Scattering matrices and Weyl functions of quasi boundary triples

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In memory of Boris Sergeevich Pavlov

Abstract. In this note a representation formula for the scattering matrix of a pair of self-adjoint extensions of a non-densely defined symmetric operator with infinite deficiency indices is proved with the help of quasi boundary triples and their Weyl functions. This result is a generalization of a classical formula by V.A. Adamyan and B.S. Pavlov.

1. Introduction

Mathematical scattering theory and its applications is a central theme in the works of B.S. Pavlov. Among his numerous contributions in this area we mention here the works [1, 3, 4, 5, 8, 26, 36, 37, 39, 40, 41, 42, 43] and we point out the famous classical paper [2], which can also be viewed as the origin of the present note on scattering matrices. In fact, in [2] V.A. Adamyan and B.S. Pavlov proved a representation formula in terms of M.G. Krein's Q-function for the scattering matrix of a pair of self-adjoint extensions A and B of a symmetric operator with finite deficiency indices (see also [6]). In this situation the resolvents of A and B differ by a finite rank operator, that is,

$$\dim\bigl(\operatorname{ran}\bigl((A-\lambda)^{-1}-(B-\lambda)^{-1}\bigr)\bigr)<\infty \tag{1.1}$$

holds for some (and hence for all) $\lambda \in \rho(A)\cap\rho(B)$, and the S-matrix becomes a matrix-valued function in a spectral representation of the absolutely continuous part of A. This important result was revisited and newly interpreted in [15] using the concept of ordinary boundary triples and their Weyl functions from extension theory of symmetric operators, see also [14, 16]. Only very recently in [17] the finite rank condition (1.1) was relaxed and, roughly speaking, replaced by the typical trace class assumption

$$(A-\lambda)^{-1}-(B-\lambda)^{-1}\in\mathfrak{S}_1 \tag{1.2}$$

for some (and hence for all) $\lambda \in \rho(A) \cap \rho(B)$. In this more general situation it is convenient to work with so-called generalized or quasi boundary triples, instead of ordinary boundary triples, in particular, this allows to apply the representation formula for the S-matrix to scattering problems involving different self-adjoint realizations of second order elliptic PDE's on unbounded domains. For related recent results we also refer the reader to [33, 34, 35].

The main objective of the present note on scattering matrices is to provide a slight generalization of the main representation formula for the scattering matrix in [17]. Here we shall extend [17, Theorem 3.1] in two directions. Firstly, we formulate and prove the representation formula in the framework of quasi boundary triples (instead of generalized boundary triples), which allows a bit more flexibility in applications to differential operators (see also [10, 17]), and secondly, we drop the assumption that the underlying symmetric operator is densely defined. We also note that the trace class condition (1.2) will follow automatically from our assumptions on the γ-field and Weyl function M of the quasi boundary triple; instead of $\mathfrak{S}_1$-regularity of the Weyl function as in [17, Theorem 3.1] we shall impose a Hilbert-Schmidt condition on the γ-field and require the values of M^{-1} to be bounded. The present generalizations lead to some technical difficulties in the proof of the representation formula for the S-matrix. More precisely, since the values of the Weyl function of a quasi boundary triple may be non-closed and unbounded operators, particular attention has to be paid in some of the main steps of the proof. Furthermore, if the domain of the underlying symmetric operator is not dense the adjoint needs to be interpreted in the sense of linear relations (multi-valued operators) and hence it is necessary to use boundary triple techniques for linear relations here. However, these additional efforts are worthwhile since problems in mathematical scattering theory naturally lead to non-densely defined symmetric defined operators. As an example we consider a scattering system consisting of one-dimensional Schrödinger operators with a real-valued bounded integrable potential in $L^2(\mathbb{R})$. Here the underlying symmetric operator is defined on all $H^2(\mathbb{R})$-functions that vanish on the support of the potential, and hence is non-densely defined. We shall illustrate how a quasi boundary triple for the adjoint relation can be chosen and derive a representation of the scattering matrix in this case from our main result Theorem 3.1.

Acknowledgement.

