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## Scattering matrices and Weyl functions

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## Abstract

For a scattering system  $\{A_\Theta, A_0\}$  consisting of selfadjoint extensions  $A_\Theta$  and  $A_0$  of a symmetric operator  $A$  with finite deficiency indices, the scattering matrix  $\{S_\Theta(\lambda)\}$  and a spectral shift function  $\xi_\Theta$  are calculated in terms of the Weyl function associated with the boundary triplet for  $A^*$  and a simple proof of the Krein-Birman formula is given. The results are applied to singular Sturm-Liouville operators with scalar and matrix potentials, to Dirac operators and to Schrödinger operators with point interactions.

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## 1 Introduction

Let  $q \in L^1_{loc}(\mathbb{R}_+)$  be a real function and consider the singular Sturm-Liouville differential expression  $-\frac{d^2}{dx^2} + q$  on  $\mathbb{R}_+$ . We assume that  $-\frac{d^2}{dx^2} + q$  is in the limit point case at  $\infty$ , i.e. the corresponding minimal operator  $L$ ,

$$Lf = -f'' + qf, \quad \text{dom}(L) = \{f \in \mathcal{D}_{max} : f(0) = f'(0) = 0\}, \quad (1.1)$$

in  $L^2(\mathbb{R}_+)$  has deficiency indices  $(1, 1)$ . Here  $\mathcal{D}_{max}$  denotes the usual maximal domain consisting of all functions  $f \in L^2(\mathbb{R}_+)$  such that  $f$  and  $f'$  are locally absolutely continuous and  $-f'' + qf$  belongs to  $L^2(\mathbb{R}_+)$ . It is well-known that the maximal operator is given by  $L^*f = -f'' + qf$ ,  $\text{dom}(L^*) = \mathcal{D}_{max}$ , and that all selfadjoint extensions of  $L$  in  $L^2(\mathbb{R}_+)$  can be parametrized in the form

$$L_\Theta = L^* \upharpoonright \text{dom}(L_\Theta), \quad \text{dom}(L_\Theta) = \{f \in \mathcal{D}_{max} : f'(0) = \Theta f(0)\}, \quad \Theta \in \overline{\mathbb{R}},$$

where  $\Theta = \infty$  corresponds to the Dirichlet boundary condition  $f(0) = 0$ .

Since the deficiency indices of  $L$  are  $(1, 1)$  the pair  $\{L_\Theta, L_\infty\}$ ,  $\Theta \in \overline{\mathbb{R}}$ , performs a complete scattering system, that is, the wave operators

$$W_\pm(L_\Theta, L_\infty) = s - \lim_{t \rightarrow \pm\infty} e^{itL_\Theta} e^{-itL_\infty} P^{ac}(L_\infty)$$

exist and their ranges coincide with the absolutely continuous subspace  $\text{ran}(P^{ac}(L_\Theta))$  of  $L_\Theta$ , cf. [6, 25, 34, 38]. Here  $P^{ac}(L_\infty)$  and  $P^{ac}(L_\Theta)$  denote the orthogonal projections onto the absolutely continuous subspace of  $L_\infty$  and  $L_\Theta$ , respectively. The scattering operator  $S_\Theta = W_+(L_\Theta, L_\infty)^* W_-(L_\Theta, L_\infty)$  commutes with  $L_\infty$  and therefore  $S_\Theta$  is unitarily equivalent to a multiplication operator induced by a family  $\{S_\Theta(\lambda)\}$  of unitary operators in the spectral representation of  $L_\infty$ . This family is usually called the scattering matrix of the scattering system  $\{L_\Theta, L_\infty\}$  and is the most important quantity in the analysis of scattering processes.

A spectral representation of the selfadjoint realizations of  $-\frac{d^2}{dx^2} + q$  and in particular of  $L_\infty$  has been obtained by H. Weyl in [35, 36, 37], see also [29, 30]. More precisely, if  $\varphi(\cdot, \lambda)$  and  $\psi(\cdot, \lambda)$  are the fundamental solutions of  $-u'' + qu = \lambda u$  satisfying

$$\varphi(0, \lambda) = 1, \quad \varphi'(0, \lambda) = 0 \quad \text{and} \quad \psi(0, \lambda) = 0, \quad \psi'(0, \lambda) = 1,$$

then there exists a scalar function  $m$  such that for each  $\lambda \in \mathbb{C} \setminus \mathbb{R}$  the function  $x \mapsto \varphi(x, \lambda) + m(\lambda)\psi(x, \lambda)$  belongs to  $L^2(\mathbb{R}_+)$ . This so-called Titchmarsh-Weyl function  $m$  is a Nevanlinna function which admits an integral representation

$$m(\lambda) = \alpha + \int_{-\infty}^{\infty} \left( \frac{1}{t - \lambda} - \frac{t}{1 + t^2} \right) d\rho(t) \quad (1.2)$$

with a measure  $\rho$  satisfying  $\int (1 + t^2)^{-1} d\rho(t) < \infty$ . Since  $L_\infty$  is unitarily equivalent to the multiplication operator in  $L^2(\mathbb{R}, d\rho)$  the spectral properties of  $L_\infty$  can be completely described with the help of the Borel measure  $\rho$ , i.e.  $L_\infty$  is absolutely continuous, singular, continuous or pure point if and only if  $\rho$  is so.

It turns out that the scattering matrix  $\{S_\Theta(\lambda)\}$  of the scattering system  $\{L_\Theta, L_\infty\}$  and the Titchmarsh-Weyl function  $m$  are connected via

$$S_\Theta(\lambda) = \frac{\Theta - \overline{m(\lambda + i0)}}{\Theta - m(\lambda + i0)} \quad (1.3)$$

for a.e.  $\lambda \in \mathbb{R}$  with  $\Im m(m(\lambda + i0)) \neq 0$ , cf. Section 5.1. For the special case  $q = 0$  in (1.1) the Titchmarsh-Weyl function is given by  $m(\lambda) = i\sqrt{\lambda}$ , where  $\sqrt{\cdot}$  is defined on  $\mathbb{C}$  with a cut along  $\mathbb{R}_+$  and fixed by  $\Im m \sqrt{\lambda} > 0$  for  $\lambda \notin \mathbb{R}_+$  and by  $\sqrt{\lambda} \geq 0$  for  $\lambda \in \mathbb{R}_+$ . In this case formula (1.3) reduces to

$$S_\Theta(\lambda) = \frac{\Theta + i\sqrt{\lambda}}{\Theta - i\sqrt{\lambda}} \quad \text{for a.e. } \lambda \in \mathbb{R}_+ \quad (1.4)$$

and was obtained in e.g. [38, §3].

The basic aim of the present paper is to generalize the correspondence (1.3) between the scattering matrix  $\{S_\Theta(\lambda)\}$  of  $\{L_\Theta, L_\infty\}$  and the Titchmarsh-Weyl function  $m$  from above to scattering systems consisting of a pair of selfadjoint operators, which both are assumed to be extensions of a symmetric operator with finite deficiency indices, and an abstract analogon of the function  $m$ .

For this we use the concept of boundary triplets and associated Weyl functions developed in [13, 14]. Namely, if  $A$  is a densely defined closed symmetric operator with equal deficiency indices  $n_\pm(A) < \infty$  in a Hilbert space  $\mathfrak{H}$  and  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  is a boundary triplet for  $A^*$ , then all selfadjoint extensions  $A_\Theta$  of  $A$  in  $\mathfrak{H}$  are labeled by the selfadjoint relations  $\Theta$  in  $\mathcal{H}$ , cf. Section 2.1. The analogon of the Sturm-Liouville operator  $L_\infty$  from above here is the selfadjoint extension  $A_0 := A^* \upharpoonright \ker(\Gamma_0)$  corresponding to the selfadjoint relation  $\left\{ \begin{pmatrix} 0 \\ h \end{pmatrix} : h \in \mathcal{H} \right\}$ . To the boundary triplet  $\Pi$  one associates an operator-valued Nevanlinna function  $M$  holomorphic on  $\rho(A_0)$  which admits an integral representation of the form (1.2) with an operator-valued measure closely connected with the spectral measure of  $A_0$ , see e.g. [2]. This function  $M$  is the abstract analogon of the Titchmarsh-Weyl function  $m$  from above and is called the Weyl function corresponding to the boundary triplet  $\Pi$ , cf. Section 2.2.

Since  $A$  is assumed to be a symmetric operator with finite deficiency indices the pair  $\{A_\Theta, A_0\}$ , where  $\Theta$  is an arbitrary selfadjoint relation in  $\mathcal{H}$ , is a complete scattering system with a corresponding scattering matrix  $\{S_\Theta(\lambda)\}$ . Our main result is Theorem 3.8, which states that the direct integral  $L^2(\mathbb{R}, \mu_L, \mathcal{H}_\lambda)$  performs a spectral representation of the absolutely continuous part  $A_0^{ac}$  of  $A_0$  such that the scattering matrix  $\{S_\Theta(\lambda)\}$  of the scattering system  $\{A_\Theta, A_0\}$  has the form

$$S_\Theta(\lambda) = I_{\mathcal{H}_\lambda} + 2i\sqrt{\Im m(M(\lambda))}(\Theta - M(\lambda))^{-1}\sqrt{\Im m(M(\lambda))} \quad (1.5)$$

for a.e.  $\lambda \in \mathbb{R}$ , where  $M(\lambda) := M(\lambda + i0)$ ,  $\mu_L$  is the Lebesgue measure and  $\mathcal{H}_\lambda := \text{ran}(\Im m(M(\lambda)))$ . If the Weyl function scalar, i.e. the deficiency indices of  $A$  are  $(1, 1)$ , then we immediately restore (1.3) from (1.5), see also Corollary 3.10. We note that in [1] (see also [4]) V.M. Adamyan and B.S. Pavlov have already obtained a different (unitarily equivalent) expression for the scattering matrix of a pair of selfadjoint extensions of a symmetric operator with finite deficiency indices.

We emphasize that the representation (1.5) in terms of the Weyl function of a fixed boundary triplet has several advantages, e.g. for Sturm-Liouville operators with matrix potentials, Schrödinger operators with point interactions and Dirac operators the high energy asymptotic of the scattering matrices can be calculated and explicit formulas can be given (see Section 5). Furthermore, since the difference of the resolvents of  $A_\Theta$  and  $A_0$  is a finite rank operator, the complete scattering system  $\{A_\Theta, A_0\}$  admits a so-called spectral shift function  $\xi_\Theta$ , cf. [27] and e.g. [9, 10]. Recall that  $\xi_\Theta$  is a real function summable with weight  $(1 + \lambda^2)^{-1}$  such that the trace formula

$$\operatorname{tr}((A_\Theta - z)^{-1} - (A_0 - z)^{-1}) = - \int_{\mathbb{R}} \frac{1}{(\lambda - z)^2} \xi_\Theta(\lambda) d\lambda$$

is valid for  $z \in \mathbb{C} \setminus \mathbb{R}$ . The spectral shift function is determined by the trace formula up to a real constant. Under the assumption that  $\Theta$  is a selfadjoint matrix, we show that the spectral shift function of  $\{A_\Theta, A_0\}$  is given (up to a real constant) by

$$\xi_\Theta(\lambda) = \frac{1}{\pi} \Im (\operatorname{tr}(\log(M(\lambda + i0) - \Theta))) \quad \text{for a.e. } \lambda \in \mathbb{R}, \quad (1.6)$$

see Theorem 4.1 and [28] for the case  $n = 1$ . With this choice of  $\xi_\Theta$  and the representation (1.5) of the scattering matrix  $\{S_\Theta(\lambda)\}$  it is easy to prove an analogue of the Birman-Krein formula (see [8])

$$\det(S_\Theta(\lambda)) = \exp(-2\pi i \xi_\Theta(\lambda)) \quad \text{for a.e. } \lambda \in \mathbb{R}$$

for scattering systems  $\{A_\Theta, A_0\}$  consisting of selfadjoint extensions of a symmetric operator with finite deficiency indices. Finally we mention that with the help of the representation (1.5) in a forthcoming paper the classical Lax-Phillips scattering theory will be extended and newly interpreted.

The paper is organized as follows. In Section 2 we briefly recall the notion of boundary triplets and associated Weyl functions and review some standard facts. Section 3 is devoted to the study of scattering systems  $\{A_\Theta, A_0\}$  consisting of selfadjoint operators which are extension of a densely defined closed simple symmetric operator  $A$  with finite deficiency indices. After some preparations we prove the representation (1.5) of the scattering matrix  $\{S_\Theta(\lambda)\}$  in Theorem 3.8. Section 4 is concerned with the spectral shift function and the Birman-Krein formula. In Section 5 we apply our general result to singular Sturm-Liouville operators with scalar and matrix potentials, to Dirac operators and to Schrödinger operators with point interactions. Finally, for the convenience of the reader we repeat some basic facts on direct integrals and spectral representations in the appendix, thus making our exposition self-contained.

**Notations.** Throughout the paper  $\mathfrak{H}$  and  $\mathcal{H}$  denote separable Hilbert spaces with scalar product  $(\cdot, \cdot)$ . The linear space of bounded linear operators defined from  $\mathfrak{H}$  to  $\mathcal{H}$  is denoted by  $[\mathfrak{H}, \mathcal{H}]$ . For brevity we write  $[\mathfrak{H}]$  instead of  $[\mathfrak{H}, \mathfrak{H}]$ . The set of closed operators in  $\mathfrak{H}$  is denoted by  $\mathcal{C}(\mathfrak{H})$ . By  $\tilde{\mathcal{C}}(\mathfrak{H})$  we denote the set of closed linear relations in  $\mathfrak{H}$ . Notice that  $\mathcal{C}(\mathfrak{H}) \subseteq \tilde{\mathcal{C}}(\mathfrak{H})$ . The resolvent set and the spectrum of a linear operator or relation are denoted by  $\rho(\cdot)$  and  $\sigma(\cdot)$ , respectively. The domain, kernel and range of a linear operator or relation are denoted by  $\operatorname{dom}(\cdot)$ ,  $\ker(\cdot)$  and  $\operatorname{ran}(\cdot)$ , respectively. By  $\mathcal{B}(\mathbb{R})$  we denote the Borel sets of  $\mathbb{R}$ . The Lebesgue measure on  $\mathcal{B}(\mathbb{R})$  is denoted by  $\mu_L(\cdot)$ .

## 2 Extension theory of symmetric operators

### 2.1 Boundary triplets and closed extensions

Let  $A$  be a densely defined closed symmetric operator with equal deficiency indices  $n_{\pm}(A) = \dim \ker(A^* \mp i) \leq \infty$  in the separable Hilbert space  $\mathfrak{H}$ . We use the concept of boundary triplets for the description of the closed extensions  $A_{\Theta} \subset A^*$  of  $A$  in  $\mathfrak{H}$ , see [12, 13, 14, 24].

**Definition 2.1** *A triplet  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  is called boundary triplet for the adjoint operator  $A^*$  if  $\mathcal{H}$  is a Hilbert space and  $\Gamma_0, \Gamma_1 : \text{dom}(A^*) \rightarrow \mathcal{H}$  are linear mappings such that*

(i) *the abstract second Green's identity,*

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

*holds for all  $f, g \in \text{dom}(A^*)$  and*

(ii) *the mapping  $\Gamma := (\Gamma_0, \Gamma_1)^{\top} : \text{dom}(A^*) \rightarrow \mathcal{H} \times \mathcal{H}$  is surjective.*

We refer to [13] and [14] 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  $A^*$  exists since the deficiency indices  $n_{\pm}(A)$  of  $A$  are assumed to be equal. Then  $n_{\pm}(A) = \dim \mathcal{H}$  holds. We note that a boundary triplet for  $A^*$  is not unique.

An operator  $\tilde{A}$  is called a *proper extension* of  $A$  if  $\tilde{A}$  is closed and satisfies  $A \subseteq \tilde{A} \subseteq A^*$ . Note that here  $A$  is a proper extension of itself. In order to describe the set of proper extensions of  $A$  with the help of a boundary triplet  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  for  $A^*$  we have to consider the set  $\tilde{\mathcal{C}}(\mathcal{H})$  of closed linear relations in  $\mathcal{H}$ , that is, the set of closed linear subspaces of  $\mathcal{H} \oplus \mathcal{H}$ . A closed linear operator in  $\mathcal{H}$  is identified with its graph, so that the set  $\mathcal{C}(\mathcal{H})$  of closed linear operators in  $\mathcal{H}$  is viewed as a subset of  $\tilde{\mathcal{C}}(\mathcal{H})$ . For the usual definitions of the linear operations with linear relations, the inverse, the resolvent set and the spectrum we refer to [15]. Recall that the adjoint relation  $\Theta^* \in \tilde{\mathcal{C}}(\mathcal{H})$  of a linear relation  $\Theta$  in  $\mathcal{H}$  is defined as

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

and  $\Theta$  is said to be *symmetric (selfadjoint)* if  $\Theta \subseteq \Theta^*$  (resp.  $\Theta = \Theta^*$ ). Note that definition (2.1) extends the definition of the adjoint operator.

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

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

A description of all proper (closed symmetric, selfadjoint) extensions of  $A$  is given in the next proposition. Note also that the selfadjointness of  $A_0$  and  $A_1$  is a consequence of Proposition 2.2 (ii).

**Proposition 2.2** *Let  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  be a boundary triplet for  $A^*$ . Then the mapping*

$$\Theta \mapsto A_{\Theta} := \Gamma^{-1}\Theta = \{f \in \text{dom}(A^*) : \Gamma f = (\Gamma_0 f, \Gamma_1 f)^{\top} \in \Theta\} \quad (2.2)$$

establishes a bijective correspondence between the set  $\widetilde{\mathcal{C}}(\mathcal{H})$  and the set of proper extensions of  $A$ . Moreover, for  $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$  the following assertions hold.

