iii) follow easily from Theorems 4.1(ii) and 4.2, respectively. □

The case that the operator A_0 has discrete spectrum is of particular importance in several applications. In this situation Theorem 5.1 reduces to the following corollary.

Corollary 5.2. *Let the assumptions and* $\{\widetilde{L}, L_0\}$ *be as in Theorem* 5.1 *and assume, in addition, that* $\sigma(A_0)$ *is discrete. Then the following holds*:

(i) L_0^{ac} *is unitarily equivalent to the multiplication operator with the free variable in* $L^2(\mathbb{R}, d\lambda, \mathcal{H}_{\tau(\lambda)})$.

(ii) *The scattering matrix* $\{S(\lambda)\}$ *of* $\{\widetilde{L}, L_0\}$ *in* $L^2(\mathbb{R}, d\lambda, \mathcal{H}_{\tau(\lambda)})$ *is given by*

$$S(\lambda) = I_{\mathcal{H}_{\tau(\lambda)}} - 2i\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\big(M(\lambda) + \tau(\lambda)\big)^{-1}\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}$$

for $\lambda \in \Sigma^M \cap \Sigma^\tau \cap \Sigma^{(M+\tau)^{-1}}$, *where* $M(\lambda) := M(\lambda + i0)$, $\tau(\lambda) = \tau(\lambda + i0)$.

(iii) *For all* $\lambda \in \Sigma^M \cap \Sigma^\tau \cap \Sigma^{(M+\tau)^{-1}}$ *with* $\ker(M(\lambda) + \Re\mathrm{e}(\tau(\lambda))) = \{0\}$ *the* R*-matrix of* $\{\widetilde{L}, L_0\}$ *is given by*

$$R(\lambda) = -\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\big(M(\lambda) + \Re\mathrm{e}\big(\tau(\lambda)\big)\big)^{-1}\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}.$$

Proof. The assumption $\sigma(A_0) = \sigma_p(A_0)$ implies $\Im\mathrm{m}(M(\lambda)) = \{0\}$ for all $\lambda \in \Sigma^M$. Therefore

$$\mathcal{H}_{(M+\tau)(\lambda)} = \mathcal{H}_{\tau(\lambda)} \quad \text{and} \quad \mathcal{H}_{M(\lambda)} = \{0\}, \quad \lambda \in \Sigma^M,$$

and the statements follow immediately from Theorem 5.1. □

From relation (4.4) we obtain the next corollary. We note that this statement can be formulated also for the case when $\sigma(A_0)$ is not discrete. However in our applications we will only make use of the more special variant below.

Corollary 5.3. *Let the assumptions be as in Corollary* 5.2. *Then for all* $\lambda \in \Sigma^M \cap \Sigma^\tau \cap \Sigma^{(M+\tau)^{-1}}$ *with* $\ker(M(\lambda) + \Re\mathrm{e}(\tau(\lambda))) = \{0\}$ *the scattering matrix* $\{S(\lambda)\}$ *of* $\{\widetilde{L}, L_0\}$ *admits the representation*

$$\begin{aligned} S(\lambda) = {} & \Big(i I_{\mathcal{H}_{\tau(\lambda)}} + \sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\big(M(\lambda) + \Re\mathrm{e}\big(\tau(\lambda)\big)\big)^{-1}\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\Big) \\ & \times \Big(i I_{\mathcal{H}_{\tau(\lambda)}} - \sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\big(M(\lambda) + \Re\mathrm{e}\big(\tau(\lambda)\big)\big)^{-1}\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\Big)^{-1} \end{aligned}$$

and, if, in particular, $\Re\mathrm{e}(\tau(\lambda)) = 0$, *then*

$$\begin{aligned} S(\lambda) = {} & \Big(i I_{\mathcal{H}_{\tau(\lambda)}} + \sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}M(\lambda)^{-1}\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\Big) \\ & \times \Big(i I_{\mathcal{H}_{\tau(\lambda)}} - \sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}M(\lambda)^{-1}\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\Big)^{-1}. \end{aligned}$$

Our next objective is to express the scattering matrix of the scattering system $\{\widetilde{L}, L_0\}$ in terms of the eigenfunctions of a family of selfadjoint extensions of A. For this let again $\tau(\cdot)$ be the Weyl function of $\Pi_T = \{\mathcal{H}, \Upsilon_0, \Upsilon_1\}$, let $\mu \in \Sigma^\tau$, and let $\Pi_A = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$ be a boundary triplet for A^* as in the beginning of this section. Then $\Re\mathrm{e}(\tau(\mu))$ is a selfadjoint matrix in $\mathcal{H}$ and therefore the operator

$$A_{-\Re\mathrm{e}(\tau(\mu))} = A^* \upharpoonright \ker\big(\Gamma_1 + \Re\mathrm{e}\big(\tau(\mu)\big)\Gamma_0\big) \tag{5.6}$$

is a selfadjoint extension of A in $\mathfrak{H}$, cf. Proposition 2.2. Note that by Theorem 2.4 a point $\lambda \in \rho(A_0)$ belongs to $\rho(A_{-\Re\mathrm{e}(\tau(\mu))})$ if and only if $0 \in \rho(M(\lambda) + \Re\mathrm{e}\,\tau(\mu))$ holds. The following corollary is a reformulation of Proposition 3.3 in our particular situation.