J.B. is most grateful to the organizers of the conferences *Spectral Theory and Applications*, March 2016, at Stockholm University, Sweden, and *OTAMP 2016*, August 2016, at the Euler Institute, St. Petersburg, Russia, for the hospitality at their institutions. This work is also supported by the Austrian Science Fund (FWF), project P 25162-N26. The authors wish to thank M.M. Malamud for numerous fruitful discussions. We are also indebted to the anonymous referee for a very careful reading of our manuscript and for pointing out various improvements.

2. Scattering systems and Weyl functions of quasi boundary triples

Let A and B be self-adjoint operators in a separable Hilbert space $\mathfrak{H}$. The pair $\{A, B\}$ may be viewed as a scattering system, where A stands for the unperturbed operator and B for the perturbed operator. In this preparatory section we do not impose any conditions on the type of the perturbation. We shall discuss in the following how (quasi) boundary triples may be used to regard A and B as self-adjoint extensions of an underlying symmetric operator and how the resolvent difference of A and B can be factorized in a convenient Krein type formula. In the following operators will often be identified with their graphs.

Let $S = A \cap B$ be the intersection (of the graphs) of A and B. Then S is given by

$$Sf := Af = Bf, \quad \operatorname{dom} S = \bigl\{ f \in \operatorname{dom} A \cap \operatorname{dom} B : Af = Bf \bigr\}. \tag{2.1}$$

In general the domain of S is not a dense subspace of $\mathfrak{H}$, and it may happen that $\operatorname{dom} S = \{0\}$. However, S is a closed operator in $\mathfrak{H}$ and since A and B are self-adjoint extensions of S it is clear that S is a symmetric operator in $\mathfrak{H}$. The adjoint S^* of S is defined as the linear relation

$$S^* = \bigl\{ \{g, g'\} : (Sf, g) = (f, g') \text{ for all } f \in \operatorname{dom} S \bigr\} \subset \mathfrak{H} \times \mathfrak{H};$$

here and in the following we write elements in linear relations (linear subspaces) in a pair notation, e.g. $\{g, g'\}$. It is clear that S^* is (the graph of) an operator if and only if $\operatorname{dom} S$ is dense in $\mathfrak{H}$, otherwise S^* has a nontrivial multivalued part (that is, there exists elements of the form $\{0, g'\} \in S^*$, $g' \neq 0$). We shall view A and B as self-adjoint restrictions of the adjoint relation S^* and use the techniques of (quasi) boundary triples from extension theory of symmetric operators and relations. We refer the reader to [7, 24, 25, 27] for more details on linear relations and to [11, 12, 20, 21, 22, 23, 29, 46] for the notion of ordinary, generalized, and quasi boundary triples for linear operators and relations. In the following we repeat a few necessary definitions from [11, 12] and provide a useful factorization of the difference of the resolvents of A and B in Proposition 2.4.

Definition 2.1. *Let T be a linear relation in the Hilbert space $\mathfrak{H}$ such that $\overline{T} = S^*$. Then $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is said to be a quasi boundary triple for S^* if $\mathcal{G}$ is a Hilbert space and $\Gamma_0, \Gamma_1 : T \to \mathcal{G}$ are linear mappings such that the following conditions* (i)–(iii) *are satisfied.*

(i) *The abstract Green's identity*

$$(f', g) - (f, g') = (\Gamma_1 \widehat{f}, \Gamma_0 \widehat{g}) - (\Gamma_0 \widehat{f}, \Gamma_1 \widehat{g})$$

holds for all $\widehat{f} = \{f, f'\}$, $\widehat{g} = \{g, g'\} \in T$;

(ii) *The range of the mapping $(\Gamma_0, \Gamma_1)^\top : T \to \mathcal{G} \times \mathcal{G}$ is dense;*

(iii) *$A_0 := \ker \Gamma_0$ is a self-adjoint relation in $\mathfrak{H}$.*

Assume that $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for $\overline{T} = S^*$ and let $A_0 = \ker \Gamma_0$. For $\lambda \in \rho(A_0)$ one verifies the direct sum decomposition

$$T = A_0 \,\widehat{+}\, \widehat{\mathcal{N}}_\lambda(T), \quad \widehat{\mathcal{N}}_\lambda(T) = \bigl\{\{f_\lambda, \lambda f_\lambda\} : f_\lambda \in \ker(T - \lambda)\bigr\}, \tag{2.2}$$

which implies that $\Gamma_0 \upharpoonright \widehat{\mathcal{N}}_\lambda(T)$ is invertible. In the decomposition (2.2) the direct sum $\mathcal{A} \widehat{+} \mathcal{N}$ of linear relations $\mathcal{A}$ and $\mathcal{N}$ such that $\mathcal{A} \cap \mathcal{N} = \{0\}$ is defined by $\mathcal{A} \widehat{+} \mathcal{N} = \{f + g, f' + g'\}$, where $\{f, f'\} \in \mathcal{A}$ and $\{g, g'\} \in \mathcal{N}$.