- (i)  $(A_\Theta)^* = A_{\Theta^*}$ .
- (ii)  $A_\Theta$  is symmetric (selfadjoint) if and only if  $\Theta$  is symmetric (resp. selfadjoint).
- (iii)  $A_\Theta$  is disjoint with  $A_0$ , that is  $\text{dom}(A_\Theta) \cap \text{dom}(A_0) = \text{dom}(A)$ , if and only if  $\Theta \in \mathcal{C}(\mathcal{H})$ . In this case the extension  $A_\Theta$  in (2.2) is given by

$$A_\Theta = A^* \upharpoonright \ker(\Gamma_1 - \Theta\Gamma_0).$$

In the following we shall often be concerned with simple symmetric operators. Recall that a symmetric operator is said to be *simple* if there is no nontrivial subspace which reduces it to a selfadjoint operator. By [26] each symmetric operator  $A$  in  $\mathfrak{H}$  can be written as the direct orthogonal sum  $\widehat{A} \oplus A_s$  of a simple symmetric operator  $\widehat{A}$  in the Hilbert space

$$\widehat{\mathfrak{H}} = \text{closan}\{\ker(A^* - \lambda) : \lambda \in \mathbb{C} \setminus \mathbb{R}\}$$

and a selfadjoint operator  $A_s$  in  $\mathfrak{H} \ominus \widehat{\mathfrak{H}}$ . Here  $\text{closan}\{\cdot\}$  denotes the closed linear span of a set. Obviously  $A$  is simple if and only if  $\widehat{\mathfrak{H}}$  coincides with  $\mathfrak{H}$ .

## 2.2 Weyl functions and resolvents of extensions

Let, as in Section 2.1,  $A$  be a densely defined closed symmetric operator in  $\mathfrak{H}$  with equal deficiency indices. If  $\lambda \in \mathbb{C}$  is a point of regular type of  $A$ , i.e.  $(A - \lambda)^{-1}$  is bounded, we denote the *defect subspace* of  $A$  by  $\mathcal{N}_\lambda = \ker(A^* - \lambda)$ . The following definition can be found in [12, 13, 14].

**Definition 2.3** 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  $\gamma(\cdot) : \rho(A_0) \rightarrow [\mathcal{H}, \mathfrak{H}]$  and  $M(\cdot) : \rho(A_0) \rightarrow [\mathcal{H}]$  defined by

$$\gamma(\lambda) := (\Gamma_0 \upharpoonright \mathcal{N}_\lambda)^{-1} \quad \text{and} \quad M(\lambda) := \Gamma_1 \gamma(\lambda), \quad \lambda \in \rho(A_0), \quad (2.3)$$

are called the  $\gamma$ -field and the Weyl function, respectively, corresponding to the boundary triplet  $\Pi$ .

It follows from the identity  $\text{dom}(A^*) = \ker(\Gamma_0) \dot{+} \mathcal{N}_\lambda$ ,  $\lambda \in \rho(A_0)$ , where as above  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ , that the  $\gamma$ -field  $\gamma(\cdot)$  in (2.3) is well defined. It is easily seen that both  $\gamma(\cdot)$  and  $M(\cdot)$  are holomorphic on  $\rho(A_0)$ . Moreover, the relations

$$\gamma(\mu) = (I + (\mu - \lambda)(A_0 - \mu)^{-1})\gamma(\lambda), \quad \lambda, \mu \in \rho(A_0), \quad (2.4)$$

and

$$M(\lambda) - M(\mu)^* = (\lambda - \bar{\mu})\gamma(\mu)^*\gamma(\lambda), \quad \lambda, \mu \in \rho(A_0), \quad (2.5)$$

are valid (see [13]). The identity (2.5) yields that  $M(\cdot)$  is a *Nevanlinna function*, that is,  $M(\cdot)$  is holomorphic on  $\mathbb{C} \setminus \mathbb{R}$  and takes values in  $[\mathcal{H}]$ ,  $M(\lambda) = M(\bar{\lambda})^*$  for all  $\lambda \in \mathbb{C} \setminus \mathbb{R}$  and



$\Im m(M(\lambda))$  is a nonnegative operator for all  $\lambda$  in the upper half plane  $\mathbb{C}_+ = \{\lambda \in \mathbb{C} : \Im m \lambda > 0\}$ . Moreover, it follows from (2.5) that  $0 \in \rho(\Im m(M(\lambda)))$  holds. It is important to note that if the operator  $A$  is simple, then the Weyl function  $M(\cdot)$  determines the pair  $\{A, A_0\}$  uniquely up to unitary equivalence, cf. [12, 13].

In the case that the deficiency indices  $n_+(A) = n_-(A)$  are finite the Weyl function  $M$  corresponding to  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  is a matrix-valued Nevanlinna function in the finite dimensional space  $\mathcal{H}$ . From [16, 18] one gets the existence of the (strong) limit

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

from the upper half-plane for a.e.  $\lambda \in \mathbb{R}$ .

Let now  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  be a boundary triplet for  $A^*$  with  $\gamma$ -field  $\gamma(\cdot)$  and Weyl function  $M(\cdot)$ . The spectrum and the resolvent set of a proper (not necessarily selfadjoint) extension of  $A$  can be described with the help of the Weyl function. If  $A_\Theta \subseteq A^*$  is the extension corresponding to  $\Theta \in \tilde{\mathcal{C}}(\mathcal{H})$  via (2.2), then a point  $\lambda \in \rho(A_0)$  ( $\lambda \in \sigma_i(A_0)$ ,  $i = p, c, r$ ) belongs to  $\rho(A_\Theta)$  if and only if  $0 \in \rho(\Theta - M(\lambda))$  (resp.  $0 \in \sigma_i(\Theta - M(\lambda))$ ,  $i = p, c, r$ ). Moreover, for  $\lambda \in \rho(A_0) \cap \rho(A_\Theta)$  the well-known resolvent formula

$$(A_\Theta - \lambda)^{-1} = (A_0 - \lambda)^{-1} + \gamma(\lambda)(\Theta - M(\lambda))^{-1}\gamma(\bar{\lambda})^* \quad (2.6)$$

holds. Formula (2.6) is a generalization of the known Krein formula for canonical resolvents. We emphasize that it is valid for any proper extension of  $A$  with a nonempty resolvent set. It is worth to note that the Weyl function can also be used to investigate the absolutely continuous and singular continuous spectrum of extensions of  $A$ , cf. [11].

### 3 Scattering matrix and Weyl function

Throughout this section let  $A$  be a densely defined closed symmetric operator with equal deficiency indices  $n_+(A) = n_-(A)$  in the separable Hilbert space  $\mathfrak{H}$ . Let  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  be a boundary triplet for  $A^*$  and let  $\gamma(\cdot)$  and  $M(\cdot)$  be the corresponding  $\gamma$ -field and Weyl function, respectively. The selfadjoint extension  $A^* \upharpoonright \ker(\Gamma_0)$  of  $A$  is denoted by  $A_0$ . Let  $A_\Theta$  be an arbitrary selfadjoint extension of  $A$  in  $\mathfrak{H}$  corresponding to the selfadjoint relation  $\Theta \in \tilde{\mathcal{C}}(\mathcal{H})$  via (2.2),  $A_\Theta = A^* \upharpoonright \Gamma^{-1}\Theta$ .

Later in this section we will assume that the deficiency indices of  $A$  are finite. In this case the *wave operators*

$$W_\pm(A_\Theta, A_0) := s\text{-}\lim_{t \rightarrow \pm\infty} e^{itA_\Theta} e^{-itA_0} P^{ac}(A_0),$$

exist and are complete, where  $P^{ac}(A_0)$  denotes the orthogonal projection onto the absolutely continuous subspace  $\mathfrak{H}^{ac}(A_0)$  of  $A_0$ . Completeness means that the ranges of  $W_\pm(A_\Theta, A_0)$  coincide with the absolutely continuous subspace  $\mathfrak{H}^{ac}(A_\Theta)$  of  $A_\Theta$ , cf. [6, 25, 34, 38]. The *scattering operator*  $S_\Theta$  of the *scattering system*  $\{A_\Theta, A_0\}$  is then defined by

$$S_\Theta := W_+(A_\Theta, A_0)^* W_-(A_\Theta, A_0). \quad (3.1)$$

Since the scattering operator commutes with  $A_0$  it follows that it is unitarily equivalent to a multiplication operator induced by a family  $\{S_\Theta(\lambda)\}$  of unitary operators in a spectral

representation of  $A_0^{ac} := A_0 \upharpoonright \text{dom}(A_0) \cap \mathfrak{H}^{ac}(A_0)$ . The aim of this section is to compute this so-called *scattering matrix*  $\{S_\Theta(\lambda)\}$  of the complete scattering system  $\{A_\Theta, A_0\}$  in a suitable chosen spectral representation of  $A_0^{ac}$  in terms of the Weyl function  $M(\cdot)$  and the extension parameter  $\Theta$ , see Theorem 3.8.

For this purpose we introduce the identification operator

$$J := -(A_\Theta - i)^{-1}(A_0 - i)^{-1} \in [\mathfrak{H}] \quad (3.2)$$

and we set

$$B := \Gamma_0(A_\Theta + i)^{-1} \quad \text{and} \quad C := \Gamma_1(A_0 - i)^{-1}. \quad (3.3)$$

**Lemma 3.1** *Let  $A$  be a densely defined closed symmetric operator in the separable Hilbert space  $\mathfrak{H}$  and let  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  be a boundary triplet for  $A^*$ . Let  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$  and let  $A_\Theta = A^* \upharpoonright \Gamma^{-1}\Theta$ ,  $\Theta \in \mathcal{C}(\mathcal{H})$ , be a selfadjoint extension of  $A$ . Then we have*

$$A_\Theta Jf - JA_0f = (A_\Theta - i)^{-1}f - (A_0 - i)^{-1}f, \quad f \in \text{dom}(A_0),$$

and the factorization

$$(A_\Theta - i)^{-1} - (A_0 - i)^{-1} = B^*C \quad (3.4)$$

holds, where  $B$  and  $C$  are given by (3.3).

**Proof.** The first assertion follows immediately. Let us prove the factorization (3.4). If  $\gamma(\cdot)$  and  $M(\cdot)$  denote the  $\gamma$ -field and Weyl function, respectively, corresponding to the boundary triplet  $\Pi$ , then the resolvent formula

$$(A_\Theta - \lambda)^{-1} = (A_0 - \lambda)^{-1} + \gamma(\lambda)(\Theta - M(\lambda))^{-1}\gamma(\bar{\lambda})^* \quad (3.5)$$

holds for all  $\lambda \in \rho(A_\Theta) \cap \rho(A_0)$ , cf. (2.6). Applying the operator  $\Gamma_0$  to (3.5), using (3.3),  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$  and the relation  $\Gamma_0\gamma(-i) = I_{\mathcal{H}}$  we obtain

$$\begin{aligned} B &= \Gamma_0(A_\Theta + i)^{-1} = \Gamma_0(A_0 + i)^{-1} + \Gamma_0\gamma(-i)(\Theta - M(-i))^{-1}\gamma(i)^* \\ &= (\Theta - M(-i))^{-1}\gamma(i)^*. \end{aligned}$$

Hence  $\Theta = \Theta^*$  and  $M(-i)^* = M(i)$  imply

$$B^* = \gamma(i)(\Theta - M(i))^{-1}. \quad (3.6)$$

Similarly, setting  $A_1 := A^* \upharpoonright \ker(\Gamma_1)$  we get from the resolvent formula (3.5)

$$(A_1 - i)^{-1} = (A_0 - i)^{-1} - \gamma(i)M(i)^{-1}\gamma(-i)^*.$$

On the other hand, by the definition of the Weyl function  $\Gamma_1\gamma(i) = M(i)$  holds. Therefore we obtain

$$C = \Gamma_1(A_0 - i)^{-1} = \gamma(-i)^* \quad \text{and} \quad C^* = \gamma(-i). \quad (3.7)$$

Combining (3.5) with (3.6) and (3.7) we arrive at the factorization (3.4).  $\square$

**Lemma 3.2** *Let  $A$  be a densely defined closed symmetric operator in the separable Hilbert space  $\mathfrak{H}$ , let  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  be a boundary triplet for  $A^*$  and let  $M(\cdot)$  be the corresponding Weyl function. Further, let  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$  and let  $A_\Theta = A^* \upharpoonright \Gamma^{-1}\Theta$ ,  $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$ , be a selfadjoint extension of  $A$ . Then the relation*

$$B(A_\Theta - \lambda)^{-1}B^* = \frac{1}{1 + \lambda^2} \left( (\Theta - M(\lambda))^{-1} - (\Theta - M(i))^{-1} \right) - \frac{1}{\lambda + i} \Im(\Theta - M(i))^{-1}$$

holds for all  $\lambda \in \mathbb{C} \setminus \{\mathbb{R} \cup \pm i\}$ , where  $B$  is given by (3.3).

**Proof.** By (3.3) we have

$$B(A_\Theta - \lambda)^{-1}B^* = \Gamma_0 \{ \Gamma_0(A_\Theta + i)^{-1}(A_\Theta - \bar{\lambda})^{-1}(A_\Theta - i)^{-1} \}^*.$$

It follows from the resolvent formula (3.5) that

$$\Gamma_0(A_\Theta - \mu)^{-1} = ((\Theta - M(\mu))^{-1} \gamma(\bar{\mu}))^*$$

holds for all  $\mu \in \mathbb{C} \setminus \mathbb{R}$ . Combining this formula with the identity

$$(A_\Theta + i)^{-1}(A_\Theta - \bar{\lambda})^{-1}(A_\Theta - i)^{-1} = \frac{1}{\bar{\lambda}^2 + 1} \{ (A_\Theta - \bar{\lambda})^{-1} - (A_\Theta + i)^{-1} \} - \frac{1}{2i(\bar{\lambda} - i)} \{ (A_\Theta - i)^{-1} - (A_\Theta + i)^{-1} \}$$

we obtain

$$B(A_\Theta - \lambda)^{-1}B^* = \Gamma_0 \left\{ \frac{1}{\bar{\lambda}^2 + 1} \left( (\Theta - M(\bar{\lambda}))^{-1} \gamma(\lambda)^* - (\Theta - M(-i))^{-1} \gamma(i)^* \right) - \frac{1}{2i(\bar{\lambda} - i)} \left( (\Theta - M(i))^{-1} \gamma(-i)^* - (\Theta - M(-i))^{-1} \gamma(i)^* \right) \right\}^*.$$

Calculating the adjoint and making use of  $\Gamma_0 \gamma(\mu) = I_{\mathcal{H}}$ ,  $\mu \in \mathbb{C} \setminus \mathbb{R}$ , and the symmetry property  $M(\bar{\lambda}) = M(\lambda)^*$  the assertion of Lemma 3.2 follows.  $\square$

From now on for the rest of this section we will assume that the deficiency indices  $n_+(A) = n_-(A)$  of the symmetric operator  $A$  are finite,  $n_\pm(A) < \infty$ . In this case the dimension of the Hilbert space  $\mathcal{H}$  in the boundary triplet  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  is also finite and coincides with the number  $n_\pm(A)$ . Let again  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$  and  $J$ ,  $B$  and  $C$  as in (3.2) and (3.3), respectively. Then the operators  $BJ$  and  $C$  are finite dimensional and hence the linear manifold

$$\mathcal{M} := \text{span} \{ \text{ran}(P^{ac}(A_0)J^*B^*), \text{ran}(P^{ac}(A_0)C^*) \} \subseteq \mathfrak{H}^{ac}(A_0) \quad (3.8)$$

is finite dimensional. Therefore there is a spectral core  $\Delta_0 \subseteq \sigma_{ac}(A_0)$  of the operator  $A_0^{ac} := A_0 \upharpoonright \mathfrak{H}^{ac}(A_0)$  such that  $\mathcal{M}$  is a spectral manifold, cf. Appendix A. The spectral measure of  $A_0$  will be denoted by  $E_0$ . We equip  $\mathcal{M}$  with the semi-scalar products

$$(f, g)_{E_0, \lambda} = \frac{d}{d\lambda} (E_0(\lambda)f, g), \quad \lambda \in \Delta_0, \quad f, g \in \mathcal{M},$$

and define the finite dimensional Hilbert spaces  $\widehat{\mathcal{M}}_\lambda$  by

$$\widehat{\mathcal{M}}_\lambda := \mathcal{M} / \ker(\|\cdot\|_{E_0, \lambda}), \quad \lambda \in \Delta_0, \quad (3.9)$$

where  $\|\cdot\|_{E_0, \lambda}$  is the semi-norm induced by the semi-scalar product  $(\cdot, \cdot)_{E_0, \lambda}$ , see Appendix A. Further, in accordance with Appendix A we introduce the linear subset  $\mathcal{D}_\lambda \subseteq \mathfrak{H}^{ac}(A_0)$ ,  $\lambda \in \mathbb{R}$ , with the semi-norm  $[\cdot]_{E_0, \lambda}$  given by (A.2). By factorization and completion of  $\mathcal{D}_\lambda$  with respect to the semi-norm  $[\cdot]_{E_0, \lambda}$  we obtain the Banach space

$$\widehat{\mathcal{D}}_\lambda := \text{clo}_{[\cdot]_{E_0, \lambda}}(\mathcal{D}_\lambda / \ker([\cdot]_{E_0, \lambda})), \quad \lambda \in \mathbb{R},$$

where  $\text{clo}_{[\cdot]_{E_0, \lambda}}$  denotes the completion with respect to  $[\cdot]_{E_0, \lambda}$ . By  $D_\lambda : \mathcal{D}_\lambda \rightarrow \widehat{\mathcal{D}}_\lambda$  we denote the canonical embedding operator. From  $\mathcal{M} \subseteq \mathcal{D}_\lambda$ ,  $\lambda \in \Delta_0$ , we have  $D_\lambda \mathcal{M} \subseteq \widehat{\mathcal{D}}_\lambda$ . Moreover, since  $\mathcal{M}$  is a spectral manifold  $D_\lambda \mathcal{M}$  coincides with the Hilbert space  $\widehat{\mathcal{M}}_\lambda$  for every  $\lambda \in \Delta_0$ , cf. Appendix A.