Corollary 5.4. *Let A, $\Pi_A = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$, $M(\cdot)$ and T, $\Pi_T = \{\mathcal{H}, \Upsilon_0, \Upsilon_1\}$, $\tau(\cdot)$ be as above and assume $\sigma(A_0)$ is discrete and that A is semibounded from below. For each $\mu \in \Sigma^\tau$ with $A_{-\Re\mathrm{e}(\tau(\mu))} \leqslant A_0$ the function $\lambda \mapsto -(\Re\mathrm{e}(\tau(\mu)) + M(\lambda))^{-1}$ admits the representation*

$$-\big(M(\lambda) + \Re\mathrm{e}\big(\tau(\mu)\big)\big)^{-1} = \sum_{k=1}^{\infty} \big(\lambda_k[\mu] - \lambda\big)^{-1} \big(\cdot, \Gamma_0 \psi_k[\mu]\big) \Gamma_0 \psi_k[\mu],$$

where $\{\lambda_k[\mu]\}$, $k = 1, 2, \ldots,$ are the eigenvalues of the selfadjoint extension $A_{-\Re\mathrm{e}(\tau(\mu))}$ in increasing order (counting multiplicities) and $\psi_k[\mu]$ are the corresponding eigenfunctions.

Setting $\mu = \lambda$ in Corollary 5.4 and taking into account Corollaries 5.2 and 5.3 we obtain the following representations of the R-matrix and scattering matrix of $\{\widetilde{L}, L_0\}$.

Theorem 5.5. *Let the assumptions be as in Corollary* 5.4. *Then for all $\lambda \in \Sigma^M \cap \Sigma^\tau \cap \Sigma^{(M+\tau)^{-1}}$ with* $\ker(M(\lambda) + \Re\mathrm{e}(\tau(\lambda))) = \{0\}$ *and $A_{-\Re\mathrm{e}(\tau(\lambda))} \leqslant A_0$ the R-matrix and the scattering matrix of $\{\widetilde{L}, L_0\}$ admit the representations*

$$R(\lambda) = \sum_{k=1}^{\infty} \big(\lambda_k[\lambda] - \lambda\big)^{-1} \Big(\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\, \cdot, \Gamma_0 \psi_k[\lambda]\Big) \sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\, \Gamma_0 \psi_k[\lambda]$$

and

$$\begin{aligned} S(\lambda) = {} & \left(i I_{\mathcal{H}_{\tau(\lambda)}} - \sum_{k=1}^{\infty} \big(\lambda_k[\lambda] - \lambda\big)^{-1} \Big(\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\, \cdot, \Gamma_0 \psi_k[\lambda]\Big) \sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\, \Gamma_0 \psi_k[\lambda] \right) \\ & \times \left(i I_{\mathcal{H}_{\tau(\lambda)}} + \sum_{k=1}^{\infty} \big(\lambda_k[\lambda] - \lambda\big)^{-1} \Big(\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\, \cdot, \Gamma_0 \psi_k[\lambda]\Big) \sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\, \Gamma_0 \psi_k[\lambda] \right)^{-1}, \end{aligned}$$

respectively, where $\{\lambda_k[\lambda]\}$, $k = 1, 2, \ldots,$ are the eigenvalues of the selfadjoint extension $A_{-\Re\mathrm{e}(\tau(\lambda))}$ in increasing order and $\psi_k[\lambda]$ are the corresponding eigenfunctions.

If $\Re\mathrm{e}(\tau(\lambda)) = 0$ for some $\lambda \in \Sigma^\tau$, then the operator $A_{-\Re\mathrm{e}(\tau(\lambda))}$ in (5.6) coincides with the selfadjoint operator $A_1 = A^* \upharpoonright \ker(\Gamma_1)$. This yields the next corollary.