We then define the γ-field and Weyl function corresponding to the quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ as operator functions on $\rho(A_0)$ by

$$\lambda \mapsto \gamma(\lambda) = \pi_1 \bigl(\Gamma_0 \upharpoonright \widehat{\mathcal{N}}_\lambda(T)\bigr)^{-1} \quad \text{and} \quad \lambda \mapsto M(\lambda) = \Gamma_1 \bigl(\Gamma_0 \upharpoonright \widehat{\mathcal{N}}_\lambda(T)\bigr)^{-1};$$

here π_1 denotes the projection onto the first component of $\mathfrak{H} \times \mathfrak{H}$. We refer the reader to [11, 12] for a detailed discussion of the properties of the γ-field and Weyl function; here we only recall [11, Proposition 2.6].

Proposition 2.2. *Let $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi-boundary triple for S^* with γ-field γ and Weyl function M. For $\lambda, \mu \in \rho(A_0)$ the following holds.*

(i) *$\gamma(\lambda)$ is a densely defined operator from $\mathcal{G}$ into $\mathfrak{H}$ with $\operatorname{dom} \gamma(\lambda) = \operatorname{ran} \Gamma_0$ such that the function $\lambda \mapsto \gamma(\lambda)\varphi$ is holomorphic on $\rho(A_0)$ for every $\varphi \in \operatorname{ran} \Gamma_0$ and*

$$\gamma(\lambda) = \bigl(I + (\lambda - \mu)(A_0 - \lambda)^{-1}\bigr)\gamma(\mu)$$

holds. Moreover, for each $\lambda \in \rho(A_0)$ the operator $\gamma(\lambda)$ is closable and its closure $\overline{\gamma(\lambda)}$ is a bounded operator from $\mathcal{G}$ into $\mathfrak{H}$.

(ii) *$\gamma(\overline{\lambda})^*$ is a bounded mapping defined on $\mathfrak{H}$ with values in $\operatorname{ran} \Gamma_1 \subset \mathcal{G}$ and for all $h \in \mathfrak{H}$ we have*

$$\gamma(\overline{\lambda})^* h = \Gamma_1 \begin{pmatrix} (A_0 - \lambda)^{-1} h \\ (I + \lambda (A_0 - \lambda)^{-1}) h \end{pmatrix}.$$

(iii) *$M(\lambda)$ is a densely defined operator in $\mathcal{G}$ with $\operatorname{dom} M(\lambda) = \operatorname{ran} \Gamma_0$ and $\operatorname{ran} M(\lambda) \subset \operatorname{ran} \Gamma_1$.*

(iv) *$M(\lambda)\Gamma_0 \widehat{f}_\lambda = \Gamma_1 \widehat{f}_\lambda$ for all $\widehat{f}_\lambda \in \widehat{\mathcal{N}}_\lambda(T)$.*

(v) *$M(\lambda) \subseteq M(\overline{\lambda})^*$ and*

$$M(\lambda)\varphi - M(\mu)^*\varphi = (\lambda - \overline{\mu})\gamma(\mu)^*\gamma(\lambda)\varphi, \quad \varphi \in \operatorname{dom} M(\lambda).$$

The function $\lambda \mapsto M(\lambda)$ is holomorphic in the sense that it can be written as $M(\lambda) = C + L(\lambda)$, where

$$C\varphi := \operatorname{Re} M(i)\varphi = \frac{1}{2}(M(i) + M(i)^*)\varphi, \quad \varphi \in \operatorname{dom} C := \operatorname{dom} M(i),$$

is a possible unbounded symmetric operator and $L(\lambda)$ is given by

$$L(\lambda) := \gamma(i)^*(\lambda + (1 + \lambda^2)(A_0 - \lambda)^{-1})\overline{\gamma(i)}, \quad \lambda \in \rho(A_0).$$

In the next lemma we show that the inclusion $\operatorname{ran} M(\lambda) \subset \operatorname{ran} \Gamma_1$ in Proposition 2.2 (iii) becomes an equality if the relation $A_1 := \ker \Gamma_1$ is assumed to be self-adjoint in $\mathfrak{H}$. Note that by Green's identity A_1 is automatically symmetric.