Following [6, §18.1.4] we introduce the linear operators  $F_{BJ}(\lambda)$  and  $F_C(\lambda)$  for every  $\lambda \in \Delta_0$  by

$$F_{BJ}(\lambda) := D_\lambda P^{ac}(A_0) J^* B^* \in [\mathcal{H}, \widehat{\mathcal{M}}_\lambda] \quad (3.10)$$

and

$$F_C(\lambda) := D_\lambda P^{ac}(A_0) C^* \in [\mathcal{H}, \widehat{\mathcal{M}}_\lambda].$$

**Lemma 3.3** *Let  $A$  be a densely defined closed symmetric operator with finite deficiency indices in the separable Hilbert space  $\mathfrak{H}$ , let  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  be a boundary triplet for  $A^*$  and let  $M(\cdot)$  be the corresponding Weyl function. Further, let  $A_\Theta = A^* \upharpoonright \ker(\Gamma_\Theta)$  and let  $A_\Theta = A^* \upharpoonright \Gamma^{-1}\Theta$ ,  $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$ , be a selfadjoint extension of  $A$ . Then*

$$F_{BJ}(\lambda) = -F_C(\lambda) \left\{ \frac{1}{\lambda + i} \Im(\Theta - M(i))^{-1} + \frac{1}{1 + \lambda^2} (\Theta - M(i))^{-1} \right\}$$

and  $\widehat{\mathcal{M}}_\lambda = \text{ran } F_C(\lambda)$  holds for all  $\lambda \in \Delta_0$ .

**Proof.** Inserting  $J$  from (3.2) into (3.10) we find

$$F_{BJ}(\lambda) = -D_\lambda P^{ac}(A_0)(A_0 + i)^{-1}(A_\Theta + i)^{-1}B^*.$$

For  $f \in \mathfrak{H}^{ac}(A_0)$  Lemma A.3 implies  $D_\lambda(A_0 + i)^{-1}f = (\lambda + i)^{-1}D_\lambda f$  and therefore

$$\begin{aligned} F_{BJ}(\lambda) &= -(\lambda + i)^{-1}D_\lambda P^{ac}(A_0)(A_\Theta + i)^{-1}B^* \\ &= -(\lambda + i)^{-1}D_\lambda P^{ac}(A_0)((A_\Theta + i)^{-1} - (A_0 + i)^{-1})B^* \\ &\quad - (\lambda + i)^{-1}D_\lambda P^{ac}(A_0)(A_0 + i)^{-1}B^*. \end{aligned} \quad (3.11)$$

By (2.5) we have  $2i\gamma(i)^*\gamma(i) = M(i) - M(-i)$ . Taking this identity into account we obtain from (3.5), (3.6) and (3.7)

$$\begin{aligned} &((A_\Theta + i)^{-1} - (A_0 + i)^{-1})B^* \\ &= \gamma(-i)(\Theta - M(-i))^{-1}\gamma(i)^*\gamma(i)(\Theta - M(i))^{-1} \\ &= C^*(\Theta - M(-i))^{-1}\Im(M(i))(\Theta - M(i))^{-1} \\ &= C^*\Im(\Theta - M(i))^{-1}. \end{aligned} \quad (3.12)$$

On the other hand, by (2.4) we have  $\gamma(i) = (A_0 + i)(A_0 - i)^{-1}\gamma(-i)$  and this identity combined with (3.7) and (3.6) yields

$$B^* = (A_0 + i)(A_0 - i)^{-1}C^*(\Theta - M(i))^{-1}. \quad (3.13)$$

Inserting (3.12) and (3.13) into (3.11) and making use of (3.7), Lemma A.3 and the definition of  $F_C(\lambda)$  we obtain

$$\begin{aligned} F_{BJ}(\lambda) &= -(\lambda + i)^{-1}D_\lambda P^{ac}(A_0)C^* \Im(\Theta - M(i))^{-1} \\ &\quad - (\lambda^2 + 1)^{-1}D_\lambda P^{ac}(A_0)C^*(\Theta - M(i))^{-1} \\ &= -F_C(\lambda) \left\{ \frac{1}{\lambda + i} \Im(\Theta - M(i))^{-1} + \frac{1}{1 + \lambda^2} (\Theta - M(i))^{-1} \right\} \end{aligned}$$

for all  $\lambda \in \Delta_0$ . Therefore  $\text{ran } F_{BJ}(\lambda) \subseteq \text{ran } F_C(\lambda)$  and it follows that  $\widehat{\mathcal{M}}_\lambda$  coincides with  $\text{ran } F_C(\lambda)$ ,  $\lambda \in \Delta_0$ . This completes the proof of Lemma 3.3.  $\square$

In the next lemma we show that the spectral manifold  $\mathcal{M}$  defined by (3.8) is generating with respect to  $A_0^{ac}$  if the symmetric operator  $A$  is assumed to be simple (cf. Section 2.1 and (A.1)). The set of all Borel subsets of the real axis is denoted by  $\mathcal{B}(\mathbb{R})$ .

**Lemma 3.4** *Let  $A$  be a densely defined closed symmetric operator in the separable Hilbert space  $\mathfrak{H}$  and let  $A_0$  be a selfadjoint extension of  $A$  with spectral measure  $E_0(\cdot)$ . If  $A$  is simple, then the condition*

$$\mathfrak{H}^{ac}(A_0) = \text{cspan}\{E_0(\Delta)f : \Delta \in \mathcal{B}(\mathbb{R}), f \in \mathcal{M}\} \quad (3.14)$$

is satisfied.

**Proof.** Since  $A$  is assumed to be simple we have  $\mathfrak{H} = \text{cspan}\{\mathcal{N}_\lambda : \lambda \in \mathbb{C} \setminus \mathbb{R}\}$ , where  $\mathcal{N}_\lambda = \ker(A^* - \lambda)$ . Hence  $\mathfrak{H}^{ac}(A_0) = \text{cspan}\{P^{ac}(A_0)\mathcal{N}_\lambda : \lambda \in \mathbb{C} \setminus \mathbb{R}\}$ . From  $C^* = \gamma(-i)$  we find  $P^{ac}(A_0)\mathcal{N}_{-i} \subset \mathcal{M}$  and by (2.4) we have

$$\mathcal{N}_\lambda = (A_0 + i)(A_0 - \lambda)^{-1}\mathcal{N}_{-i}$$

which yields

$$\mathcal{N}_\lambda \subseteq \text{cspan}\{E_0(\Delta)\text{ran}(C^*) : \Delta \in \mathcal{B}(\mathbb{R})\}$$

for  $\lambda \in \mathbb{C} \setminus \mathbb{R}$ . Therefore

$$P^{ac}(A_0)\mathcal{N}_\lambda \subseteq \text{cspan}\{E_0(\Delta)P^{ac}(A_0)\text{ran}(C^*) : \Delta \in \mathcal{B}(\mathbb{R})\} \subseteq \mathfrak{H}^{ac}(A_0)$$

for  $\lambda \in \mathbb{C} \setminus \mathbb{R}$ . Since  $\mathfrak{H}^{ac}(A_0) = \text{cspan}\{P^{ac}(A_0)\mathcal{N}_\lambda : \lambda \in \mathbb{C} \setminus \mathbb{R}\}$  holds we find

$$\mathfrak{H}^{ac}(A_0) = \text{cspan}\{E_0(\Delta)P^{ac}(A_0)\text{ran}(C^*) : \Delta \in \mathcal{B}(\mathbb{R})\}$$

which proves relation (3.14).  $\square$

In accordance with Appendix A we can perform a direct integral representation  $L^2(\Delta_0, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})$  of  $\mathfrak{H}^{ac}(A_0)$  with respect to the absolutely continuous part  $A_0^{ac}$  of

$A_0$ , where  $\widehat{\mathcal{M}}_\lambda$ ,  $\lambda \in \Delta_0$ , is defined by (3.9),  $\mu_L$  is the Lebesgue measure and  $\mathcal{S}_\mathcal{M}$  is the admissible system from Lemma A.2. We recall that in this representation  $A_0^{ac}$  is unitarily equivalent to the multiplication operator  $M$ ,

$$(M\widehat{f})(\lambda) := \lambda\widehat{f}(\lambda), \quad \widehat{f} \in \text{dom}(M),$$

where

$$\text{dom}(M) := \{\widehat{f} \in L^2(\Delta_0, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M}) : \lambda \mapsto \lambda\widehat{f}(\lambda) \in L^2(\Delta_0, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})\}.$$

Since the scattering operator  $S_\Theta$  (see (3.1)) of the scattering system  $\{A_\Theta, A_0\}$  commutes with  $A_0$  and  $A_0^{ac}$  Proposition 9.57 of [6] implies that there exists a family  $\{\widehat{S}_\Theta(\lambda)\}_{\lambda \in \Delta_0}$  of unitary operators in  $\{\widehat{\mathcal{M}}_\lambda\}_{\lambda \in \Delta_0}$  such that the scattering operator  $S_\Theta$  is unitarily equivalent to the multiplication operator  $\widehat{S}_\Theta$  induced by this family in the Hilbert space  $L^2(\Delta_0, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})$ . We note that this family is determined up to a set of Lebesgue measure zero and is called the *scattering matrix*. The scattering matrix defines the *scattering amplitude*  $\{\widehat{T}_\Theta(\lambda)\}_{\lambda \in \Delta_0}$  by

$$\widehat{T}_\Theta(\lambda) := \widehat{S}_\Theta(\lambda) - I_{\widehat{\mathcal{M}}_\lambda}, \quad \lambda \in \Delta_0.$$

Obviously, the scattering amplitude induces a multiplication operator  $\widehat{T}_\Theta$  in the Hilbert space  $L^2(\Delta_0, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})$  which is unitarily equivalent to the *T-operator*

$$T_\Theta := S_\Theta - P^{ac}(A_0). \quad (3.15)$$

The scattering amplitude is also determined up to a set of Lebesgue measure zero. Making use of results from [6, §18] we calculate the scattering amplitude of  $\{A_\Theta, A_0\}$  in terms of the Weyl function  $M(\cdot)$  and the parameter  $\Theta$ . Recall that the limit  $M(\lambda + i0)$  exists for a.e.  $\lambda \in \mathbb{R}$ , cf. Section 2.2.

**Theorem 3.5** *Let  $A$  be a densely defined closed simple symmetric operator with finite deficiency indices in the separable Hilbert space  $\mathfrak{H}$ , let  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  be a boundary triplet for  $A^*$  and let  $M(\cdot)$  be the corresponding Weyl function. Further, let  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$  and let  $A_\Theta = A^* \upharpoonright \Gamma^{-1}\Theta$ ,  $\Theta \in \widetilde{\mathcal{C}}(\mathcal{H})$ , be a selfadjoint extension of  $A$ . Then  $L^2(\Delta_0, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})$  is a spectral representation of  $A_0^{ac}$  such that scattering amplitude  $\{\widehat{T}_\Theta(\lambda)\}_{\lambda \in \Delta_0}$  of the scattering system  $\{A_\Theta, A_0\}$  admits the representation*

$$\widehat{T}_\Theta(\lambda) = 2\pi i(1 + \lambda^2)F_C(\lambda)(\Theta - M(\lambda + i0))^{-1}F_C(\lambda)^* \in [\widehat{\mathcal{M}}_\lambda]$$

for a.e.  $\lambda \in \Delta_0$ .

**Proof.** Besides the scattering system  $\{A_\Theta, A_0\}$  and the corresponding scattering operator  $S_\Theta$  and  $T$ -operator  $T_\Theta$  defined in (3.1) and (3.15), respectively, we consider the scattering system  $\{A_\Theta, A_0, J\}$ , where  $J$  is defined by (3.2). The wave operators of  $\{A_\Theta, A_0, J\}$  are defined by

$$W_\pm(A_\Theta, A_0; J) := s\text{-}\lim_{t \rightarrow \pm\infty} e^{itA_\Theta} J e^{-itA_0} P^{ac}(A_0);$$

they exist and are complete since  $A$  has finite deficiency indices. Note that

$$\begin{aligned} W_\pm(A_\Theta, A_0; J) &= -(A_\Theta - i)^{-1} W_\pm(A_\Theta, A_0) (A_0 - i)^{-1} \\ &= -W_\pm(A_\Theta, A_0) (A_0 - i)^{-2} \end{aligned} \quad (3.16)$$

holds. The scattering operator  $S_J$  and the  $T$ -operator  $T_J$  of the scattering system  $\{A_\Theta, A_0; J\}$  are defined by

$$S_J := W_+(A_\Theta, A_0; J)^* W_-(A_\Theta, A_0; J)$$

and

$$\begin{aligned} T_J &:= S_J - W_+(A_\Theta, A_0; J)^* W_+(A_\Theta, A_0; J) \\ &= S_J - (I + A_0^2)^{-2} P^{ac}(A_0), \end{aligned} \quad (3.17)$$

respectively. The second equality in (3.17) follows from (3.16). Since the scattering operator  $S_\Theta$  commutes with  $A_0$  we obtain

$$S_J = (I + A_0^2)^{-2} S_\Theta \quad (3.18)$$

from (3.16). Note that  $S_J$  and  $T_J$  both commute with  $A_0$  and therefore by [6, Proposition 9.57] there are families  $\{\widehat{S}_J(\lambda)\}_{\lambda \in \Delta_0}$  and  $\{\widehat{T}_J(\lambda)\}_{\lambda \in \Delta_0}$  such that the operators  $S_J$  and  $T_J$  are unitarily equivalent to the multiplication operators  $\widehat{S}_J$  and  $\widehat{T}_J$  induced by these families in  $L^2(\Delta_0, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})$ . From (3.1) and (3.17) we obtain

$$\widehat{T}_\Theta(\lambda) = \widehat{S}_\Theta(\lambda) - I_{\widehat{\mathcal{M}}_\lambda} \quad \text{and} \quad \widehat{T}_J(\lambda) = \widehat{S}_J(\lambda) - \frac{1}{(1 + \lambda^2)^2} I_{\widehat{\mathcal{M}}_\lambda}$$

for  $\lambda \in \Delta_0$ . As (3.18) implies  $\widehat{S}_J(\lambda) = (1 + \lambda^2)^{-2} \widehat{S}_\Theta(\lambda)$ ,  $\lambda \in \Delta_0$ , we conclude

$$\widehat{T}_J(\lambda) = \frac{1}{(1 + \lambda^2)^2} \widehat{T}_\Theta(\lambda), \quad \lambda \in \Delta_0. \quad (3.19)$$

In order to apply [6, Corollary 18.9] we have to verify that

$$\lim_{\epsilon \rightarrow +0} B(A_\Theta - \lambda - i\epsilon)^{-1} B^* \quad (3.20)$$

exists for a.e.  $\lambda \in \Delta_0$  in the operator norm and that

$$s\text{-}\lim_{\delta \rightarrow +0} C((A_0 - \lambda - i\delta)^{-1} - (A_0 - \lambda + i\delta)^{-1}) f \quad (3.21)$$

exist for a.e.  $\lambda \in \Delta_0$  and all  $f \in \mathcal{M}$ , cf. [6, Theorem 18.7 and Remark 18.8], where  $C$  is given by (3.3). Since  $\mathcal{H}$  is a finite dimensional space it follows from [16, 18] that the (strong) limit

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

of the  $[\mathcal{H}]$ -valued Nevanlinna function  $\lambda \mapsto -(\Theta - M(\lambda))^{-1}$  exists for a.e.  $\lambda \in \Delta_0$ , cf. Section 2.2. Combining this fact with Lemma 3.2 we obtain that (3.20) holds. Condition (3.21) is fulfilled since  $C$  is a finite dimensional operator and  $\mathcal{M}$  is a finite dimensional linear manifold. Hence, by [6, Corollary 18.9] we have

$$\widehat{T}_J(\lambda) = 2\pi i \{ -F_{BJ}(\lambda) F_C(\lambda)^* + F_C(\lambda) B(A_\Theta - \lambda - i0)^{-1} B^* F_C(\lambda)^* \}$$

for a.e.  $\lambda \in \Delta_0$ . Making use of Lemma 3.3 and Lemma 3.2 we obtain

$$\begin{aligned} \widehat{T}_J(\lambda) &= 2\pi i F_C(\lambda) \left\{ \frac{1}{\lambda + i} \Im(\Theta - M(i))^{-1} + \frac{1}{1 + \lambda^2} (\Theta - M(i))^{-1} \right. \\ &\quad \left. + \frac{1}{1 + \lambda^2} ((\Theta - M(\lambda + i0))^{-1} - (\Theta - M(i))^{-1}) \right. \\ &\quad \left. - \frac{1}{\lambda + i} \Im(\Theta - M(i))^{-1} \right\} F_C(\lambda)^*. \end{aligned}$$

Combining this relation with (3.19) we conclude

$$\frac{1}{1+\lambda^2} \widehat{T}_\Theta(\lambda) = 2\pi i F_C(\lambda) (\Theta - M(\lambda + i0))^{-1} F_C(\lambda)^*$$

for a.e.  $\lambda \in \Delta_0$  which completes the proof.  $\square$

In the following we are going to replace the direct integral  $L^2(\Delta_0, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})$  by a more convenient one. To this end we prove the following lemma.