Corollary 5.6. *Let the assumptions be as in Corollary* 5.4. *Then for all $\lambda \in \Sigma^M \cap \Sigma^\tau \cap \Sigma^{(M+\tau)^{-1}}$ with $\Re\mathrm{e}(\tau(\lambda)) = 0$,* $\ker(M(\lambda)) = \{0\}$ *and $A_1 \leqslant A_0$ the R-matrix and the scattering matrix of $\{\widetilde{L}, L_0\}$ admit the representations*

$$R(\lambda) = \sum_{k=1}^{\infty} (\lambda_k - \lambda)^{-1} \Big(\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\, \cdot, \Gamma_0 \psi_k\Big) \sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\, \Gamma_0 \psi_k$$

and

$$S(\lambda) = \left(i I_{\mathcal{H}_{\tau(\lambda)}} - \sum_{k=1}^{\infty} (\lambda_k - \lambda)^{-1} \bigl(\sqrt{\Im\mathrm{m}\bigl(\tau(\lambda)\bigr)}\,\cdot, \Gamma_0\psi_k\bigr) \sqrt{\Im\mathrm{m}\bigl(\tau(\lambda)\bigr)}\,\Gamma_0\psi_k \right)$$
$$\times \left(i I_{\mathcal{H}_{\tau(\lambda)}} + \sum_{k=1}^{\infty} (\lambda_k - \lambda)^{-1} \bigl(\sqrt{\Im\mathrm{m}\bigl(\tau(\lambda)\bigr)}\,\cdot, \Gamma_0\psi_k\bigr) \sqrt{\Im\mathrm{m}\bigl(\tau(\lambda)\bigr)}\,\Gamma_0\psi_k \right)^{-1},$$

respectively, where $\{\lambda_k\}$, $k = 1, 2, \ldots,$ *are the eigenvalues of the selfadjoint extension* A_1 *in increasing order and* ψ_k *are the corresponding eigenfunctions.*

Remark 5.7. The assumption $A_1 \leqslant A_0$ in Corollary 5.6 above is necessary. Indeed, let us assume that $A_0 \leqslant A_1$ and that A_1 is the Friedrichs extension. Let us show that in this case the sum

$$\sum_{k=1}^{\infty} (\lambda_k - \lambda)^{-1} (\cdot, \Gamma_0\psi_k)\Gamma_0\psi_k \tag{5.7}$$

cannot converge, where $\{\lambda_k\}$ and $\{\psi_k\}$ are the eigenvalues and eigenfunctions of A_1. For this consider the boundary triplet $\{\mathcal{H}, \Gamma_0', \Gamma_1'\}$, $\Gamma_0' = \Gamma_1$ and $\Gamma_1' = -\Gamma_0$. Obviously $A_0' = A^* \upharpoonright \ker(\Gamma_0') = A_1$, $A_1' = A^* \upharpoonright \ker(\Gamma_1') = A_0$ and A_0' is the Friedrichs extension. By Proposition 3.5 we obtain that the sum

$$\sum_{k=1}^{\infty} (\lambda - \lambda_k)^{-1} \bigl(\cdot, \Gamma_1'\psi_k\bigr)\Gamma_1'\psi_k$$

diverges, where $\{\lambda_k\}$ and $\{\psi_k\}$ are the eigenvalues and eigenfunctions of $A_0' = A_1$. Using $\Gamma_1' = -\Gamma_0$ one gets that the sum (5.7) diverges.

6. Scattering systems of differential operators

In this section we illustrate the general results from the previous sections for scattering systems which consist of regular and singular second order differential operators, see Section 2.3.

6.1. Coupling of differential operators

Let the symmetric operators $A = -\frac{1}{2}\frac{d}{dx}\frac{1}{m}\frac{d}{dx} + v$ and

$$T = T_l \oplus T_r = \left(-\frac{1}{2}\frac{d}{dx}\frac{1}{m_l}\frac{d}{dx} + v_l \right) \oplus \left(-\frac{1}{2}\frac{d}{dx}\frac{1}{m_r}\frac{d}{dx} + v_r \right)$$

in $\mathfrak{H} = L^2((x_l, x_r))$ and $\mathfrak{K} = L^2((-\infty, x_l)) \oplus L^2((x_r, \infty))$ and the boundary triplets $\Pi_A = \{\mathbb{C}^2, \Gamma_0, \Gamma_1\}$ and $\Pi_T = \{\mathbb{C}^2, \Upsilon_0, \Upsilon_1\}$ be as in Sections 2.3.1 and 2.3.2, respectively. By Theorem 5.1(i) the operator

$$\widetilde{L} := A^* \oplus T^* \upharpoonright \left\{ f \oplus g \in \mathrm{dom}(A^* \oplus T^*) \colon \begin{array}{l} \Gamma_0 f - \Upsilon_0 g = 0 \\ \Gamma_1 f + \Upsilon_1 g = 0 \end{array} \right\} \tag{6.1}$$

is a selfadjoint extension of $L = A \oplus T$ in $\mathfrak{H} \oplus \mathfrak{K}$. We can identify $\mathfrak{H} \oplus \mathfrak{K}$ with

$$L^2\big((x_l, x_r)\big) \oplus L^2\big((-\infty, x_l)\big) \oplus L^2\big((x_r, \infty)\big) \cong L^2(\mathbb{R}).$$