Lemma 2.3. *Let* $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ *be a quasi-boundary triple for* S^* *with Weyl function* M *and assume, in addition, that* $A_1 = \ker \Gamma_1$ *is a self-adjoint relation in* $\mathfrak{H}$. *Then for all* $\lambda \in \rho(A_0) \cap \rho(A_1)$ *the operator* $M(\lambda)$ *maps* $\operatorname{ran} \Gamma_0$ *onto* $\operatorname{ran} \Gamma_1$ *and* $M(\lambda)^{-1}$ *exist and is defined on* $\operatorname{ran} \Gamma_1$.

Proof. The assumption that $A_1 = \ker \Gamma_1$ is self-adjoint implies that the transposed triple $\Pi^\top = \{\mathcal{G}, \Gamma_1, -\Gamma_0\}$ is also quasi-boundary triple for S^*. The corresponding Weyl function $M^\top(\lambda)$, $\lambda \in \rho(A_1)$, is defined on $\operatorname{ran} \Gamma_1$ and has values in $\operatorname{ran} \Gamma_0$. One easily checks that $M^\top(\lambda) M(\lambda) g = -g$, $g \in \operatorname{ran} \Gamma_0$, and $M(\lambda) M^\top(\lambda) h = -h$, $h \in \operatorname{ran} \Gamma_1$, $\lambda \in \rho(A_0) \cap \rho(A_1)$. Hence $M(\lambda)$ maps $\operatorname{ran} \Gamma_0$ onto $\operatorname{ran} \Gamma_1$ and is invertible. □

The next result will be used in the formulation and proof of our abstract representation formula for the scattering matrix in the next section. The statement on the existence of a quasi boundary triple follows for the case that S is densely defined also from [17, Proposition 2.9 (i)] and the Krein-type resolvent formula in (2.4) is a special case of [12, Corollary 6.17] or [13, Corollary 3.9].

Proposition 2.4. *Let* A *and* B *be self-adjoint operators in* $\mathfrak{H}$ *and consider the closed symmetric operator* $S = A \cap B$. *Then the closure of the linear relation* $T = A \widehat{+} B$ *coincides with the adjoint relation* S^* *and there exists a quasi boundary triple* $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ *for* $T \subset S^*$ *such that*

$$A = \ker \Gamma_0 \quad \text{and} \quad B = \ker \Gamma_1. \tag{2.3}$$

Furthermore, if γ *and* M *are the corresponding* γ*-field and Weyl function then*

$$(B - \lambda)^{-1} - (A - \lambda)^{-1} = -\gamma(\lambda) M(\lambda)^{-1} \gamma(\overline{\lambda})^*, \quad \lambda \in \rho(A) \cap \rho(B). \tag{2.4}$$

Proof. Since A and B are self-adjoint extensions of the closed symmetric operator $S = A \cap B$ (see also (2.1)) there exists an ordinary boundary triple $\Pi' = \{\mathcal{G}, \Lambda_0, \Lambda_1\}$ for S^* and a self-adjoint operator Θ in $\mathcal{G}$ such that

$$A = \ker \Lambda_0 \ \text{and} \ B = \ker(\Lambda_1 - \Theta \Lambda_0). \tag{2.5}$$