**Lemma 3.6** *Let  $A$  be a densely defined closed simple symmetric operator with 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  $M(\cdot)$ . Further, let  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ , let  $A_\Theta = A^* \upharpoonright \Gamma^{-1}\Theta$ ,  $\Theta \in \widehat{\mathcal{C}}(\mathcal{H})$ , be a selfadjoint extension of  $A$  and let  $\Delta_0$  be a spectral core of  $A_0^{ac}$  such that  $\mathcal{M}$  in (3.8) is a spectral manifold. Then*

$$F_C(\lambda)^* F_C(\lambda) = \frac{1}{\pi(1+\lambda^2)} \Im m(M(\lambda + i0)) \quad (3.22)$$

holds for a.e.  $\lambda \in \Delta_0$ .

**Proof.** Let  $B$  and  $C$  be as in (3.3) and let  $\Delta_0$  be a spectral core for  $A_0^{ac}$  such that  $\mathcal{M}$  defined by (3.8) is a spectral manifold. By definition of the operator  $D_\lambda$  we have

$$(F_C(\lambda)^* F_C(\lambda)u, v) = \frac{d}{d\lambda} (E_0(\lambda)C^*u, P^{ac}(A_0)C^*v), \quad u, v \in \mathcal{H},$$

for  $\lambda \in \Delta_0$ . It is not difficult to see that

$$\begin{aligned} (E_0(\delta)C^*u, P^{ac}(A_0)C^*v) &= \int_\delta \frac{d}{d\lambda} (E_0(\lambda)C^*u, P^{ac}(A_0)C^*v) d\mu_L(\lambda) \\ &= \int_\delta \frac{d}{d\lambda} (E_0(\lambda)C^*u, C^*v) d\mu_L(\lambda) \end{aligned}$$

holds for all  $u, v \in \mathcal{H}$  and any Borel set  $\delta \subseteq \mathbb{R}$ . Hence, we find

$$\frac{d}{d\lambda} (E_0(\lambda)C^*u, P^{ac}(A_0)C^*v) = \frac{d}{d\lambda} (E_0(\lambda)C^*u, C^*v)$$

for a.e.  $\lambda \in \Delta_0$  and  $u, v \in \mathcal{H}$ , which yields

$$\begin{aligned} &(F_C(\lambda)^* F_C(\lambda)u, v) \\ &= \lim_{\delta \rightarrow +0} \frac{1}{2\pi i} (\{(A_0 - \lambda - i\delta)^{-1} - (A_0 - \lambda + i\delta)^{-1}\} C^*u, C^*v) \end{aligned}$$

for a.e.  $\lambda \in \Delta_0$  and  $u, v \in \mathcal{H}$ . From  $C = \Gamma_1(A_0 - i)^{-1} = \gamma(-i)^*$  (see (3.3) and (3.7)) and the relation  $\Gamma_1(A_0 - \lambda)^{-1} = \gamma(\bar{\lambda})^*$ ,  $\lambda \in \mathbb{C} \setminus \mathbb{R}$ , we obtain

$$\begin{aligned} &C\{(A_0 - \lambda - i\delta)^{-1} - (A_0 - \lambda + i\delta)^{-1}\}C^* \\ &= \frac{1}{i - \lambda - i\delta} \{\gamma(-i)^*\gamma(-i) - \gamma(\lambda - i\delta)^*\gamma(-i)\} \\ &\quad - \frac{1}{i - \lambda + i\delta} \{\gamma(-i)^*\gamma(-i) - \gamma(\lambda + i\delta)^*\gamma(-i)\}. \end{aligned}$$



With the help of (2.5) it follows that the right hand side can be written as

$$\begin{aligned} & \frac{1}{i - \lambda - i\delta} \left\{ \Im m (M(i)) + \frac{M(-i) - M(\lambda + i\delta)}{i + \lambda + i\delta} \right\} \\ & - \frac{1}{i - \lambda + i\delta} \left\{ \Im m (M(i)) + \frac{M(-i) - M(\lambda - i\delta)}{i + \lambda - i\delta} \right\} \end{aligned}$$

and we conclude

$$(F_C(\lambda)^* F_C(\lambda) u, v) = \frac{1}{2\pi i} \frac{1}{1 + \lambda^2} ((M(\lambda + i0) - M(\lambda - i0)) u, v)$$

for a.e.  $\lambda \in \Delta_0$  and  $u, v \in \mathcal{H}$  which immediately yields (3.22).  $\square$

In order to formulate the main result we introduce the usual Hilbert spaces  $L^2(\Delta_0, \mu_L, \mathcal{H})$  and  $L^2(\mathbb{R}, \mu_L, \mathcal{H})$  of square integrable  $\mathcal{H}$ -valued functions on the spectral core  $\Delta_0$  of  $A_0^{ac}$  and on  $\mathbb{R}$ , respectively. Note that  $L^2(\Delta_0, \mu_L, \mathcal{H})$  is subspace of  $L^2(\mathbb{R}, \mu_L, \mathcal{H})$ . Let us define the family  $\{\mathcal{H}_\lambda\}_{\lambda \in \Lambda^M}$  of Hilbert spaces  $\mathcal{H}_\lambda$  by

$$\mathcal{H}_\lambda := \text{ran} (\Im m (M(\lambda + i0))) \subseteq \mathcal{H}, \quad \lambda \in \Lambda^M,$$

where  $M(\lambda + i0) = \lim_{\epsilon \rightarrow 0} M(\lambda + i\epsilon)$  and

$$\Lambda^M := \{\lambda \in \mathbb{R} : M(\lambda + i0) \text{ exists}\}.$$

We note that  $\mathcal{H}_\lambda = \{0\}$  is quite possible and we recall that  $\mathbb{R} \setminus \Lambda^M$  has Lebesgue measure zero. By  $\{Q(\lambda)\}_{\lambda \in \Lambda^M}$  we denote the family of orthogonal projections from  $\mathcal{H}$  onto  $\mathcal{H}_\lambda$ . One easily verifies that the family  $\{Q(\lambda)\}_{\lambda \in \Lambda^M}$  is measurable. This family induces an orthogonal projection  $Q_0$ ,

$$(Q_0 f)(\lambda) := Q(\lambda) f(\lambda), \quad \text{for a.e. } \lambda \in \Delta_0, \quad f \in L^2(\Delta_0, \mu_L, \mathcal{H}),$$

in  $L^2(\Delta_0, \mu_L, \mathcal{H})$ . The range of the projection  $Q_0$  is denoted by  $L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda)$ . Similarly, the family  $\{Q(\lambda)\}_{\lambda \in \Lambda^M}$  induces an orthogonal projection  $Q$  in  $L^2(\mathbb{R}, \mu_L, \mathcal{H})$ , the range of  $Q$  is denoted by  $L^2(\mathbb{R}, \mu_L, \mathcal{H}_\lambda)$ . We note that  $L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda) \subseteq L^2(\mathbb{R}, \mu_L, \mathcal{H}_\lambda)$  holds.

**Lemma 3.7** *Let  $A$  be a densely defined closed simple symmetric operator with finite deficiency indices in the separable Hilbert space  $\mathfrak{H}$ , let  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  be a boundary triplet for  $A^*$ ,  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ , and let  $M(\cdot)$  be the corresponding Weyl function. If the Borel set  $\Delta_0 \subseteq \sigma_{ac}(A_0)$  is a spectral core of  $A_0^{ac}$ , then  $L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda) = L^2(\mathbb{R}, \mu_L, \mathcal{H}_\lambda)$ .*

**Proof.** Define the set  $\Lambda_0^M$  by

$$\Lambda_0^M := \{\lambda \in \Lambda^M : \mathcal{H}_\lambda \neq \{0\}\}. \quad (3.23)$$

Then we have to verify that  $\mu_L(\Lambda_0^M \setminus \Delta_0) = 0$  holds. From (2.5) we obtain

$$\Im m (M(\lambda)) = \Im m (\lambda) \gamma(\lambda)^* \gamma(\lambda), \quad \lambda \in \mathbb{C}_+.$$

and from (2.4) we conclude that  $\Im m (M(\lambda))$  coincides with

$$\Im m (\lambda) \gamma(i)^* \{I + (\bar{\lambda} + i)(A_0 - \bar{\lambda})^{-1}\} \{I + (\lambda - i)(A_0 - \lambda)^{-1}\} \gamma(i).$$

Hence we have

$$\Im(M(\lambda)) = \Im(\lambda)\gamma(i)^*(A_0 + i)(A_0 - \bar{\lambda})^{-1}(A_0 - i)(A_0 - \lambda)^{-1}\gamma(i)$$

for  $\lambda \in \mathbb{C}_+$  and if  $\lambda$  tends to  $\mathbb{R}$  from the upper half-plan we get

$$\Im(M(\lambda)) = \pi(1 + \lambda^2) \frac{\gamma(i)^* E_0(d\lambda)\gamma(i)}{d\lambda}$$

for a.e.  $\lambda \in \mathbb{R}$ . Here  $E_0(\cdot)$  is the spectral measure of  $A_0$ . Hence for any bounded Borel set  $\delta \in \mathcal{B}(\mathbb{R})$  we obtain

$$\int_{\delta} \frac{1}{1 + \lambda^2} \Im(M(\lambda)) d\mu_L(\lambda) = \pi\gamma(i)^* E_0^{ac}(\delta)\gamma(i).$$

Since  $\Delta_0$  is a spectral core of  $A_0^{ac}$  one has  $E_0^{ac}(\Delta_0) = E_0^{ac}(\mathbb{R})$  which implies  $E_0^{ac}(\mathbb{R} \setminus \Delta_0) = 0$  and therefore

$$\int_{\mathbb{R} \setminus \Delta_0} \frac{1}{1 + \lambda^2} \Im(M(\lambda)) d\mu_L(\lambda) = 0.$$

Hence we have  $\Im(M(\lambda)) = 0$  for a.e.  $\lambda \in \mathbb{R} \setminus \Delta_0$  and thus  $\mathcal{H}_\lambda = \{0\}$  for a.e.  $\lambda \in \mathbb{R} \setminus \Delta_0$ . Consequently  $\mu_L(\Lambda_0^M \setminus \Delta_0) = 0$  and Lemma 3.7 is proved.  $\square$

We note that the so-called absolutely continuous closure  $\text{cl}_{ac}(\Lambda_0^M)$  of the set  $\Lambda_0^M$  (see (3.23)),

$$\text{cl}_{ac}(\Lambda_0^M) := \{x \in \mathbb{R} : \mu_L((x - \epsilon, x + \epsilon) \cap \Lambda_0^M) > 0 \quad \forall \epsilon > 0\},$$

coincides with the absolutely continuous spectrum  $\sigma_{ac}(A_0)$  of  $A_0$ , cf. [11, Proposition 4.2].

The following theorem is the main result of this section, we calculate the scattering matrix of  $\{A_\Theta, A_0\}$  in terms of the Weyl function  $M(\cdot)$  and the parameter  $\Theta$  in the direct integral  $L^2(\mathbb{R}, \mu_L, \mathcal{H}_\lambda)$ .

**Theorem 3.8** *Let  $A$  be a densely defined closed simple symmetric operator with 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  $M(\cdot)$ . Further, let  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$  and let  $A_\Theta = A^* \upharpoonright \Gamma^{-1}\Theta$ ,  $\Theta \in \tilde{\mathcal{C}}(\mathcal{H})$ , be a selfadjoint extension of  $A$ . Then  $L^2(\mathbb{R}, \mu_L, \mathcal{H}_\lambda)$  performs a spectral representation of  $A_0^{ac}$  such that the scattering matrix  $\{S_\Theta(\lambda)\}_{\lambda \in \mathbb{R}}$  of the scattering system  $\{A_\Theta, A_0\}$  admits the representation*

$$S_\Theta(\lambda) = I_{\mathcal{H}_\lambda} + 2i\sqrt{\Im(M(\lambda))}(\Theta - M(\lambda))^{-1}\sqrt{\Im(M(\lambda))} \in [\mathcal{H}_\lambda] \quad (3.24)$$

for a.e.  $\lambda \in \mathbb{R}$ , where  $M(\lambda) := M(\lambda + i0)$  and  $\mathcal{H}_\lambda := \text{ran}(\Im(M(\lambda)))$ .

**Proof.** From the polar decomposition of  $F_C(\lambda) \in [\mathcal{H}, \widehat{\mathcal{M}}_\lambda]$  we obtain a family of partial isometries  $V(\lambda) \in [\widehat{\mathcal{M}}_\lambda, \mathcal{H}]$  defined for a.e.  $\lambda \in \Delta_0$  which map  $\widehat{\mathcal{M}}_\lambda = \text{ran } F_C(\lambda)$  isometrically onto  $\mathcal{H}_\lambda$  such that

$$V(\lambda)F_C(\lambda) = \frac{1}{\sqrt{\pi(1 + \lambda^2)}} \sqrt{\Im(M(\lambda + i0))}$$

holds for a.e.  $\lambda \in \Delta_0$ . Let us introduce the admissible system

$$\mathcal{S} := \left\{ \sum_{l=1}^n \alpha_l(\lambda) V(\lambda) J_\lambda f_l \mid f_l \in \mathcal{M}, \alpha_l \in L^\infty(\Delta_0, \mu_L), n \in \mathbb{N} \right\} \subseteq X_{\lambda \in \Delta_0} \widehat{\mathcal{H}}_\lambda.$$

Since  $V\mathcal{S}_\mathcal{M} = \mathcal{S}$  one easily verifies that the operator

$$V : L^2(\Delta_0, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M}) \longrightarrow L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda, \mathcal{S}),$$

$$(V\widehat{f})(\lambda) := V(\lambda)\widehat{f}(\lambda), \quad \lambda \in \Delta_0,$$

defines an isometry acting from  $L^2(\Delta_0, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})$  onto  $L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda, \mathcal{S})$  such that the multiplication operators induced by the independent variable in  $L^2(\Delta_0, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})$  and  $L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda, \mathcal{S})$  are unitarily equivalent. Hence  $L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda, \mathcal{S})$  is a spectral representation of  $A_0^{qc}$ , too. In the spectral representation  $L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda, \mathcal{S})$  the operator  $T_\Theta = S_\Theta - P^{ac}(A_0)$  is unitarily equivalent to the multiplication operator induced by  $\{T_\Theta(\lambda)\}_{\lambda \in \Delta_0}$ ,

$$T_\Theta(\lambda) = V(\lambda)\widehat{T}_\Theta(\lambda)V(\lambda)^*, \quad \lambda \in \Delta_0,$$

in  $L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda, \mathcal{S})$ . Using Theorem 3.5 and Lemma 3.6 we find the representation

$$T_\Theta(\lambda) = 2i\sqrt{\Im m(M(\lambda + i0))}(\Theta - M(\lambda + i0))^{-1}\sqrt{\Im m(M(\lambda + i0))}$$

for a.e.  $\lambda \in \Delta_0$  and therefore the scattering matrix  $\{S_\Theta(\lambda)\}_{\lambda \in \Delta_0}$  has the form (3.24).

A straightforward computation shows that the direct integral  $L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda, \mathcal{S})$  is equal to the subspace  $L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda) \subseteq L^2(\Delta_0, \mu_L, \mathcal{H})$ . Taking into account Lemma 3.7 we find  $L^2(\Delta_0, \mu_L, \mathcal{H}_\lambda, \mathcal{S}) = L^2(\mathbb{R}, \mu_L, \mathcal{H}_\lambda)$  which shows that  $L^2(\mathbb{R}, \mu_L, \mathcal{H}_\lambda)$  performs a spectral representation of  $A_0^{qc}$  such that the scattering matrix is given by (3.24).  $\square$

**Remark 3.9** Note that the scattering matrix  $\{S_\Theta(\lambda)\}$  in (3.24) is defined for a.e.  $\lambda \in \mathbb{R}$  and not only on a spectral core of  $A_0$ . In particular, if  $\Im m(M(\lambda)) = 0$  for some  $\lambda \in \mathbb{R}$ , then  $\mathcal{H}_\lambda = \{0\}$  and  $S_\Theta(\lambda) = I_{\{0\}}$ . In this case we set  $\det S_\Theta(\lambda) = 1$ .

**Corollary 3.10** *Let  $A, \Pi, A_0$  and  $A_\Theta$  be as in Theorem 3.8 and assume, in addition, that the Weyl function  $M(\cdot)$  is of scalar type, i.e.  $M(\cdot) = m(\cdot)I_\mathcal{H}$  with a scalar Nevanlinna function  $m(\cdot)$ . Then  $L^2(\mathbb{R}, \mu_L, \mathcal{H}_\lambda)$  performs a spectral representation of  $A_0^{qc}$  such that the scattering matrix  $\{S_\Theta(\lambda)\}_{\lambda \in \mathbb{R}}$  of the scattering system  $\{A_\Theta, A_0\}$  admits the representation*

$$S_\Theta(\lambda) = I_{\mathcal{H}_\lambda} + 2i\Im m(m(\lambda))(\Theta - m(\lambda) \cdot I_\mathcal{H})^{-1} \in [\mathcal{H}_\lambda]$$

for a.e.  $\lambda \in \mathbb{R}$ . Here  $\mathcal{H}_\lambda = \mathcal{H}$  if  $\Im m(m(\lambda)) \neq 0$  and  $\mathcal{H}_\lambda = \{0\}$  otherwise. If, in addition  $\Theta \in [\mathcal{H}]$ , then

$$S_\Theta(\lambda) = (\Theta - \overline{m(\lambda)} \cdot I_\mathcal{H})(\Theta - m(\lambda) \cdot I_\mathcal{H})^{-1}. \quad (3.25)$$

for a.e.  $\lambda \in \mathbb{R}$  with  $\Im m(m(\lambda)) \neq 0$ .