The elements $f \oplus g$ in $\mathfrak{H} \oplus \mathfrak{K}$, $f \in \mathfrak{H}$, $g = g_l \oplus g_r \in \mathfrak{K}$, will be written as $f \oplus g_l \oplus g_r$. Here the conditions $\Gamma_0 f = \Upsilon_0 g$ and $\Gamma_1 f = -\Upsilon_1 g$, $f \in \mathrm{dom}(A^*)$, $g \in \mathrm{dom}(T^*)$, explicitly mean

$$g_l(x_l) = f(x_l) \quad \text{and} \quad f(x_r) = g_r(x_r),$$

and

$$\left(\frac{1}{m} f'\right)(x_l) = \left(\frac{1}{m_l} g_l'\right)(x_l) \quad \text{and} \quad \left(\frac{1}{m} f'\right)(x_r) = \left(\frac{1}{m_r} g_r'\right)(x_r).$$

Hence the selfadjoint operator (6.1) has the form

$$\widetilde{L}(f \oplus g_l \oplus g_r) = \begin{pmatrix} -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx} f + v f & 0 & 0 \\ 0 & -\frac{1}{2}\frac{d}{dx}\frac{1}{m_l}\frac{d}{dx} g_l + v_l g_l & 0 \\ 0 & 0 & -\frac{1}{2}\frac{d}{dx}\frac{1}{m_r}\frac{d}{dx} g_r + v_r g_r \end{pmatrix}$$

and coincides with the usual Schrödinger operator

$$-\frac{1}{2}\frac{d}{dx}\frac{1}{\widetilde{m}}\frac{d}{dx} + \widetilde{v} \upharpoonright \left\{ f \in L^2(\mathbb{R}) \colon\ f, \frac{1}{\widetilde{m}} f' \in W^{1,2}(\mathbb{R}) \right\},$$

where

$$\widetilde{m}(x) := \begin{cases} m(x), & x \in (x_l, x_r), \\ m_l(x), & x \in (-\infty, x_l), \\ m_r(x), & x \in (x_r, \infty), \end{cases}$$

and

$$\widetilde{v}(x) := \begin{cases} v(x), & x \in (x_l, x_r), \\ v_l(x), & x \in (-\infty, x_l), \\ v_r(x), & x \in (x_r, \infty). \end{cases}$$

The selfadjoint operator $L_0 = A_0 \oplus T_0$, where $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ and $T_0 = T^* \upharpoonright \ker(\Upsilon_0)$, is defined on

$$\mathrm{dom}(L_0) = \left\{ f \oplus g_l \oplus g_r \in \mathrm{dom}(A^*) \oplus \mathrm{dom}\big(T_l^*\big) \oplus \mathrm{dom}\big(T_r^*\big) \colon\ \begin{matrix} f(x_l) = f(x_r) = 0 \\ g_l(x_l) = g_r(x_r) = 0 \end{matrix} \right\}$$

and can be identified with the selfadjoint Schrödinger operator

$$-\frac{1}{2}\frac{d}{dx}\frac{1}{\widetilde{m}}\frac{d}{dx} + \widetilde{v} \upharpoonright \left\{ f \in L^2(\mathbb{R}) \colon\ f, \frac{1}{\widetilde{m}} f' \in W^{1,2}\big(\mathbb{R} \setminus \{x_l, x_r\}\big),\ f(x_l) = f(x_r) = 0 \right\}.$$

6.2. S and R-matrix representation

It is well known that all selfadjoint extensions of the differential operator A in $L^2((x_l,x_r))$ have discrete spectrum. Hence according to Theorem 5.1 and Corollary 5.2 the selfadjoint Schrödinger operators $\widetilde{L}$ and L_0 form a complete scattering system $\{\widetilde{L},L_0\}$ in $L^2(\mathbb{R})$ and the scattering matrix $\{S(\lambda)\}$ is given by

$$S(\lambda)=I_{\mathcal{H}_{\tau(\lambda)}}-2i\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)}\big(M(\lambda)+\tau(\lambda)\big)^{-1}\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)} \tag{6.2}$$

for $\lambda\in\Sigma^M\cap\Sigma^\tau\cap\Sigma^{(M+\tau)^{-1}}$. Here $M(\cdot)$ is the Weyl function corresponding to the boundary triplet $\Pi_A=\{\mathbb{C}^2,\Gamma_0,\Gamma_1\}$ and