We note that in the present situation the self-adjoint parameter Θ in $\mathcal{G}$ is an operator (and not a linear relation) since $S = A \cap B$, that is, A and B are disjoint self-adjoint extensions of S (cf. [20, 22, 23, 29]). Now consider the restriction $T := A \widehat{+} B$ of S^*. Since A and B are disjoint self-adjoint extensions of S it follows that $\overline{T} = S^*$, see [17, Proposition 2.9]. We claim that $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$, where

$$\Gamma_0 \widehat{f} := \Lambda_0 \widehat{f} \ \text{and} \ \Gamma_1 \widehat{f} := \Lambda_1 \widehat{f} - \Theta \Lambda_0 \widehat{f}, \quad \widehat{f} \in T,$$

is a quasi boundary triple for $T \subset S^*$ such that (2.3) holds. In fact, (2.3) is clear from (2.5) and the definition of Γ_0 and Γ_1, and hence it remains to check items (i)–(iii) in Definition 2.1. For $\widehat{f} = \{f, f'\}, \widehat{g} = \{g, g'\} \in T$ one computes

$$\begin{aligned}(\Gamma_1\widehat{f},\Gamma_0\widehat{g})-(\Gamma_0\widehat{f},\Gamma_1\widehat{g}) &= \bigl(\Lambda_1\widehat{f}-\Theta\Lambda_0\widehat{f},\Lambda_0\widehat{g}\bigr)-\bigl(\Lambda_0\widehat{f},\Lambda_1\widehat{g}-\Theta\Lambda_0\widehat{g}\bigr)\\ &= (\Lambda_1\widehat{f},\Lambda_0\widehat{g})-(\Lambda_0\widehat{f},\Lambda_1\widehat{g})\\ &= (f',g)-(f,g')\end{aligned}$$

and hence the abstract Green's identity is valid. Next, assume that

$$0=\left(\begin{pmatrix}\varphi\\ \psi\end{pmatrix},\begin{pmatrix}\Gamma_0\widehat{f}\\ \Gamma_1\widehat{f}\end{pmatrix}\right)=\bigl(\varphi,\Lambda_0\widehat{f}\bigr)+\bigl(\psi,\Lambda_1\widehat{f}-\Theta\Lambda_0\widehat{f}\bigr)$$

holds for some $\varphi,\psi\in\mathcal{G}$ and all $\widehat{f}\in T$. Since $\Pi'=\{\mathcal{G},\Lambda_0,\Lambda_1\}$ is an ordinary boundary triple the map $(\Lambda_0,\Lambda_1)^\top: S^*\to\mathcal{G}\times\mathcal{G}$ is surjective. It follows that $\Lambda_1\upharpoonright\ker\Lambda_0$ maps onto $\mathcal{G}$ and hence for $\widehat{f}\in A=\ker\Lambda_0$ one has $0=(\psi,\Lambda_1\widehat{f})$, and therefore, $\psi=0$. Now $(\varphi,\Lambda_0\widehat{f})=0$ for $\widehat{f}\in T$, and the fact that the range of the restriction of Λ_0 onto T is dense in $\mathcal{G}$ (this follows since $\Lambda_0: S^*\to\mathcal{G}$ is surjective, continuous with respect to the norm on $S^*\subset\mathfrak{H}\times\mathfrak{H}$ and T is dense in S^*), yield $\varphi=0$. Therefore, the range of the mapping $(\Gamma_0,\Gamma_1)^\top: T\to\mathcal{G}\times\mathcal{G}$ is dense and hence condition (ii) in Definition 2.1 holds. Condition (iii) is clear from (2.3). Thus, we have shown that $\Pi=\{\mathcal{G},\Gamma_0,\Gamma_1\}$ is a quasi boundary triple for $\overline{T}=S^*$.

Next, we verify the Krein-type resolvent formula (2.4). To this end we note that the right-hand side of (2.3) makes sense by Proposition 2.2 and Lemma 2.3. It remains to show the equality of the left- and right-hand side. Let $g\in\mathfrak{H}$ and define $\widehat{f}=\{f,f'\}\in T=A_0\widehat{+}\widehat{\mathcal{N}}_\lambda(T)$ by

$$\begin{aligned}f &:= (A-\lambda)^{-1}g-\gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*g,\\ f' &:= (1+\lambda(A-\lambda)^{-1})g-\lambda\gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*g.\end{aligned}\tag{2.6}$$