**Remark 3.11** It follows from (3.24) that if  $\Theta \in [\mathcal{H}]$ , then the scattering matrix  $\{S_\Theta(\lambda)\}$  admits the representation

$$S_\Theta(\lambda) = (\Im m(M(\lambda)))^{-1/2} S(\lambda) (\Im m(M(\lambda)))^{1/2} \in [\mathcal{H}_\lambda] \quad (3.26)$$

for a.e.  $\lambda \in \mathbb{R}$  with  $\Im m(M(\lambda)) \neq 0$ , where

$$S(\lambda) := (\Theta - M(\lambda - i0))(\Theta - M(\lambda + i0))^{-1}. \quad (3.27)$$

Here the operator  $(\Im m(M(\lambda)))^{-1/2}$  is well defined in  $\mathcal{H}_\lambda$  for a.e.  $\lambda \in \mathbb{R}$ . It is worth to note that the first (second) factor of  $S(\cdot)$  admits a holomorphic continuation to the lower (resp. upper) half-plane.

If the Weyl function  $M(\cdot) = m(\cdot)I_{\mathcal{H}}$  is of scalar type and  $\Theta \in [\mathcal{H}]$ , then we have  $S_\Theta(\lambda) = S(\lambda)$  and relations (3.26) and (3.27) turn into (3.25). In this case  $S_\Theta(\cdot)$  itself can be factorized such that both factors can be continued holomorphically in  $\mathbb{C}_-$  and  $\mathbb{C}_+$ , respectively.

## 4 Spectral shift function

M.G. Krein's spectral shift function introduced in [27] is an important tool in the spectral and perturbation theory of self-adjoint operators, in particular scattering theory. A detailed review on the spectral shift function can be found in e.g. [9, 10]. Furthermore we mention [20, 21, 22] as some recent papers on the spectral shift function and its various applications.

Recall that for any pair of selfadjoint operators  $H_1, H_0$  in a separable Hilbert space  $\mathfrak{H}$  such that the resolvents differ by a trace class operator,

$$(H_1 - \lambda)^{-1} - (H_0 - \lambda)^{-1} \in \mathfrak{S}_1(\mathfrak{H}) \quad (4.1)$$

for some (and hence for all)  $\lambda \in \rho(H_1) \cap \rho(H_0)$ , there exists a real valued function  $\xi(\cdot) \in L^1_{loc}(\mathbb{R})$  satisfying the conditions

$$\mathrm{tr}((H_1 - \lambda)^{-1} - (H_0 - \lambda)^{-1}) = - \int_{\mathbb{R}} \frac{1}{(t - \lambda)^2} \xi(t) dt, \quad (4.2)$$

$\lambda \in \rho(H_1) \cap \rho(H_0)$ , and

$$\int_{\mathbb{R}} \frac{1}{1 + t^2} \xi(t) dt < \infty, \quad (4.3)$$

cf. [9, 10, 27]. Such a function  $\xi$  is called a *spectral shift function* of the pair  $\{H_1, H_0\}$ . We emphasize that  $\xi$  is not unique, since simultaneously with  $\xi$  a function  $\xi + c$ ,  $c \in \mathbb{R}$ , also satisfies both conditions (4.2) and (4.3). Note that the converse also holds, namely, any two spectral shift functions for a pair of selfadjoint operators  $\{H_1, H_0\}$  satisfying (4.1) differ by a real constant. We remark that (4.2) is a special case of the general formula

$$\mathrm{tr}(\phi(H_1) - \phi(H_0)) = \int_{\mathbb{R}} \phi'(t) \xi(t) dt, \quad (4.4)$$

which is valid for a wide class of smooth functions. A very large class of such functions  $\phi(\cdot)$  has been described in terms of the Besov classes by V.V. Peller in [31].

In Theorem 4.1 below we find a representation for the spectral shift function  $\xi_\Theta$  of a pair of selfadjoint operators  $A_\Theta$  and  $A_0$  which are both assumed to be extensions of a densely defined closed simple symmetric operator  $A$  with finite deficiency indices. For that purpose we use the definition

$$\log(T) := -i \int_0^\infty ((T + it)^{-1} - (1 + it)^{-1}I_{\mathcal{H}}) dt \quad (4.5)$$

for an operator  $T$  on a finite dimensional Hilbert space  $\mathcal{H}$  satisfying  $\Im m(T) \geq 0$  and  $0 \notin \sigma(T)$ , see e.g. [20, 32]. A straightforward calculation shows that the relation

$$\det(T) = \exp(\operatorname{tr}(\log(T))) \quad (4.6)$$

holds. Next we choose a special spectral shift function  $\xi_\Theta$  for the pair  $\{A_\Theta, A_0\}$  in terms of the Weyl function  $M$  and the parameter  $\Theta$ , see also [28] for the case of defect one. Making use of Theorem 3.8 we give a simple proof of the Birman-Krein formula, cf. [8].

**Theorem 4.1** *Let  $A$  be a densely defined closed simple symmetric operator in the separable Hilbert space  $\mathfrak{H}$  with finite deficiency indices  $n_\pm(A) = n$ , let  $\Pi = \{\mathcal{H}, \Gamma_0, \Gamma_1\}$  be a boundary triplet for  $A^*$  and let  $M(\cdot)$  be the corresponding Weyl function. Further, let  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$  and let  $A_\Theta = A^* \upharpoonright \Gamma^{-1}\Theta$ ,  $\Theta \in [\mathcal{H}]$ , be a selfadjoint extension of  $A$ . Then the following holds:*

- (i) *The limit  $\lim_{\epsilon \rightarrow +0} \log(M(\lambda + i\epsilon) - \Theta)$  exists for a.e.  $\lambda \in \mathbb{R}$  and the function*

$$\xi_\Theta(\lambda) := \frac{1}{\pi} \Im m(\operatorname{tr}(\log(M(\lambda + i0) - \Theta))) \quad \text{for a.e. } \lambda \in \mathbb{R} \quad (4.7)$$

*is a spectral shift function for the pair  $\{A_\Theta, A_0\}$  with  $0 \leq \xi_\Theta(\lambda) \leq n$ .*

- (ii) *The scattering matrix  $\{S_\Theta(\lambda)\}_{\lambda \in \mathbb{R}}$  of the pair  $\{A_\Theta, A_0\}$  and the spectral shift function  $\xi_\Theta$  in (4.7) are connected via the Birman-Krein formula*

$$\det S_\Theta(\lambda) = \exp(-2\pi i \xi_\Theta(\lambda)) \quad (4.8)$$

*for a.e.  $\lambda \in \mathbb{R}$  (cf. Remark 3.9).*

**Proof.** (i) Since  $\lambda \mapsto M(\lambda) - \Theta$  is a Nevanlinna function with values in  $[\mathcal{H}]$  and  $0 \in \rho(\Im m(M(\lambda)))$  for all  $\lambda \in \mathbb{C}_+$ , it follows that  $\log(M(\lambda) - \Theta)$  is well-defined for all  $\lambda \in \mathbb{C}_+$  by (4.5). According to [20, Lemma 2.8] the function  $\lambda \mapsto \log(M(\lambda) - \Theta)$ ,  $\lambda \in \mathbb{C}_+$ , is a  $[\mathcal{H}]$ -valued Nevanlinna function such that

$$0 \leq \Im m(\log(M(\lambda) - \Theta)) \leq \pi I_{\mathcal{H}}$$

holds for all  $\lambda \in \mathbb{C}_+$ . Hence the limit  $\lim_{\epsilon \rightarrow +0} \log(M(\lambda + i\epsilon) - \Theta)$  exists for a.e.  $\lambda \in \mathbb{R}$  (see [16, 18] and Section 2.2) and  $\lambda \mapsto \operatorname{tr}(\log(M(\lambda) - \Theta))$ ,  $\lambda \in \mathbb{C}_+$ , is a scalar Nevanlinna function with the property

$$0 \leq \Im m(\operatorname{tr}(\log(M(\lambda) - \Theta))) \leq n\pi, \quad \lambda \in \mathbb{C}_+,$$

that is, the function  $\xi_\Theta$  in (4.7) satisfies  $0 \leq \xi_\Theta(\lambda) \leq n$  for a.e.  $\lambda \in \mathbb{R}$ .

In order to show that (4.2) holds with  $H_1, H_0$  and  $\xi$  replaced by  $A_\Theta, A_0$  and  $\xi_\Theta$ , respectively, we first verify that the relation

$$\frac{d}{d\lambda} \operatorname{tr}(\log(M(\lambda) - \Theta)) = \operatorname{tr} \left( (M(\lambda) - \Theta)^{-1} \frac{d}{d\lambda} M(\lambda) \right) \quad (4.9)$$

is true for all  $\lambda \in \mathbb{C}_+$ . Indeed, for  $\lambda \in \mathbb{C}_+$  we have

$$\log(M(\lambda) - \Theta) = -i \int_0^\infty ((M(\lambda) - \Theta + it)^{-1} - (1 + it)^{-1} I_{\mathcal{H}}) dt$$

by (4.5) and this yields

$$\frac{d}{d\lambda} \log(M(\lambda) - \Theta) = i \int_0^\infty (M(\lambda) - \Theta + it)^{-1} \left( \frac{d}{d\lambda} M(\lambda) \right) (M(\lambda) - \Theta + it)^{-1} dt.$$

Hence we obtain

$$\frac{d}{d\lambda} \operatorname{tr}(\log(M(\lambda) - \Theta)) = i \int_0^\infty \operatorname{tr} \left( (M(\lambda) - \Theta + it)^{-2} \frac{d}{d\lambda} M(\lambda) \right) dt$$

and since  $\frac{d}{dt}(M(\lambda) - \Theta + it)^{-1} = -i(M(\lambda) - \Theta + it)^{-2}$  for  $t \in (0, \infty)$  we conclude

$$\frac{d}{d\lambda} \operatorname{tr}(\log(M(\lambda) - \Theta)) = - \int_0^\infty \frac{d}{dt} \operatorname{tr} \left( (M(\lambda) - \Theta + it)^{-1} \frac{d}{d\lambda} M(\lambda) \right) dt$$

for all  $\lambda \in \mathbb{C}_+$ , that is, relation (4.9) holds.

From (2.5) we find

$$\gamma(\bar{\mu})^* \gamma(\lambda) = \frac{M(\lambda) - M(\bar{\mu})^*}{\lambda - \mu}, \quad \lambda, \mu \in \mathbb{C} \setminus \mathbb{R}, \lambda \neq \mu, \quad (4.10)$$

and passing in (4.10) to the limit  $\mu \rightarrow \lambda$  one gets

$$\gamma(\bar{\lambda})^* \gamma(\lambda) = \frac{d}{d\lambda} M(\lambda).$$

Making use of formula (2.6) for canonical resolvents together with (4.9) this implies

$$\begin{aligned} \operatorname{tr} \left( (A_\Theta - \lambda)^{-1} - (A_0 - \lambda)^{-1} \right) &= -\operatorname{tr} \left( (M(\lambda) - \Theta)^{-1} \gamma(\bar{\lambda})^* \gamma(\lambda) \right) \\ &= -\frac{d}{d\lambda} \operatorname{tr}(\log(M(\lambda) - \Theta)) \end{aligned} \quad (4.11)$$

for all  $\lambda \in \mathbb{C}_+$ .

Further, by [20, Theorem 2.10] there exists a  $[\mathcal{H}]$ -valued measurable function  $t \mapsto \Xi_\Theta(t)$ ,  $t \in \mathbb{R}$ , such that

$$\Xi_\Theta(t) = \Xi_\Theta(t)^* \quad \text{and} \quad 0 \leq \Xi_\Theta(t) \leq I_{\mathcal{H}}$$

for a.e.  $\lambda \in \mathbb{R}$  and the representation

$$\log(M(\lambda) - \Theta) = C + \int_{\mathbb{R}} \Xi_\Theta(t) \left( (t - \lambda)^{-1} - t(1 + t^2)^{-1} \right) dt, \quad \lambda \in \mathbb{C}_+,$$

holds with some bounded selfadjoint operator  $C$ . Hence

$$\operatorname{tr}(\log(M(\lambda) - \Theta)) = \operatorname{tr}(C) + \int_{\mathbb{R}} \operatorname{tr}(\Xi_\Theta(t)) \left( (t - \lambda)^{-1} - t(1 + t^2)^{-1} \right) dt$$

for  $\lambda \in \mathbb{C}_+$  and we conclude from

$$\begin{aligned} \xi_\Theta(\lambda) &= \lim_{\epsilon \rightarrow +0} \frac{1}{\pi} \Im \left( \operatorname{tr}(\log(M(\lambda + i\epsilon) - \Theta)) \right) \\ &= \lim_{\epsilon \rightarrow +0} \frac{1}{\pi} \int_{\mathbb{R}} \operatorname{tr}(\Xi_\Theta(t)) \epsilon (t - \lambda)^2 + \epsilon^2)^{-1} dt \end{aligned}$$

that  $\xi_\Theta(\lambda) = \text{tr}(\Xi_\Theta(\lambda))$  is true for a.e.  $\lambda \in \mathbb{R}$ . Therefore we have

$$\frac{d}{d\lambda} \text{tr}(\log(M(\lambda) - \Theta)) = \int_{\mathbb{R}} (t - \lambda)^{-2} \xi_\Theta(t) dt$$

and together with (4.11) we immediately get the trace formula

$$\text{tr}((A_\Theta - \lambda)^{-1} - (A_0 - \lambda)^{-1}) = - \int_{\mathbb{R}} \frac{1}{(t - \lambda)^2} \xi_\Theta(t) dt.$$

The integrability condition (4.3) holds because of [20, Theorem 2.10]. This completes the proof of assertion (i).

(ii) To verify the Birman-Krein formula note that by (4.6)

$$\begin{aligned} & \exp(-2i\Im(\text{tr}(\log(M(\lambda) - \Theta)))) \\ &= \exp(-\text{tr}(\log(M(\lambda) - \Theta))) \exp(\overline{\text{tr}(\log(M(\lambda) - \Theta))}) \\ &= \frac{\det(M(\lambda) - \Theta)}{\det(M(\lambda) - \Theta)} = \frac{\det(M(\lambda)^* - \Theta)}{\det(M(\lambda) - \Theta)} \end{aligned}$$

holds for all  $\lambda \in \mathbb{C}_+$ . Hence we find

$$\exp(-2\pi i \xi_\Theta(\lambda)) = \frac{\det(M(\lambda + i0)^* - \Theta)}{\det(M(\lambda + i0) - \Theta)} \quad (4.12)$$

for a.e.  $\lambda \in \mathbb{R}$ , where  $M(\lambda + i0) := \lim_{\epsilon \rightarrow +0} M(\lambda + i\epsilon)$  exists for a.e.  $\lambda \in \mathbb{R}$ . It follows from the representation of the scattering matrix in (3.24) and the identity  $\det(I + AB) = \det(I + BA)$  that

$$\begin{aligned} \det S(\lambda) &= \det \left( I_{\mathcal{H}} + 2i(\Im(M(\lambda + i0))) (\Theta - M(\lambda + i0))^{-1} \right) \\ &= \det \left( I_{\mathcal{H}} + (M(\lambda + i0) - M(\lambda + i0)^*) (\Theta - M(\lambda + i0))^{-1} \right) \\ &= \det \left( (\Theta - M(\lambda + i0)^*) \cdot (\Theta - M(\lambda + i0))^{-1} \right) \\ &= \frac{\det(\Theta - M(\lambda + i0)^*)}{\det(\Theta - M(\lambda + i0))} \end{aligned} \quad (4.13)$$

holds for a.e.  $\lambda \in \mathbb{R}$ . Comparing (4.12) with (4.13) we obtain (4.8).  $\square$

We note that for singular Sturm-Liouville operators a definition for the spectral shift function similar to (4.7) was already used in [19].

## 5 Scattering systems of differential operators

In this section the results from Section 3 and Section 4 are illustrated for some differential operators. In Section 5.1 we consider a Sturm-Liouville differential expression, in Section 5.2 we investigate Sturm-Liouville operators with matrix potentials satisfying certain integrability conditions and Section 5.3 deals with scattering systems consisting of Dirac operators. Finally, Section 5.4 is devoted to Schrödinger operators with point interactions.

## 5.1 Sturm-Liouville operators

Let  $p, q$  and  $r$  be real valued functions on  $(a, b)$ ,  $-\infty < a < b \leq \infty$ , such that  $p(x) \neq 0$  and  $r(x) > 0$  for a.e.  $x \in (a, b)$  and  $p^{-1}, q, r \in L^1((a, c))$  for all  $c \in (a, b)$ . Moreover we assume that either  $b = \infty$  or at least one of the functions  $p^{-1}, q, r$  does not belong to  $L^1((a, b))$ . The Hilbert space of all equivalence classes of measurable functions  $f$  defined on  $(a, b)$  for which  $|f|^2 r \in L^1((a, b))$  equipped with the usual inner product

$$(f, g) := \int_a^b f(x) \overline{g(x)} r(x) dx$$

will be denoted by  $L_r^2((a, b))$ . By our assumptions the differential expression

$$\frac{1}{r} \left( -\frac{d}{dx} \left( p \frac{d}{dx} \right) + q \right) \quad (5.1)$$

is regular at the left endpoint  $a$  and singular at the right endpoint  $b$ . In addition we assume that the limit point case prevails at  $b$ , that is, the equation

$$-(pf')' + qf = \lambda r f, \quad \lambda \in \mathbb{C},$$

has a unique solution  $\phi(\cdot, \lambda)$  (up to scalar multiples) in  $L_r^2((a, b))$ . We refer to [17, 34] for sufficient conditions on the coefficients  $r, p, q$  such that (5.1) is limit point at  $b$ .