$$\lambda\mapsto\tau(\lambda)=\begin{pmatrix}\mathfrak{m}_l(\lambda)&0\\0&\mathfrak{m}_r(\lambda)\end{pmatrix},\quad\lambda\in\rho(T_0),$$

is the Weyl function of $\Pi_T=\{\mathbb{C}^2,\Upsilon_0,\Upsilon_1\}$, cf. Section 2.3.2. It follows from [19] that for $\lambda\in\Sigma^\tau$ with $\Im\mathrm{m}(\tau(\lambda))\neq 0$ the maximal dissipative differential operator

$$A_{-\tau(\lambda)}=A^*\upharpoonright\ker\big(\Gamma_1+\tau(\lambda)\Gamma_0\big),$$

that is,

$$(A_{-\tau(\lambda)}f)(x)=-\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}f(x)+v(x)f(x),$$
$$\mathrm{dom}(A_{-\tau(\lambda)})=\left\{f\in L^2\big((x_l,x_r)\big):\ \begin{array}{c}f,\frac{1}{m}f'\in W^{1,2}((x_l,x_r))\\ \big(\frac{1}{2m}f'\big)(x_l)=-\mathfrak{m}_l(\lambda)f(x_l)\\ \big(\frac{1}{2m}f'\big)(x_r)=\mathfrak{m}_r(\lambda)f(x_r)\end{array}\right\},$$

has no real eigenvalues, i.e. $\mathbb{R}\subset\rho(A_{-\tau(\lambda)})$, so that each $\lambda\in\Sigma^M=\rho(A_0)\cap\mathbb{R}$ necessarily belongs to the set $\Sigma^{(M+\tau)^{-1}}$ by Theorem 2.4. Therefore the representation (6.2) is valid for all $\lambda\in\{t\in\Sigma^\tau:\ \Im\mathrm{m}(\tau(t))\neq 0\}\cap\rho(A_0)$. Moreover, for $\lambda\in\Sigma^\tau$ with $\Im\mathrm{m}(\tau(\lambda))=0$ we have $S(\lambda)=\{0\}$.

It is well known that the symmetric operator A given by (2.9) is semibounded from below and that the extension $A_0=A^*\upharpoonright\ker(\Gamma_0)$, cf. (2.10), is the Friedrichs extension of A. In particular, this yields $A_\Theta\leqslant A_0$ for any other selfadjoint extension A_Θ of A.

The selfadjoint operator $A_{-\Re\mathrm{e}(\tau(\lambda))}$, $\lambda\in\Sigma^\tau=\Sigma^{\mathfrak{m}_l}\cap\Sigma^{\mathfrak{m}_r}$, is given by

$$(A_{-\Re\mathrm{e}(\tau(\lambda))}f)(x)=-\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx}f(x)+v(x)f(x),$$
$$\mathrm{dom}(A_{-\Re\mathrm{e}(\tau(\lambda))})=\left\{f\in L^2\big((x_l,x_r)\big):\ \begin{array}{c}f,\frac{1}{m}f'\in W^{1,2}((x_l,x_r))\\ \big(\frac{1}{2m}f'\big)(x_l)=-\Re\mathrm{e}(\mathfrak{m}_l(\lambda))f(x_l)\\ \big(\frac{1}{2m}f'\big)(x_r)=\Re\mathrm{e}(\mathfrak{m}_r(\lambda))f(x_r)\end{array}\right\}$$

and clearly $\sigma(A_{-\Re\mathrm{e}(\tau(\lambda))})$ is discrete and semibounded from below for all $\lambda\in\Sigma^\tau$.

Taking into account Theorem 5.5 it follows that the R-matrix of $\{\widetilde{L},L_0\}$ has the form

$$R(\lambda) = \sum_{k=1}^{\infty} \big(\lambda_k[\lambda] - \lambda\big)^{-1} \left(\begin{pmatrix} \sqrt{\Im m(\mathfrak{m}_l(\lambda))}\,\cdot \\ \sqrt{\Im m(\mathfrak{m}_r(\lambda))}\,\cdot \end{pmatrix}, \begin{pmatrix} \psi_k[\lambda](x_l) \\ \psi_k[\lambda](x_r) \end{pmatrix} \right) \begin{pmatrix} \sqrt{\Im m(\mathfrak{m}_l(\lambda))}\psi_k[\lambda](x_l) \\ \sqrt{\Im m(\mathfrak{m}_r(\lambda))}\psi_k[\lambda](x_r) \end{pmatrix}$$

for all $\lambda \in \Sigma^\tau \cap \Sigma^M$ with the property $\ker(M(\lambda) + \Re e(\tau(\lambda))) = \{0\}$ and $\Im m(\tau(\lambda)) \neq 0$. Here $\{\lambda_k[\lambda]\}$, $k = 1, 2, \ldots$, denote the eigenvalues of the selfadjoint operator $A_{-\Re e(\tau(\lambda))}$ in increasing order and $\psi_k[\lambda]$ are the corresponding eigenfunctions. Furthermore we have again used $\mathbb{R} \subset \rho(A_{-\tau(\lambda)})$ if $\Im m(\tau(\lambda)) \neq 0$, and moreover, $R(\lambda) = \{0\}$ if $\Im m(\tau(\lambda)) = 0$.