Proposition 2.2 (ii) and the definition of the Weyl function yield

$$\Gamma_1\widehat{f}=\Gamma_1\bigl\{(A-\lambda)^{-1}g,(1+\lambda(A-\lambda)^{-1})g\bigr\}-M(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*g=0$$

and hence $\widehat{f}\in\ker\Gamma_1=B$. From (2.6), $A,B\subset T$, and $\operatorname{ran}\gamma(\lambda)=\ker(T-\lambda)$ one infers

$$(B-\lambda)f=(T-\lambda)(A-\lambda)^{-1}g-(T-\lambda)\gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*g=g$$

and together with (2.6) this yields the resolvent formula (2.4). □

3. Main result

Let again A and B be self-adjoint operators in a separable Hilbert space $\mathfrak{H}$, and assume first that

$$(B-\lambda)^{-1}-(A-\lambda)^{-1}\in\mathfrak{S}_1(\mathfrak{H})\tag{3.1}$$

holds for some, and hence for all, $\lambda\in\rho(A)\cap\rho(B)$. Here the symbol $\mathfrak{S}_1$ is used for the ideal of trace class operators. The ideal of Hilbert-Schmidt operators will be denoted in a similar way by $\mathfrak{S}_2$. The trace class condition

(3.1) will follow in Theorem 3.1 and Theorem 3.2 from other assumptions automatically. Denote the absolutely continuous subspaces of A and B by $\mathfrak{H}^{ac}(A)$ and $\mathfrak{H}^{ac}(B)$, respectively, let $P^{ac}(A)$ be the orthogonal projection onto $\mathfrak{H}^{ac}(A)$ and let $A^{ac} = A \upharpoonright (\operatorname{dom} A \cap \mathfrak{H}^{ac}(A))$ be the absolutely continuous part of A. It is well known (see, e.g., [9, 32, 45, 48, 49]) that under the trace class condition (3.1) the wave operators

$$W_\pm(B,A) := s - \lim_{t\to\pm\infty} e^{itB}e^{-itA}P^{ac}(A)$$

exist and are complete, i.e. $\operatorname{ran}(W_\pm(B,A)) = \mathfrak{H}^{ac}(B)$. The scattering operator is defined as $S(A,B) := W_+(B,A)^*W_-(B,A)$ and it follows that $S(A,B)$ is a unitary operator in $\mathfrak{H}^{ac}(A)$. In the following we discuss a representation formula for the scattering matrix $\{S_{AB}(\lambda)\}_{\lambda\in\mathbb{R}}$, a family of unitary operators in a spectral representation of the absolutely continuous part A^{ac} of A (see, e.g., [9, Chapter 4]), which is unitarily equivalent to the scattering operator $S(A,B)$.

The next theorem is a generalization of [17, Theorem 3.1] (see also [15, Theorem 3.8]). Instead of generalized boundary triples the result is formulated for quasi boundary triples here, and the assumption that the intersection of A and B is densely defined is dropped. The proof is similar to the one in [17], although more technical. For the convenience of the reader we give a self-contained complete proof in Section 4.

Theorem 3.1. *Let A and B be self-adjoint operators in $\mathfrak{H}$, suppose that the closed symmetric operator $S = A\cap B$ is simple, choose a quasi boundary triple $\{\mathcal{G},\Gamma_0,\Gamma_1\}$ for $\overline{T} = S^*$ such that $A = \ker\Gamma_0$ and $B = \ker\Gamma_1$ as in Proposition 2.4, and let γ and M be the corresponding γ-field and Weyl function M, respectively. Assume that*

$$\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2(\mathcal{G},\mathfrak{H}) \quad \textit{for some} \quad \lambda_0 \in \rho(A),$$

and that $\overline{M(\lambda_1)}$ is boundedly invertible in $\mathcal{G}$ for some $\lambda_1 \in \rho(A)\cap\rho(B)$. Then the following holds.

(i) *The resolvent difference of B and A is a trace class operator, that is,*

$$(B-\lambda)^{-1} - (A-\lambda)^{-1} \in \mathfrak{S}_1(\mathfrak{H}), \qquad \lambda\in\rho(A)\cap\rho(B).$$

(ii) *For all $\lambda\in\rho(A)\cap\rho(B)$ the closure of the Weyl function $\overline{M(\lambda)}$ exists and is boundedly invertible. Moreover, $L(\lambda) := \overline{M(\lambda) - \operatorname{Re} M(i)}$, $\lambda\in\rho(A)$, is a Nevanlinna function such that the limit $\overline{L(\lambda+i0)} = \lim_{y\downarrow 0}\overline{L(\lambda+iy)}$ exists in the operator norm for a.e. $\lambda\in\mathbb{R}$ and*

$$\overline{M(\lambda+i0)} := \overline{\operatorname{Re} M(i)} + L(\lambda+i0)$$