In  $L_r^2((a, b))$  we consider the operator

$$(Af)(x) := \frac{1}{r(x)} \left( -(pf')'(x) + q(x)f(x) \right)$$

$$\text{dom}(A) := \{f \in \mathcal{D}_{max} : f(a) = (pf')(a) = 0\},$$

where  $\mathcal{D}_{max}$  denotes the set of all  $f \in L_r^2((a, b))$  such that  $f$  and  $pf'$  are locally absolutely continuous and  $\frac{1}{r}(-(pf')' + qf)$  belongs to  $L_r^2((a, b))$ . It is well known that  $A$  is a densely defined closed simple symmetric operator with deficiency indices  $(1, 1)$ , see e.g. [17, 34] and [23] for the fact that  $A$  is simple. The adjoint operator  $A^*$  is

$$(A^*f)(x) = \frac{1}{r(x)} \left( -(pf')'(x) + q(x)f(x) \right), \quad \text{dom}(A^*) = \mathcal{D}_{max}.$$

If we choose  $\Pi = \{\mathbb{C}, \Gamma_0, \Gamma_1\}$ ,

$$\Gamma_0 f := f(a) \quad \text{and} \quad \Gamma_1 f := (pf')(a), \quad f \in \text{dom}(A^*),$$

then  $\Pi$  is a boundary triplet for  $A^*$  such that the corresponding Weyl function coincides with the classical Titchmarsh-Weyl coefficient  $m(\cdot)$ , cf. [33, 35, 36, 37]. In fact, if  $\varphi(\cdot, \lambda)$  and  $\psi(\cdot, \lambda)$  denote the fundamental solutions of the differential equation  $-(pf')' + qf = \lambda r f$  satisfying

$$\varphi(a, \lambda) = 1, \quad (p\varphi')(a, \lambda) = 0 \quad \text{and} \quad \psi(a, \lambda) = 0, \quad (p\psi')(a, \lambda) = 1,$$

then  $\text{sp} \{ \varphi(\cdot, \lambda) + m(\lambda)\psi(\cdot, \lambda) \} = \ker(A^* - \lambda)$ ,  $\lambda \in \mathbb{C} \setminus \mathbb{R}$ , and by applying  $\Gamma_0$  and  $\Gamma_1$  to the defect elements it follows that  $m(\cdot)$  is the Weyl function corresponding to the boundary triplet  $\Pi$ .



Let us consider the scattering system  $\{A_\Theta, A_0\}$ , where  $A_0 := A^* \upharpoonright \ker(\Gamma_0)$  and

$$A_\Theta = A^* \upharpoonright \ker(\Gamma_1 - \Theta\Gamma_0) = A^* \upharpoonright \{f \in \text{dom}(A^*) \mid (pf')(a) = \Theta f(a)\}$$

for some  $\Theta \in \mathbb{R}$ . By Corollary 3.10 the scattering matrix has the form

$$S_\Theta(\lambda) = \frac{\Theta - \overline{m(\lambda)}}{\Theta - m(\lambda)}$$

for a.e.  $\lambda \in \mathbb{R}$  with  $\Im m(m(\lambda + i0)) \neq 0$ , where  $m(\lambda) := m(\lambda + i0)$ , cf. (1.3).

Notice, that in the special case  $A^* = -d^2/dx^2$ ,  $\text{dom}(A^*) = W_2^2(\mathbb{R}_+)$ , i.e.

$$r(x) = p(x) = 1, \quad q(x) = 0, \quad a = 0 \quad \text{and} \quad b = \infty,$$

the defect subspaces  $\ker(A^* - \lambda)$ ,  $\lambda \in \mathbb{C} \setminus \mathbb{R}$ , are spanned by  $x \mapsto e^{i\sqrt{\lambda}x}$ , where the square root is defined on  $\mathbb{C}$  with a cut along  $[0, \infty)$  and fixed by  $\Im \sqrt{\lambda} > 0$  for  $\lambda \notin [0, \infty)$  and by  $\sqrt{\lambda} \geq 0$  for  $\lambda \in [0, \infty)$ . Therefore the Weyl function corresponding to  $\Pi$  is  $m(\lambda) = i\sqrt{\lambda}$  and hence the scattering matrix of the scattering system  $\{A_\Theta, A_0\}$  is

$$S_\Theta(\lambda) = 1 + 2i\sqrt{\lambda}(\Theta - i\sqrt{\lambda})^{-1} = \frac{\Theta + i\sqrt{\lambda}}{\Theta - i\sqrt{\lambda}}, \quad \lambda \in \mathbb{R}_+,$$

where  $\Theta \in \mathbb{R}$ , see [38, §3] and (1.4). In this case the spectral shift function  $\xi_\Theta(\cdot)$  of the pair  $\{A_\Theta, A_0\}$  is given by

$$\xi_\Theta(\lambda) = \begin{cases} 1 - \chi_{[0, \infty)}(\lambda) \frac{1}{\pi} \arctan\left(\frac{\sqrt{|\lambda|}}{\Theta}\right), & \Theta > 0, \\ 1 - \frac{1}{2} \chi_{[0, \infty)}, & \Theta = 0, \\ \chi_{(-\infty, -\Theta^2)}(\lambda) - \chi_{[0, \infty)}(\lambda) \frac{1}{\pi} \arctan\left(\frac{\sqrt{|\lambda|}}{\Theta}\right), & \Theta < 0, \end{cases} \quad (5.2)$$

for a.e.  $\lambda \in \mathbb{R}$ .

## 5.2 Sturm-Liouville operators with matrix potentials

Let  $Q \in L^\infty(\mathbb{R}_+, [\mathbb{C}^n])$  be a matrix valued function such that  $Q(\cdot) = Q(\cdot)^*$  and the functions  $x \mapsto Q(x)$  and  $x \mapsto xQ(x)$  belong to  $L^1(\mathbb{R}_+, [\mathbb{C}^n])$ . We consider the operator

$$A := -\frac{d^2}{dx^2} + Q, \quad \text{dom}(A) := \{f \in W_2^2(\mathbb{R}_+, \mathbb{C}^n) : f(0) = f'(0) = 0\},$$

in  $L^2(\mathbb{R}_+, \mathbb{C}^n)$ . Then  $A$  is a densely defined closed simple symmetric operator with deficiency indices  $n_\pm(A)$  both equal to  $n$  and we have  $A^* = -d^2/dx^2 + Q$ ,  $\text{dom}(A^*) = W_2^2(\mathbb{R}_+, \mathbb{C}^n)$ . Setting

$$\Gamma_0 f = f(0), \quad \Gamma_1 f = f'(0), \quad f \in \text{dom}(A^*) = W_2^2(\mathbb{R}_+, \mathbb{C}^n), \quad (5.3)$$

we obtain a boundary triplet  $\Pi = \{\mathbb{C}^n, \Gamma_0, \Gamma_1\}$  for  $A^*$ . Note that the extension  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$  corresponds to Dirichlet boundary conditions at 0,

$$A_0 = -\frac{d^2}{dx^2} + Q, \quad \text{dom}(A_0) = \{f \in W_2^2(\mathbb{R}_+, \mathbb{C}^n) : f(0) = 0\}. \quad (5.4)$$

**Proposition 5.1** *Let  $A = -d^2/dx^2 + Q$  and  $\Pi$  be as above and denote the corresponding Weyl function by  $M(\cdot)$ . Then the following holds.*

- (i) *The function  $M(\cdot)$  has poles on  $(-\infty, 0)$  with zero as the only possible accumulation point. Moreover,  $M(\cdot)$  admits a continuous continuation from  $\mathbb{C}_+$  onto  $\mathbb{R}_+$  and the asymptotic relation*

$$M(\lambda + i0) = i\sqrt{\lambda} I_{\mathbb{C}^n} + o(1) \quad \text{as } \lambda = \bar{\lambda} \rightarrow +\infty \quad (5.5)$$

*holds. Here the cut of the square root  $\sqrt{\cdot}$  is along the positive real axis as in Section 5.1.*

- (ii) *If  $\Theta \in [\mathbb{C}^n]$  is self-adjoint, then the scattering matrix  $\{S_\Theta(\lambda)\}$  of the scattering system  $\{A_\Theta, A_0\}$  behaves asymptotically like*

$$S_\Theta(\lambda) = I_{\mathbb{C}^n} + 2i\sqrt{\lambda}(\Theta - i\sqrt{\lambda} \cdot I_{\mathbb{C}^n})^{-1} + o(1) \quad (5.6)$$

*as  $\lambda \rightarrow +\infty$ , which yields  $S_\Theta(\lambda) \sim -I_{\mathbb{C}^n}$  as  $\lambda \rightarrow +\infty$ .*

**Proof.** (i) Since the spectrum of  $A_0$  (see (5.4)) is discrete in  $(-\infty, 0)$  with zero as only possible accumulation point (and purely absolutely continuous in  $(0, \infty)$ ) it follows that the Weyl function  $M(\cdot)$  has only poles in  $(-\infty, 0)$  possibly accumulating to zero. To prove the asymptotic properties of  $M(\cdot)$  we recall that under the condition  $x \mapsto xQ(x) \in L^1(\mathbb{R}_+, [\mathbb{C}^n])$  the equation  $A^*y = \lambda y$  has an  $n \times n$ -matrix solution  $E(\cdot, \lambda)$  which solves the integral equation

$$E(x, \lambda) = e^{ix\sqrt{\lambda}} I_{\mathbb{C}^n} + \int_x^\infty \frac{\sin(\sqrt{\lambda}(t-x))}{\sqrt{\lambda}} Q(t) E(t, \lambda) dt, \quad (5.7)$$

$\lambda \in \overline{\mathbb{C}}_+$ ,  $x \in \mathbb{R}_+$ , see [5]. By [5, Theorem 1.3.1] the solution  $E(x, \lambda)$  is continuous and uniformly bounded for  $\lambda \in \overline{\mathbb{C}}_+$  and  $x \in \mathbb{R}_+$ . Moreover, the derivative  $E'(x, \lambda) = \frac{d}{dx} E(x, \lambda)$  exists, is continuous and uniformly bounded for  $\lambda \in \overline{\mathbb{C}}_+$  and  $x \in \mathbb{R}_+$ , too. From (5.7) we immediately get the relation

$$E(0, \lambda) = I_{\mathbb{C}^n} + \frac{1}{\sqrt{\lambda}} o(1) \quad \text{as } \Re(\lambda) \rightarrow +\infty, \quad \lambda \in \overline{\mathbb{C}}_+. \quad (5.8)$$

Since

$$E'(x, \lambda) = i\sqrt{\lambda} e^{ix\sqrt{\lambda}} I_{\mathbb{C}^n} - \int_x^\infty \cos(\sqrt{\lambda}(t-x)) Q(t) E(t, \lambda) dt,$$

$\lambda \in \overline{\mathbb{C}}_+$ ,  $x \in \mathbb{R}_+$ , we get

$$E'(0, \lambda) = i\sqrt{\lambda} I_n + o(1) \quad \text{as } \Re(\lambda) \rightarrow +\infty, \quad \lambda \in \overline{\mathbb{C}}_+. \quad (5.9)$$

In particular, the asymptotic relations (5.8) and (5.9) hold as  $\lambda \rightarrow +\infty$  along the real axis. Since  $A^*E(x, \lambda)\xi = \lambda E(x, \lambda)\xi$ ,  $\xi \in \mathbb{C}^n$ , one gets

$$\mathcal{N}_\lambda = \ker(A^* - \lambda) = \{E(\cdot, \lambda)\xi : \xi \in \mathbb{C}^n\}, \quad \lambda \in \mathbb{C}_+.$$

Therefore using expressions (5.3) for  $\Gamma_0$  and  $\Gamma_1$  we obtain

$$M(\lambda) = E'(0, \lambda) \cdot E(0, \lambda)^{-1}, \quad \lambda \in \mathbb{C}_+, \quad (5.10)$$

where the existence of  $E(0, \lambda)^{-1}$  for  $\lambda \in \mathbb{C}_+ \cup (0, \infty)$  follows from the surjectivity of the map  $\Gamma_0$  and the fact that the operator  $A_0$  has no eigenvalues in  $(0, \infty)$ . Further, by continuity of  $E(0, \lambda)$  and  $E'(0, \lambda)$  in  $\lambda \in \overline{\mathbb{C}_+}$  we conclude that the Weyl function  $M(\cdot)$  admits a continuous continuation to  $\mathbb{R}_+$ . Therefore combining (5.10) with (5.8) and (5.9) we arrive at the asymptotic relation

$$M(\lambda + i0) = E'(0, \lambda + i0) \cdot E(0, \lambda + i0)^{-1} = i\sqrt{\lambda} I_{\mathbb{C}^n} + o(1)$$

as  $\lambda = \bar{\lambda} \rightarrow +\infty$  which proves (5.5)

(ii) Let now  $\Theta = \Theta^* \in [\mathbb{C}^n]$  and let  $A_\Theta = A^* \upharpoonright \ker(\Gamma_1 - \Theta\Gamma_0)$  be the corresponding selfadjoint extension of  $A$ ,

$$A_\Theta = -\frac{d^2}{dx^2} + Q, \quad \text{dom}(A_\Theta) = \{f \in W_2^2(\mathbb{R}_+, \mathbb{C}^n) : \Theta f(0) = f'(0)\},$$

and consider the scattering system  $\{A_\Theta, A_0\}$ , where  $A_0$  is given by (5.4). Combining the formula for the scattering matrix  $\{S_\Theta(\lambda)\}$ ,

$$S_\Theta(\lambda) = I_{\mathbb{C}^n} + 2i\sqrt{\Im(M(\lambda))}(\Theta - M(\lambda))^{-1}\sqrt{\Im(M(\lambda))}$$

for a.e.  $\lambda \in \mathbb{R}_+$ , from Theorem 3.8 with the asymptotic behaviour (5.5) of the Weyl function  $M(\cdot)$  a straightforward calculation implies relation (5.6) as  $\lambda \rightarrow +\infty$ . Therefore the scattering matrix of the scattering system  $\{A_\Theta, A_0\}$  satisfies  $S_\Theta(\lambda) \sim -I_{\mathbb{C}^n}$  as  $\lambda \rightarrow +\infty$ .  $\square$

We note that with the help of the asymptotic behaviour (5.5) of the Weyl function  $M(\cdot)$  also the asymptotic behaviour of the spectral shift function  $\xi_\Theta(\cdot)$  of the pair  $\{A_\Theta, A_0\}$  can be calculated. The details are left to the reader.

**Remark 5.2** The high energy asymptotic (5.6) is quite different from the one for the usually considered scattering system  $\{A_0, L_0\}$ , where  $A_0$  is as in (5.4),

$$L_0 = -\frac{d^2}{dx^2}, \quad \text{dom}(L_0) = \{f \in W_2^2(\mathbb{R}_+, \mathbb{C}^n) : f(0) = 0\},$$

and  $Q$  is rapidly decreasing. In this case the scattering matrix  $\{\tilde{S}(\lambda)\}_{\lambda \in \mathbb{R}_+}$  obeys the relation  $\lim_{\lambda \rightarrow \infty} \tilde{S}(\lambda) = I_{\mathbb{C}^n}$ , see [5], whereas by Proposition 5.1 the scattering matrix  $\{S_\Theta(\lambda)\}$  of the scattering system  $\{A_\Theta, A_0\}$ ,  $\Theta \in [\mathbb{C}^n]$  selfadjoint, satisfies  $\lim_{\lambda \rightarrow +\infty} S_\Theta(\lambda) = -I_{\mathbb{C}^n}$ .

Let us now consider the special case  $Q = 0$ . Instead of  $A$  and  $A^*$  we denote the minimal and maximal operator by  $L$  and  $L^*$  and we choose the boundary triplet  $\Pi$  from (5.3). Then the defect subspace is

$$\mathcal{N}_\lambda = \{x \mapsto e^{i\sqrt{\lambda}x}\xi : \xi \in \mathbb{C}^n, x \in \mathbb{R}_+\}, \quad \lambda \in \mathbb{C}_+ \cup \mathbb{C}_-,$$

and the Weyl function  $M(\cdot)$  is given by

$$M(\lambda) = i\sqrt{\lambda} \cdot I_{\mathbb{C}^n}, \quad \lambda \notin \mathbb{R}_+.$$

Let  $L_\Theta$  be the selfadjoint extension corresponding to  $\Theta = \Theta^* \in \tilde{\mathcal{C}}(\mathbb{C}^n)$  and let  $L_0 = L^* \upharpoonright \ker \Gamma_0$ . By Corollary 3.10 the scattering matrix  $\{S_\Theta(\lambda)\}_{\lambda \in \mathbb{R}_+}$  of the scattering system  $\{L_\Theta, L_0\}$  admits the representation

$$S_\Theta(\lambda) = I_{\mathbb{C}^n} + 2i\sqrt{\lambda}(\Theta - i\sqrt{\lambda} \cdot I_{\mathbb{C}^n})^{-1} \quad \text{for a.e. } \lambda \in \mathbb{R}_+. \quad (5.11)$$

Moreover, if  $\Theta \in [\mathbb{C}^n]$  formula (5.11) directly yields the asymptotic relation

$$\lim_{\lambda \rightarrow +\infty} S_\Theta(\lambda) = -I_{\mathbb{C}^n}.$$

If, in particular  $\Theta = 0$ , then  $L_\Theta = L^* \upharpoonright \ker(\Gamma_1)$  is the operator  $-d^2/dx^2$  subject to Neumann boundary conditions  $f'(0) = 0$ , and we have  $S_\Theta(\lambda) = -I_{\mathbb{C}^n}$ ,  $\lambda \in \mathbb{R}_+$ .

We note that the spectral shift function  $\xi_\Theta(\cdot)$  of the pair  $\{L_\Theta, L_0\}$  is given by

$$\xi_\Theta(\lambda) = \sum_{k=1}^n \xi_{\Theta_k}(\lambda) \quad \text{for a.e. } \lambda \in \mathbb{R}, \quad (5.12)$$

where  $\Theta_k$ ,  $k = 1, 2, \dots, n$ , are the eigenvalues of  $\Theta = \Theta^* \in [\mathbb{C}^n]$  and the functions  $\xi_{\Theta_k}(\cdot)$  are defined by (5.2).