The scattering matrix $\{S(\lambda)\}$ of $\{\widetilde{L}, L_0\}$ can be represented in the form

$$\begin{aligned} S(\lambda) = \Bigg\{ i I_{\mathcal{H}_{\tau(\lambda)}} - \sum_{k=1}^{\infty} \big(\lambda_k[\lambda] - \lambda\big)^{-1} &\left(\begin{pmatrix} \sqrt{\Im m(\mathfrak{m}_l(\lambda))}\,\cdot \\ \sqrt{\Im m(\mathfrak{m}_r(\lambda))}\,\cdot \end{pmatrix}, \begin{pmatrix} \psi_k[\lambda](x_l) \\ \psi_k[\lambda](x_r) \end{pmatrix} \right) \\ &\times \begin{pmatrix} \sqrt{\Im m(\mathfrak{m}_l(\lambda))}\psi_k[\lambda](x_l) \\ \sqrt{\Im m(\mathfrak{m}_r(\lambda))}\psi_k[\lambda](x_r) \end{pmatrix} \Bigg\} \\ \times \Bigg\{ i I_{\mathcal{H}_{\tau(\lambda)}} + \sum_{k=1}^{\infty} \big(\lambda_k[\lambda] - \lambda\big)^{-1} &\left(\begin{pmatrix} \sqrt{\Im m(\mathfrak{m}_l(\lambda))}\,\cdot \\ \sqrt{\Im m(\mathfrak{m}_r(\lambda))}\,\cdot \end{pmatrix}, \begin{pmatrix} \psi_k[\lambda](x_l) \\ \psi_k[\lambda](x_r) \end{pmatrix} \right) \\ &\times \begin{pmatrix} \sqrt{\Im m(\mathfrak{m}_l(\lambda))}\psi_k[\lambda](x_l) \\ \sqrt{\Im m(\mathfrak{m}_r(\lambda))}\psi_k[\lambda](x_r) \end{pmatrix} \Bigg\}^{-1} \end{aligned}$$

for all $\lambda \in \Sigma^\tau \cap \Sigma^M$ with $\ker(M(\lambda) + \Re e(\tau(\lambda))) = \{0\}$ and $\Im m(\tau(\lambda)) \neq 0$.

6.2.1. Constant potentials v_l and v_r

Let us assume that the potentials $v_l(\cdot)$ and $v_r(\cdot)$ as well as the mass functions $m_l(\cdot)$ and $m_r(\cdot)$ are constant, that is, $v_l(x) = v_l \in \mathbb{R}$, $m_l(x) = m_l > 0$ for $x \in (-\infty, x_l)$ and $v_r(x) = v_r \in \mathbb{R}$, $m_r(x) = m_r > 0$ for $x \in (v_r, \infty)$. The Titchmarsh–Weyl functions $\mathfrak{m}_l(\cdot)$ and $\mathfrak{m}_r(\cdot)$ can be calculated explicitly in this simple case. One gets

$$\mathfrak{m}_l(\lambda) = i\sqrt{\frac{\lambda - v_l}{2m_l}} \quad \text{and} \quad \mathfrak{m}_r(\lambda) = i\sqrt{\frac{\lambda - v_r}{2m_r}}$$

for $\lambda \in \mathbb{C}_+$, where the square root is defined on $\mathbb{C}$ with a cut along $[0, \infty)$ and fixed by $\Im m(\sqrt{\lambda}) > 0$ for $\lambda \notin [0, \infty)$ and by $\sqrt{\lambda} \geqslant 0$ for $\lambda \in [0, \infty)$. It is clear that

$$\Sigma^\tau = \Sigma^{\mathfrak{m}_l} \cap \Sigma^{\mathfrak{m}_r} = \mathbb{R}$$

and it is not difficult to check

$$\big\{\lambda \in \Sigma^\tau \colon \Im m\big(\tau(\lambda)\big) \neq 0\big\} = \big(\min\{v_l, v_r\}, \infty\big).$$

Furthermore

$$\Re e\big(\mathfrak{m}_l(\lambda)\big) = \begin{cases} -\sqrt{\frac{v_l - \lambda}{2m_l}}, & \lambda \leqslant v_l, \\ 0, & \lambda > v_l, \end{cases}$$

and

$$\Re\mathrm{e}\big(\mathfrak{m}_r(\lambda)\big) = \begin{cases} -\sqrt{\frac{v_r-\lambda}{2m_r}}, & \lambda \leqslant v_r, \\ 0, & \lambda > v_r. \end{cases}$$

If $\lambda \in (\max\{v_l, v_r\}, \infty)$, then $\Re\mathrm{e}(\tau(\lambda)) = 0$ and it follows from Corollary 5.6 and the above considerations that the R-matrix of $\{\widetilde{L}, L_0\}$ has the form

$$R(\lambda) = \sum_{k=1}^{\infty} (\lambda_k - \lambda)^{-1} \left(\begin{pmatrix} \sqrt{\Im\mathrm{m}(\mathfrak{m}_l(\lambda))}\,\cdot \\ \sqrt{\Im\mathrm{m}(\mathfrak{m}_r(\lambda))}\,\cdot \end{pmatrix}, \begin{pmatrix} \psi_k(x_l) \\ \psi_k(x_r) \end{pmatrix} \right) \begin{pmatrix} \sqrt{\Im\mathrm{m}(\mathfrak{m}_l(\lambda))}\psi_k(x_l) \\ \sqrt{\Im\mathrm{m}(\mathfrak{m}_r(\lambda))}\psi_k(x_r) \end{pmatrix} \tag{6.3}$$

for all $\lambda \in \Sigma^M$ with the property $\ker(M(\lambda)) = \{0\}$. Here $\{\lambda_k\}$, $k = 1, 2, \ldots$, denote the eigenvalues of the selfadjoint operator A_1 in increasing order and ψ_k are the corresponding eigenfunctions. Note that A_1 is the usual Schrödinger operator in $L^2((x_l, x_r))$ which corresponds to Neumann boundary conditions, cf. (2.11), and that $\lambda \in \Sigma^M$ has the property $\ker(M(\lambda)) = \{0\}$ if and only if $\lambda \in \rho(A_0) \cap \rho(A_1)$, cf. Theorem 2.4.

Analogously the scattering matrix $\{S(\lambda)\}$ of $\{\widetilde{L}, L_0\}$ has the form

$$S(\lambda) = \left\{ iI_{\mathcal{H}_{\tau(\lambda)}} - \sum_{k=1}^{\infty} (\lambda_k - \lambda)^{-1} \left(\begin{pmatrix} \sqrt{\Im\mathrm{m}(\mathfrak{m}_l(\lambda))}\,\cdot \\ \sqrt{\Im\mathrm{m}(\mathfrak{m}_r(\lambda))}\,\cdot \end{pmatrix}, \begin{pmatrix} \psi_k(x_l) \\ \psi_k(x_r) \end{pmatrix} \right) \begin{pmatrix} \sqrt{\Im\mathrm{m}(\mathfrak{m}_l(\lambda))}\psi_k(x_l) \\ \sqrt{\Im\mathrm{m}(\mathfrak{m}_r(\lambda))}\psi_k(x_r) \end{pmatrix} \right\}$$

$$\times \left\{ iI_{\mathcal{H}_{\tau(\lambda)}} + \sum_{k=1}^{\infty} (\lambda_k - \lambda)^{-1} \left(\begin{pmatrix} \sqrt{\Im\mathrm{m}(\mathfrak{m}_l(\lambda))}\,\cdot \\ \sqrt{\Im\mathrm{m}(\mathfrak{m}_r(\lambda))}\,\cdot \end{pmatrix}, \begin{pmatrix} \psi_k(x_l) \\ \psi_k(x_r) \end{pmatrix} \right) \begin{pmatrix} \sqrt{\Im\mathrm{m}(\mathfrak{m}_l(\lambda))}\psi_k(x_l) \\ \sqrt{\Im\mathrm{m}(\mathfrak{m}_r(\lambda))}\psi_k(x_r) \end{pmatrix} \right\}^{-1}$$

for all $\lambda \in (\max\{v_l, v_r\}, \infty) \cap \rho(A_0) \cap \rho(A_1)$.