### 5.3 Dirac operator

Let  $a > 0$  and let  $A$  be a symmetric Dirac operator on  $\mathbb{R}$  defined by

$$Af = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \frac{d}{dx} f + \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix} f, \\ \text{dom}(A) = \{f = (f_1, f_2)^\top \in W_2^1(\mathbb{R}, \mathbb{C}^2) : f(0) = 0\}.$$

The deficiency indices of  $A$  are  $(2, 2)$  and  $A^*$  is given by

$$A^*f = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \frac{d}{dx} f + \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix} f, \\ \text{dom}(A^*) = W_2^1(\mathbb{R}_-, \mathbb{C}^2) \oplus W_2^1(\mathbb{R}_+, \mathbb{C}^2).$$

Moreover, setting

$$\Gamma_0 f = \begin{pmatrix} f_2(0-) \\ f_1(0+) \end{pmatrix}, \quad \Gamma_1 f = \begin{pmatrix} f_1(0-) \\ f_2(0+) \end{pmatrix}, \quad f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix},$$

$f_1, f_2 \in W_2^1(\mathbb{R}_-, \mathbb{C}) \oplus W_2^1(\mathbb{R}_+, \mathbb{C})$ , we obtain a boundary triplet  $\Pi = \{\mathbb{C}^2, \Gamma_0, \Gamma_1\}$  for  $A^*$ , cf. [11]. Let the square root  $\sqrt{\cdot}$  be defined as in the previous sections and let  $k(\lambda) := \sqrt{\lambda - a}\sqrt{\lambda + a}$ ,  $\lambda \in \mathbb{C}$ . One verifies as in [11] that  $\ker(A^* - \lambda)$ ,  $\lambda \in \mathbb{C}_+$ , is spanned by the functions

$$f_{\lambda, \pm}(x) := \begin{pmatrix} \mp i \frac{\sqrt{\lambda+a}}{\sqrt{\lambda-a}} e^{\pm ik(\lambda)x} \\ e^{\pm ik(\lambda)x} \end{pmatrix} \chi_{\mathbb{R}_\pm}(x), \quad x \in \mathbb{R}, \lambda \in \mathbb{C}_+,$$

and hence for  $\lambda \in \mathbb{C}_+$  the Weyl function  $M$  corresponding to the boundary triplet  $\Pi$  is given by

$$M(\lambda) = \begin{pmatrix} i\sqrt{\frac{\lambda+a}{\lambda-a}} & 0 \\ 0 & i\sqrt{\frac{\lambda-a}{\lambda+a}} \end{pmatrix}, \quad \lambda \in \mathbb{C}_+. \quad (5.13)$$

If  $\Theta = \Theta^*$  is a selfadjoint relation in  $\mathbb{C}^2$  and  $A_\Theta = A^* \upharpoonright \Gamma^{-1}\Theta$  is the corresponding extension,

$$A_\Theta f = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \frac{d}{dx} f + \begin{pmatrix} a & 0 \\ 0 & -a \end{pmatrix} f,$$

$$\text{dom}(A_\Theta) = \left\{ f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \in \text{dom}(A^*) : \begin{pmatrix} (f_2(0-), f_1(0+))^\top \\ (f_1(0-), f_2(0+))^\top \end{pmatrix} \in \Theta \right\},$$

then it follows from Theorem 3.8 that the scattering matrix  $\{S_\Theta(\lambda)\}_{\lambda \in \Omega_a}$ , where  $\Omega_a := (-\infty, -a) \cup (a, \infty)$ , of the Dirac scattering system  $\{A_\Theta, A_0\}$ ,  $A_0 = A^* \upharpoonright \ker(\Gamma_0)$ , is given by

$$S_\Theta(\lambda) = I_{\mathbb{C}^2} + 2i\sqrt{\Im(M(\lambda))}(\Theta - M(\lambda))^{-1}\sqrt{\Im(M(\lambda))} \quad (5.14)$$

for a.e.  $\lambda \in \Omega_a$ , where

$$\Im(M(\lambda)) = \begin{pmatrix} \sqrt{|\frac{\lambda+a}{\lambda-a}|} & 0 \\ 0 & \sqrt{|\frac{\lambda-a}{\lambda+a}|} \end{pmatrix}, \quad \lambda \in \Omega_a. \quad (5.15)$$

Note that for  $\lambda \in (-a, a)$  we have  $\Im(M(\lambda)) = 0$ .

**Remark 5.3** We note that the parameter  $\Theta = \Theta^* \in [\mathbb{C}^2]$ , i.e. the boundary conditions of the perturbed Dirac operator  $A_\Theta$ , can be recovered from the limit of the scattering matrix  $S_\Theta(\lambda)$ ,  $|\lambda| \rightarrow +\infty$ , corresponding to the scattering system  $\{A_\Theta, A_0\}$ . In fact, it follows from (5.14), (5.15) and (5.13) that

$$S_\Theta(\infty) := \lim_{|\lambda| \rightarrow +\infty} S_\Theta(\lambda) = I_{\mathbb{C}^2} + 2i(\Theta - i)^{-1}$$

holds. Therefore the extension parameter  $\Theta$  is given by

$$\Theta = i(S_\Theta(\infty) + I_{\mathbb{C}^2})(S_\Theta(\infty) - I_{\mathbb{C}^2})^{-1}.$$

Assume now that  $\Theta = \begin{pmatrix} \theta_1 & 0 \\ 0 & \theta_2 \end{pmatrix}$ ,  $\theta_1, \theta_2 \in \mathbb{R}$ . Then

$$\text{dom}(A_\Theta) = \left\{ f = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \in \text{dom}(A^*) : \begin{matrix} \theta_1 f_2(0-) = f_1(0-) \\ \theta_2 f_1(0+) = f_2(0+) \end{matrix} \right\}$$

and the scattering matrix  $\{S_\Theta(\lambda)\}_{\lambda \in \Omega_a}$  has the form

$$S_\Theta(\lambda) = \begin{pmatrix} \frac{\theta_1 + i\sqrt{|\frac{\lambda+a}{\lambda-a}|}}{\theta_1 - i\sqrt{|\frac{\lambda+a}{\lambda-a}|}} & 0 \\ 0 & \frac{\theta_2 + i\sqrt{|\frac{\lambda-a}{\lambda+a}|}}{\theta_2 - i\sqrt{|\frac{\lambda-a}{\lambda+a}|}} \end{pmatrix}, \quad \lambda \in \Omega_a.$$

In this case the spectral shift function  $\xi_\Theta$  of the pair  $\{A_\Theta, A_0\}$  is given by

$$\xi_\Theta(\lambda) = \eta_{\theta_1}(\lambda) + \eta_{\theta_2}(\lambda) \quad \text{for a.e. } \lambda \in \mathbb{R},$$

where

$$\eta_{\theta_i}(\lambda) := \begin{cases} 1 - \chi_{\Omega_a}(\lambda) \frac{1}{\pi} \arctan\left(\frac{1}{\theta_i} \sqrt{\left|\frac{\lambda+a}{\lambda-a}\right|}\right), & \theta_i > 0, \\ 1 - \frac{1}{2} \chi_{\Omega_a}(\lambda), & \theta_i = 0, \\ \chi_{(\vartheta_i, a)}(\lambda) - \chi_{\Omega_a}(\lambda) \frac{1}{\pi} \arctan\left(\frac{1}{\theta_i} \sqrt{\left|\frac{\lambda+a}{\lambda-a}\right|}\right), & \theta_i < 0, \end{cases}$$

$i = 1, 2$ , and the real constants  $\vartheta_1, \vartheta_2 \in (-a, a)$  are given by

$$\vartheta_1 = a \frac{\theta_1^2 - 1}{\theta_1^2 + 1} \quad \text{and} \quad \vartheta_2 = a \frac{1 - \theta_2^2}{1 + \theta_2^2}.$$

## 5.4 Schrödinger operators with point interactions

As a further example we consider the matrix Schrödinger differential expression  $-\Delta + Q$  in  $L^2(\mathbb{R}^3, \mathbb{C}^n)$  with a bounded selfadjoint matrix potential  $Q(x) = Q(x)^*$ ,  $x \in \mathbb{R}^3$ . This expression determines a minimal symmetric operator

$$H := -\Delta + Q, \quad \text{dom}(H) := \{f \in W_2^2(\mathbb{R}^3, \mathbb{C}^n) : f(0) = 0\}, \quad (5.16)$$

in  $L^2(\mathbb{R}^3, \mathbb{C}^n)$ . Notice that  $H$  is closed, since for any  $x \in \mathbb{R}^3$  the linear functional  $l_x : f \rightarrow f(x)$  is bounded in  $W_2^2(\mathbb{R}^3, \mathbb{C}^n)$  due to the Sobolev embedding theorem. Moreover, it is easily seen that the deficiency indices of  $H$  are  $n_{\pm}(H) = n$ . We note that if  $Q = 0$  the self-adjoint extensions of  $H$  in  $L^2(\mathbb{R}^3, \mathbb{C}^n)$  are used to model so-called point interactions or singular potentials, see e.g. [3, 4, 7].

In the next proposition we define a boundary triplet for the adjoint  $H^*$ . For  $x = (x_1, x_2, x_3)^{\top} \in \mathbb{R}^3$  we agree to write  $r := |x| = (x_1^2 + x_2^2 + x_3^2)^{1/2}$ .

**Proposition 5.4** *Let  $H$  be the minimal Schrödinger operator (5.16) with a matrix potential  $Q = Q^* \in L^\infty(\mathbb{R}^3, [\mathbb{C}^n])$ . Then the following assertions hold.*

(i) *The domain of  $H^* = -\Delta + Q$  is given by*

$$\text{dom}(H^*) = \left\{ f \in L^2(\mathbb{R}^3, \mathbb{C}^n) : \begin{array}{l} f = \xi_0 \frac{e^{-r}}{r} + \xi_1 e^{-r} + f_H, \\ \xi_0, \xi_1 \in \mathbb{C}^n, f_H \in \text{dom}(H) \end{array} \right\}. \quad (5.17)$$

(ii) *A boundary triplet  $\Pi = \{\mathbb{C}^n, \Gamma_0, \Gamma_1\}$  for  $H^*$  is defined by*

$$\Gamma_j f := 2\sqrt{\pi} \xi_j, \quad f = \xi_0 \frac{e^{-r}}{r} + \xi_1 e^{-r} + f_H \in \text{dom}(H^*), \quad j = 0, 1. \quad (5.18)$$

(iii) *The operator  $H_0 = H^* \upharpoonright \ker(\Gamma_0)$  is the usual selfadjoint Schrödinger operator  $-\Delta + Q$  with domain  $W_2^2(\mathbb{R}^3, \mathbb{C}^n)$ .*

**Proof.** (i) Since  $Q \in L^\infty(\mathbb{R}^3, [\mathbb{C}^n])$  the domain of  $H^*$  does not depend on  $Q$ . Therefore it suffices to consider the case  $Q = 0$ . Here it is well-known, that

$$\text{dom}(H^*) = \{f \in L^2(\mathbb{R}^3, \mathbb{C}^n) \cap W_{2, \text{loc}}^2(\mathbb{R}^3 \setminus \{0\}, \mathbb{C}^n) : \Delta f \in L^2(\mathbb{R}^3, \mathbb{C}^n)\}$$

holds, see e.g. [3, 4], and therefore the functions  $x \mapsto e^{-r}/r$  and  $x \mapsto e^{-r}$ ,  $r = |x| = (x_1^2 + x_2^2 + x_3^2)^{1/2}$ , belong to  $\text{dom}(H^*)$ . The linear span of the functions

$$x \mapsto \xi_0 \frac{e^{-r}}{r} + \xi_1 e^{-r} \quad \xi_0, \xi_1 \in \mathbb{C}^n,$$

is a  $2n$ -dimensional subspace in  $\text{dom}(H^*)$  and the intersection with  $\text{dom}(H)$  is trivial. Since  $\dim(\text{dom}(H^*)/\text{dom}(H)) = 2n$  it follows that  $\text{dom}(H^*)$  has the form (5.17).

(ii) Let  $f, g \in \text{dom}(H^*)$ . By assertion (i) we have

$$f = h + f_H, \quad h = \xi_0 \frac{e^{-r}}{r} + \xi_1 e^{-r}, \quad \text{and} \quad g = k + g_H, \quad k = \eta_0 \frac{e^{-r}}{r} + \eta_1 e^{-r},$$

with some functions  $f_H, g_H \in \text{dom}(H)$  and  $\xi_0, \xi_1, \eta_0, \eta_1 \in \mathbb{C}^n$ . Using polar coordinates we obtain

$$\begin{aligned} (H^* f, g) - (f, H^* g) &= (H^* h, k) - (h, H^* k) \\ &= 4\pi \int_0^\infty h(r) \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} \overline{k(r)} dr - 4\pi \int_0^\infty \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} h(r) \overline{k(r)} dr \\ &= 4\pi \left[ r^2 h(r) \frac{\partial}{\partial r} \overline{k(r)} - r^2 \frac{\partial}{\partial r} h(r) \overline{k(r)} \right]_0^\infty \end{aligned}$$

and with the help of the relations

$$r^2 \frac{\partial}{\partial r} k(r) = -e^{-r} \{ (1+r)\eta_0 + r^2\eta_1 \}$$

and

$$r^2 \frac{\partial}{\partial r} h(r) = -e^{-r} \{ (1+r)\xi_0 + r^2\xi_1 \}$$

this implies

$$\begin{aligned} (H^* f, g) - (f, H^* g) &= 4\pi \left[ e^{-2r} (\xi_0 + r\xi_0 + r^2\xi_1) \left( \frac{\overline{\eta_0}}{r} + \overline{\eta_1} \right) \right. \\ &\quad \left. - e^{-2r} \left( \frac{\xi_0}{r} + \xi_1 \right) (\overline{\eta_0} + r\overline{\eta_0} + r^2\overline{\eta_1}) \right]_0^\infty. \end{aligned}$$

This leads to

$$(H^* f, g) - (f, H^* g) = 4\pi(\xi_1, \eta_0) - 4\pi(\xi_0, \eta_1) = (\Gamma_1 f, \Gamma_0 g) - (\Gamma_1 f, \Gamma_0 g)$$

and therefore Green's identity is satisfied. It follows from (5.17) that the mapping  $\Gamma = (\Gamma_0, \Gamma_1)^\top$  is surjective and hence assertion (ii) is proved.

(iii) Combining (5.16) and (5.17) we see that any  $f \in W_2^2(\mathbb{R}^3, \mathbb{C}^n)$  admits a representation  $f = \xi_1 e^{-r} + f_H$  with  $\xi_1 := f(0)$  and  $f_H = f - \xi_1 e^{-r} \in \text{dom}(H)$  which proves (iii).  $\square$

It is important to note that the symmetric operator  $H$  in (5.16) is in general not simple (see e.g. [3]), hence  $H$  admits a decomposition into a simple part  $\widehat{H}$  and a selfadjoint part  $H_s$ , that is,  $H = \widehat{H} \oplus H_s$ , cf. Section 2.2. It is not difficult to see that the boundary triplet from

Proposition 5.4 is also a boundary triplet for  $\widehat{H}^*$ . Then obviously the Schrödinger operator  $H_0$  from Proposition 5.4 (iii) can be written as  $H_0 = \widehat{H}_0 \oplus H_s$ , where  $\widehat{H}_0 = \widehat{H}^* \upharpoonright \ker(\Gamma_0)$ .

Let us now consider the case where the potential  $Q$  is spherically symmetric, that is,  $Q(x) = Q(r)$ ,  $r = (x_1^2 + x_2^2 + x_3^2)^{1/2}$ . In this case the simple part  $\widehat{H}$  of  $H$  becomes unitarily equivalent to the symmetric Sturm-Liouville operator

$$A = -\frac{d^2}{dr^2} + Q, \quad \text{dom}(A) = \{f \in W_2^2(\mathbb{R}_+, \mathbb{C}^n) : f(0) = f'(0) = 0\},$$

cf. Section 5.2, and the extension  $\widehat{H}_0$  becomes unitarily equivalent to the selfadjoint extension  $A_0$  of  $A$  subject to Dirichlet boundary conditions at 0.

**Proposition 5.5** *Let  $H$  be the minimal Schrödinger operator with a spherically symmetric matrix potential  $Q = Q^* \in L^\infty(\mathbb{R}^3, [\mathbb{C}^n])$  from (5.16) and assume that  $r \mapsto Q(r)$  and  $r \mapsto rQ(r)$  belong to  $L^1(\mathbb{R}_+, [\mathbb{C}^n])$ . Let  $\Pi_H$  and  $\Pi_A$  be the boundary triplets for  $H^*$  and  $A^*$  defined by (5.18) and (5.3), respectively. Then the corresponding Weyl functions  $M_H(\cdot)$  and  $M_A(\cdot)$  are connected via*

$$M_H(\lambda) = I_{\mathbb{C}^n} + M_A(\lambda), \quad \lambda \in \mathbb{C} \setminus \mathbb{R}, \quad (5.19)$$

and the pairs  $\{\widehat{H}, \widehat{H}_0\}$  and  $\{A, A_0\}$  are unitarily equivalent. If, in particular,  $Q = 0$ , then  $M_H(\lambda) = (i\sqrt{\lambda} + 1) \cdot I_{\mathbb{C}^n}$ .

**Proof.** Let  $E(\cdot, \lambda)$ ,  $\lambda \in \mathbb{C}_+$ , be the  $n \times n$ -matrix solution of the equation  $A^*E(r, \lambda) = \lambda E(r, \lambda)$  from Section 5.2. Since  $E(\cdot, \lambda)\xi \in L^2(\mathbb{R}_+, [\mathbb{C}^n])$ ,  $\xi \in \mathbb{C}^n$ , we see that

$$U(x, \lambda) := \frac{1}{r}E(r, \lambda), \quad r = (x_1^2 + x_2^2 + x_3^2)^{1/2} \neq 0,$$

satisfies  $U(x, \lambda)\xi \in L^2(\mathbb{R}^3, [\mathbb{C}^n])$ ,  $\xi \in \mathbb{C}^n$ ,  $\lambda \in \mathbb{C}_+$ , and

$$\begin{aligned} H^*U(x, \lambda)\xi &= -\Delta U(x, \lambda)\xi + Q(r)U(x, \lambda)\xi \\ &= \frac{1}{r}(-E''(\lambda, r) + Q(r)E(r, \lambda))\xi = \frac{1}{r}A^*E(r, \lambda)\xi = \lambda U(x, \lambda)\xi. \end{aligned}$$

Therefore  $\ker(H^* - \lambda) = \{U(\cdot, \lambda)\xi : \xi \in \mathbb{C}^n\}$ ,  $\lambda \in \mathbb{C}_+$ . It follows from (5.18) that  $U(\cdot, \lambda)\xi$  can be decomposed in the form

$$U(x, \lambda)\xi = \frac{1}{r}E(r, \lambda)\xi = \Xi_0(\lambda)\xi \frac{e^{-r}}{r} + \Xi_1(\lambda)\xi e^{-r} + U_H(x, \lambda)\xi, \quad (5.20)$$

where

$$\Xi_0(\lambda) = E(0, \lambda), \quad \Xi_1(\lambda) = E(0, \lambda) + E'(0, \lambda), \quad (5.21)$$

and  $U_H(\cdot, \lambda) \in \text{dom } H$ .

Note that according to (5.10) the Weyl function  $M_A(\cdot)$  corresponding to  $\Pi_A$  is  $M_A(\lambda) = E'(0, \lambda) \cdot E(0, \lambda)^{-1}$ ,  $\lambda \in \mathbb{C}_+$ . On the other hand, (5.20) and (5.21) imply

$$M_H(\lambda) = \Xi_1(\lambda) \cdot \Xi_0(\lambda)^{-1} = (E(0, \lambda) + E'(0, \lambda)) \cdot E(0, \lambda)^{-1} = I_{\mathbb{C}^n} + M_A(\lambda).$$



The unitary equivalence of the simple operators  $\widehat{H}$  and  $A$  as well as of the selfadjoint extensions  $\widehat{H}_0$  and  $A_0$  is a consequence of Corollary 1 and Lemma 2 of [13].  $\square$

Let now  $H = \widehat{H} \oplus H_s$  and  $Q$  be as in Proposition 5.5 and consider the scattering system  $\{H_\Theta, H_0\}$ , where  $H_\Theta = H^* \upharpoonright \Gamma^{-1}\Theta$  for some selfadjoint  $\Theta \in \widetilde{\mathcal{C}}(\mathbb{C}^n)$ . Then in fact one considers the scattering system  $\{\widehat{H}_\Theta, \widehat{H}_0\}$ ,  $H_\Theta = \widehat{H}_\Theta \oplus H_s$ . In accordance with Theorem 3.8 the scattering matrix  $\{\widehat{S}_\Theta(\lambda)\}_{\lambda \in \mathbb{R}_+}$  of the scattering system  $\{\widehat{H}_\Theta, \widehat{H}_0\}$  is given by

$$\widehat{S}_\Theta(\lambda) = I_{\mathbb{C}^n} + 2i\sqrt{\Im m(M_A(\lambda))}(\Theta - (M_A(\lambda) + I_{\mathbb{C}^n}))^{-1}\sqrt{\Im m(M_A(\lambda))}$$

for a.e.  $\lambda \in \mathbb{R}_+$ , where  $M_A(\cdot)$  is the Weyl function of the boundary triplet  $\Pi_A$ , cf. (5.10). If, in particular  $Q = 0$ , then  $\widehat{S}_\Theta(\lambda)$  takes the form

$$\widehat{S}_\Theta(\lambda) = I_{\mathbb{C}^n} + 2i\sqrt{\lambda}(\Theta - (i\sqrt{\lambda} + 1) \cdot I_{\mathbb{C}^n})^{-1}.$$

In this case the spectral shift function  $\widehat{\xi}_\Theta(\cdot)$  of the scattering system  $\{\widehat{H}_\Theta, \widehat{H}_0\}$  is given by

$$\widehat{\xi}_\Theta(\lambda) = \xi_{\Theta-I}(\lambda) \quad \text{for a.e. } \lambda \in \mathbb{R},$$

where  $\xi_{\Theta-I}(\cdot)$  is the spectral shift function of the scattering system  $\{L_{\Theta-I}, L_0\}$  (see the end of Section 5.2) defined by (5.12).

## A Direct integrals and spectral representations

Following the lines of [6] we give a short introduction to direct integrals of Hilbert spaces and to spectral representations of selfadjoint operators.

Let  $\Lambda$  be a Borel subset of  $\mathbb{R}$  and let  $\mu$  be a Borel measure on  $\mathbb{R}$ . Further, let  $\{\mathcal{H}_\lambda, (\cdot, \cdot)_{\mathcal{H}_\lambda}\}_{\lambda \in \Lambda}$  be a family of separable Hilbert spaces. A subset  $\mathcal{S}$  of the Cartesian product  $\prod_{\lambda \in \Lambda} \mathcal{H}_\lambda$  is called an *admissible system* if the following conditions are satisfied (see [6]):

1. The set  $\mathcal{S}$  is linear and  $\mathcal{S}$  is closed with respect to multiplication by functions from  $L^\infty(\Lambda, \mu)$ .
2. For every  $f \in \mathcal{S}$  the function  $\lambda \mapsto \|f(\lambda)\|_{\mathcal{H}_\lambda}$  is Borel measurable and  $\int_\Lambda \|f(\lambda)\|_{\mathcal{H}_\lambda}^2 d\mu(\lambda) < \infty$ .
3.  $\text{span}\{f(\lambda) \mid f \in \mathcal{S}\}$  is dense in  $\mathcal{H}_\lambda \pmod{\mu}$ .
4. If for a Borel subset  $\Delta \subseteq \Lambda$  one has  $\int_\Delta \|f(\lambda)\|_{\mathcal{H}_\lambda}^2 d\mu(\lambda) = 0$  for all  $f \in \mathcal{S}$ , then  $\mu(\Delta) = 0$ .

A function  $f \in \prod_{\lambda \in \Lambda} \mathcal{H}_\lambda$  is *strongly measurable with respect to  $\mathcal{S}$*  if there exists a sequence  $t_n \in \mathcal{S}$  such that  $\lim_{n \rightarrow \infty} \|f(\lambda) - t_n(\lambda)\|_{\mathcal{H}_\lambda} = 0 \pmod{\mu}$  is valid. On the set of all strongly measurable functions  $f, g \in \prod_{\lambda \in \Lambda} \mathcal{H}_\lambda$  with the property

$$\int_\Lambda \|f(\lambda)\|_{\mathcal{H}_\lambda}^2 d\mu(\lambda) < \infty \quad \text{and} \quad \int_\Lambda \|g(\lambda)\|_{\mathcal{H}_\lambda}^2 d\mu(\lambda) < \infty$$

we introduce the semi-scalar product

$$(f, g) := \int_{\Lambda} (f(\lambda), g(\lambda))_{\mathcal{H}_{\lambda}} d\mu(\lambda).$$

By completion of the corresponding factor space one obtains the Hilbert space  $L^2(\Lambda, \mu, \mathcal{H}_{\lambda}, \mathcal{S})$  which is called the *direct integral of the family  $\mathcal{H}_{\lambda}$  with respect to  $\Lambda$ ,  $\mu$  and  $\mathcal{S}$* .

Let in the following  $A_0$  be a selfadjoint operator in the separable Hilbert space  $\mathfrak{H}$ , let  $E_0$  be the orthogonal spectral measure of  $A_0$ , denote the absolutely continuous subspace of  $A_0$  by  $\mathfrak{H}^{ac}(A_0)$  and let  $\mu_L$  be the Lebesgue measure.

**Definition A.1** *We call a Borel set  $\Lambda \subseteq \sigma_{ac}(A_0)$  a spectral core of the operator  $A_0^{ac} := A_0 \upharpoonright \text{dom}(A_0) \cap \mathfrak{H}^{ac}(A_0)$  if  $E_0(\Lambda)\mathfrak{H}^{ac}(A_0) = \mathfrak{H}^{ac}(A_0)$  and  $\mu_L(\Lambda)$  is minimal. A linear manifold  $\mathcal{M} \subseteq \mathfrak{H}^{ac}(A_0)$  is called a spectral manifold if there exists a spectral core  $\Lambda$  of  $A_0^{ac}$  such that the derivative  $\frac{d}{d\lambda}(E_0(\lambda)f, f)$  exists for all  $f \in \mathcal{M}$  and all  $\lambda \in \Lambda$ .*

Note that every finite dimensional linear manifold  $\mathcal{M}$  in  $\mathfrak{H}^{ac}(A_0)$  is a spectral manifold. Let us assume that  $\mathcal{M} \subseteq \mathfrak{H}^{ac}(A_0)$  is a spectral manifold which is *generating with respect to  $A_0^{ac}$* , that is,

$$\mathfrak{H}^{ac}(A_0) = \text{closan}\{E_0(\Delta)f : \Delta \in \mathcal{B}(\mathbb{R}), f \in \mathcal{M}\} \quad (\text{A.1})$$

holds and let  $\Lambda$  be a corresponding spectral core of  $A_0^{ac}$ . We define a family of semi-scalar products  $(\cdot, \cdot)_{E_0, \lambda}$  by

$$(f, g)_{E_0, \lambda} := \frac{d}{d\lambda}(E_0(\lambda)f, g), \quad \lambda \in \Lambda, f, g \in \mathcal{M},$$

and denote the corresponding semi-norms by  $\|\cdot\|_{E_0, \lambda}$ . We remark, that the family  $\{(\cdot, \cdot)_{E_0, \lambda}\}_{\lambda \in \Lambda}$  is an example of a so-called *spectral form* with respect to the spectral measure  $E_0^{ac} := E_0 \upharpoonright \mathfrak{H}^{ac}(A_0)$  of  $A_0^{ac}$  (see [6, Section 4.5.1]). By  $\widehat{\mathcal{M}}_{\lambda}$ ,  $\lambda \in \Lambda$ , we denote the completion of the factor space

$$\mathcal{M} / \ker(\|\cdot\|_{E_0, \lambda})$$

with respect to  $\|\cdot\|_{E_0, \lambda}$ . The canonical embedding operator mapping  $\mathcal{M}$  into the Hilbert space  $\widehat{\mathcal{M}}_{\lambda}$ ,  $\lambda \in \Lambda$ , is denoted by  $J_{\lambda}$ ,

$$J_{\lambda} : \mathcal{M} \rightarrow \widehat{\mathcal{M}}_{\lambda}, \quad k \mapsto J_{\lambda}k.$$

**Lemma A.2** *The set*

$$\mathcal{S}_{\mathcal{M}} := \left\{ \sum_{l=1}^n \alpha_l(\lambda) J_{\lambda} f_l : f_l \in \mathcal{M}, \alpha_l \in L^{\infty}(\Lambda, \mu), n \in \mathbb{N} \right\} \subseteq X_{\lambda \in \Lambda} \widehat{\mathcal{M}}_{\lambda}$$

*is an admissible system.*

**Proof.** Obviously  $\mathcal{S}_{\mathcal{M}}$  is linear and closed with respect to multiplication by functions from  $L^{\infty}(\Lambda, \mu)$ . For  $f(\lambda) = J_{\lambda}f$ ,  $f \in \mathcal{M}$ ,  $\lambda \in \Lambda$ , we find from

$$\|f(\lambda)\|_{\widehat{\mathcal{M}}_{\lambda}}^2 = \|f\|_{E_0, \lambda}^2 = \frac{d}{d\lambda}(E_0(\lambda)f, f)$$

that  $\lambda \mapsto \|f(\lambda)\|_{\widehat{\mathcal{M}}_\lambda}$  is Borel measurable and that

$$\int_{\Lambda} \|f(\lambda)\|_{\widehat{\mathcal{M}}_\lambda}^2 d\mu_L(\lambda) = (E_0(\Lambda)f, f) = (f, f) < \infty$$

holds. Hence it follows that condition (2) is satisfied. For each  $\lambda \in \Lambda$  the set  $\{J_\lambda f : f \in \mathcal{M}\}$  is dense in  $\widehat{\mathcal{M}}_\lambda$ , thus (3) holds. Finally, if for some  $\Delta \in \mathcal{B}(\Lambda)$  and all  $f \in \mathcal{S}_\mathcal{M}$

$$0 = \int_{\Delta} \|f(\lambda)\|_{\widehat{\mathcal{M}}_\lambda}^2 d\mu_L(\lambda) = (E_0(\Delta)f, f) = \|E_0(\Delta)f\|^2$$

holds, the assumption that  $\mathcal{M}$  is generating implies  $E_0(\Delta)g = 0$  for every  $g \in \mathfrak{H}^{ac}(A_0)$ , hence  $E_0(\Delta) = 0$ . As  $\Lambda$  is a spectral core we conclude  $\mu_L(\Delta) = 0$ .  $\square$

Then the direct integral  $L^2(\Lambda, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})$  of the family  $\widehat{\mathcal{M}}_\lambda$  with respect to the spectral core  $\Lambda$ , the Lebesgue measure and the admissible system  $\mathcal{S}_\mathcal{M}$  in Lemma A.2 can be defined. By [6, Proposition 4.21] there exists an isometric operator from  $\mathfrak{H}^{ac}(A_0)$  onto  $L^2(\Lambda, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})$  such that  $E_0(\Delta)$  corresponds to the multiplication operator induced by the characteristic function  $\chi_\Delta$  for any  $\Delta \in \mathcal{B}(\Lambda)$ , that is, the direct integral  $L^2(\Lambda, \mu_L, \widehat{\mathcal{M}}_\lambda, \mathcal{S}_\mathcal{M})$  performs a *spectral representation* of the spectral measure  $E_0^{ac}$  of  $A_0^{ac}$ .

According to [6, Section 3.5.5] we introduce the semi-norm  $[\cdot]_{E_0, \lambda}$ ,

$$[f]_{E_0, \lambda}^2 := \limsup_{h \rightarrow 0} \frac{1}{h} (E_0([\lambda, \lambda + h])f, f), \quad \lambda \in \mathbb{R}, \quad f \in \mathfrak{H}^{ac}(A_0),$$

and we set

$$\mathcal{D}_\lambda := \{f \in \mathfrak{H}^{ac}(A_0) : [f]_{E_0, \lambda} < \infty\}, \quad \lambda \in \mathbb{R}. \quad (\text{A.2})$$

If  $\mathcal{M}$  is a spectral manifold and  $\Lambda$  is an associated spectral core, then  $\mathcal{M} \subseteq \mathcal{D}_\lambda$  holds for all  $\lambda \in \Lambda$ . Moreover, we have

$$(f, f)_{E_0, \lambda} = [f]_{E_0, \lambda}^2, \quad f \in \mathcal{M}, \quad \lambda \in \Lambda.$$

By  $\widehat{\mathcal{D}}_\lambda$  we denote the Banach space which is obtained from  $\mathcal{D}_\lambda$  by factorization and completion with respect to the semi-norm  $[\cdot]_{E_0, \lambda}$ , i.e.

$$\widehat{\mathcal{D}}_\lambda := \text{clo}_{[\cdot]_{E_0, \lambda}}(\mathcal{D}_\lambda / \ker([\cdot]_{E_0, \lambda})).$$

For  $\lambda \in \Lambda$  we will regard  $\widehat{\mathcal{M}}_\lambda$  as a subspace of  $\widehat{\mathcal{D}}_\lambda$ . By  $D_\lambda$  we denote the canonical embedding operator from  $\mathcal{D}_\lambda$  into  $\widehat{\mathcal{D}}_\lambda$ . Note that  $\text{clo } D_\lambda \mathcal{M} = \widehat{\mathcal{M}}_\lambda$ ,  $\lambda \in \Lambda$ , where the closure is taken with respect to the topology of  $\widehat{\mathcal{D}}_\lambda$ .

**Lemma A.3** *For a continuous function  $\varphi$  on  $\sigma(A_0)$  the relation*

$$D_\lambda \varphi(A_0) f = \varphi(\lambda) D_\lambda f$$

*holds for all  $\lambda \in \mathbb{R}$  and all  $f \in \mathcal{D}_\lambda$ .*

**Proof.** We have to check that

$$\begin{aligned} 0 &= [\varphi(A_0)f - \varphi(\lambda)f]_{E_0, \lambda}^2 \\ &= \limsup_{h \rightarrow 0} \frac{1}{h} \left( E_0([\lambda, \lambda + h]) (\varphi(A_0) - \varphi(\lambda))f, (\varphi(A_0) - \varphi(\lambda))f \right) \\ &= \limsup_{h \rightarrow 0} \frac{1}{h} \int_{\lambda}^{\lambda+h} d \left( E_0(t) (\varphi(A_0) - \varphi(\lambda))f, (\varphi(A_0) - \varphi(\lambda))f \right) \end{aligned}$$

holds for  $\lambda \in \mathbb{R}$  and  $f \in \mathcal{D}_{\lambda}$ . From

$$\left( E_0(t) (\varphi(A_0) - \varphi(\lambda))f, (\varphi(A_0) - \varphi(\lambda))f \right) = \int_{-\infty}^t |\varphi(s) - \varphi(\lambda)|^2 d(E_0(s)f, f)$$

we find

$$[\varphi(A_0)f - \varphi(\lambda)f]_{E_0, \lambda}^2 = \limsup_{h \rightarrow 0} \frac{1}{h} \int_{\lambda}^{\lambda+h} |\varphi(t) - \varphi(\lambda)|^2 d(E_0(t)f, f).$$

As  $f$  belongs to  $D_{\lambda}$  and  $\varphi$  is continuous on  $\sigma(A_0)$  we obtain that this expression is zero.  $\square$

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