The situation is slightly more complicated if $\lambda \in (\min\{v_l, v_r\}, \max\{v_l, v_r\})$. Assume e.g. $v_l > v_r$ and let $\lambda \in (v_r, v_l)$. In this case $\Im\mathrm{m}(\tau(\lambda)) \neq 0$, but the condition $\Re\mathrm{e}(\tau(\lambda)) = 0$ is not satisfied since

$$\Re\mathrm{e}\big(\mathfrak{m}_l(\lambda)\big) = -\sqrt{\frac{v_l - \lambda}{2m_l}} \quad \text{and} \quad \Re\mathrm{e}\big(\mathfrak{m}_r(\lambda)\big) = 0.$$

The operator $A_{-\Re\mathrm{e}(\tau(\lambda))}$ is given by

$$(A_{-\Re\mathrm{e}(\tau(\lambda))} f)(x) = -\frac{1}{2}\frac{d}{dx}\frac{1}{m(x)}\frac{d}{dx} f(x) + v(x) f(x),$$

$$\mathrm{dom}(A_{-\Re\mathrm{e}(\tau(\lambda))}) = \left\{ f \in L^2\big((x_l, x_r)\big)\colon \begin{array}{c} f, \frac{1}{m} f' \in W^{1,2}((x_l, x_r)) \\ \big(\frac{1}{2m} f'\big)(x_l) = \sqrt{\frac{v_l-\lambda}{2m_l}} f(x_l) \\ \big(\frac{1}{2m} f'\big)(x_r) = 0 \end{array} \right\}.$$

Since

$$\sqrt{\Im\mathrm{m}\big(\tau(\lambda)\big)} = \begin{pmatrix} 0 & 0 \\ 0 & \big(\frac{\lambda - v_r}{2m_r}\big)^{1/4} \end{pmatrix}, \quad \lambda \in (v_r, v_l),$$

the representations of the R and S-matrix of $\{\widetilde{L}, L_0\}$ from the previous subsections become

$$R(\lambda) = \sum_{k=1}^{\infty} \big(\lambda_k[\lambda] - \lambda\big)^{-1} \Big(\sqrt{\Im\mathrm{m}\big(\mathfrak{m}_r(\lambda)\big)}\,\cdot, \psi_k[\lambda](x_r)\Big) \sqrt{\Im\mathrm{m}\big(\mathfrak{m}_r(\lambda)\big)}\,\psi_k[\lambda](x_r)$$

and

$$S(\lambda) = \frac{i - \sum_{k=1}^{\infty} (\lambda_k[\lambda] - \lambda)^{-1} (\sqrt{\Im\mathrm{m}(\mathfrak{m}_r(\lambda))}\,\cdot, \psi_k[\lambda](x_r)) \sqrt{\Im\mathrm{m}(\mathfrak{m}_r(\lambda))}\,\psi_k[\lambda](x_r)}{i + \sum_{k=1}^{\infty} (\lambda_k[\lambda] - \lambda)^{-1} (\sqrt{\Im\mathrm{m}(\mathfrak{m}_r(\lambda))}\,\cdot, \psi_k[\lambda](x_r)) \sqrt{\Im\mathrm{m}(\mathfrak{m}_r(\lambda))}\,\psi_k[\lambda](x_r)},$$

respectively, for $\lambda \in (v_r, v_l) \cap \rho(A_0) \cap \rho(A_{-\Re\mathrm{e}(\tau(\lambda))})$, see Theorem 5.5. Here $\{\lambda_k[\lambda]\}$, $k = 1, 2, \ldots,$ are the eigenvalues of the selfadjoint extension $A_{-\Re\mathrm{e}(\tau(\lambda))}$ in increasing order and $\psi_k[\lambda]$ are the corresponding eigenfunctions.

Remark 6.1. One might guess that the sum

$$\sum_{k=1}^{\infty} (\lambda_k - \lambda)^{-1} \left(\cdot, \begin{pmatrix} \psi_k(x_l) \\ \psi_k(x_r) \end{pmatrix}\right) \begin{pmatrix} \psi_k(x_l) \\ \psi_k(x_r) \end{pmatrix}$$

in the representation of the scattering matrix in (6.3), where $\{\lambda_k\}$ and $\{\psi_k\}$ are the eigenvalues and eigenfunctions of the Schrödinger operator with Neumann boundary conditions, can be replaced by the sum

$$\sum_{k=1}^{\infty} (\mu_k - \lambda)^{-1} \left(\cdot, \begin{pmatrix} \big(\frac{1}{2m}\phi_k'\big)(x_l) \\ -\big(\frac{1}{2m}\phi_k'\big)(x_r) \end{pmatrix}\right) \begin{pmatrix} \big(\frac{1}{2m}\phi_k'\big)(x_l) \\ -\big(\frac{1}{2m}\phi_k'\big)(x_r) \end{pmatrix},$$

where $\{\mu_k\}$ and $\{\phi_k\}$ are the eigenvalues and eigenfunctions of the Schrödinger operator with Dirichlet boundary conditions. However, this is not possible since by Proposition 3.5 the last sum does not converge. We note that this can easily be verified directly for the case $v(x) = 0$ and $m(x) = \text{constant}$.

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