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

(iii) *The space $L^2(\mathbb{R},d\lambda,\mathcal{G}_\lambda)$, where $\mathcal{G}_\lambda := \overline{\operatorname{ran}\big(\operatorname{Im} M(\lambda+i0)\big)}$ for a.e. $\lambda\in\mathbb{R}$, forms a spectral representation of A^{ac} such that the scattering matrix $\{S_{AB}(\lambda)\}_{\lambda\in\mathbb{R}}$ of the scattering system $\{A,B\}$ admits the representation*

$$S_{AB}(\lambda) = I_{\mathcal{G}_\lambda} - 2i\sqrt{\overline{\operatorname{Im} M(\lambda+i0)}}\,\Big(\overline{M(\lambda+i0)}\Big)^{-1}\sqrt{\overline{\operatorname{Im} M(\lambda+i0)}}$$

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

In Theorem 3.1 it is assumed that the closed symmetric operator $S = A \cap B$ is simple. This assumption can be dropped and Theorem 3.1 admits a natural generalization, which will be explained next. If S is not simple then there is a nontrivial orthogonal decomposition of $\mathfrak{H} = \mathfrak{H}_1 \oplus \mathfrak{H}_2$ such that

$$S = H_1 \oplus H_2,$$

where H_1 is a simple symmetric operator in $\mathfrak{H}_1$ and H_2 is a self-adjoint operator in $\mathfrak{H}_2$. Then there exist self-adjoint extensions A_1 and B_1 of H_1 in $\mathfrak{H}_1$ such that

$$A = A_1 \oplus H_2 \qquad \text{and} \qquad B = B_1 \oplus H_2.$$

Let $L^2(\mathbb{R}, d\lambda, \mathcal{H}_\lambda)$ be a spectral representation of the absolutely continuous part H_2^{ac} of the self-adjoint operator H_2 in $\mathfrak{H}_2$. Then the following variant of Theorem 3.1 holds.

Theorem 3.2. *Let A and B be self-adjoint operators in $\mathfrak{H}$, let $S = A \cap B$, choose a quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ for $\overline{T} = S^*$ such that $A = \ker \Gamma_0$ and $B = \ker \Gamma_1$ as in Proposition 2.4, and let γ and M be the corresponding γ-field and Weyl function M, respectively. Assume that*

$$\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2(\mathcal{G}, \mathfrak{H}) \quad \textit{for some} \ \ \lambda_0 \in \rho(A),$$

and that $\overline{M(\lambda_1)}$ is boundedly invertible in $\mathcal{G}$ for some $\lambda_1 \in \rho(A) \cap \rho(B)$. Then the conclusions (i) *and* (ii) *of Theorem* 3.1 *are valid and instead* (iii) *the following holds.*

(iii') *The space $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda \oplus \mathcal{H}_\lambda)$, where $\mathcal{G}_\lambda := \overline{\operatorname{ran}\bigl(\overline{\operatorname{Im} M(\lambda + i0)}\bigr)}$ for a.e. $\lambda \in \mathbb{R}$ forms a spectral representation of A^{ac} and the scattering matrix $\{S_{AB}(\lambda)\}_{\lambda \in \mathbb{R}}$ of the scattering system $\{A, B\}$ admits the representation*

$$S_{AB}(\lambda) = \begin{pmatrix} S_{A_1 B_1}(\lambda) & 0 \\ 0 & I_{\mathcal{H}_\lambda} \end{pmatrix}$$

for a.e. $\lambda \in \mathbb{R}$, where $\{S_{A_1 B_1}(\lambda)\}_{\lambda \in \mathbb{R}}$ given in Theorem 3.1 (iii) *is the scattering matrix of the scattering system $\{A_1, B_1\}$.*

4. Proof of Theorem 3.1

The proof of Theorem 3.1 is split into steps. First we make clear in Lemma 4.1 and Lemma 4.2 in which sense the limits $M(\lambda \pm i0)$ and $\operatorname{Im} M(\lambda \pm i0)$ of the Weyl function M and its imaginary part are understood; cf. Theorem 3.1 (ii) and (iii).

Lemma 4.1. *Let M be the Weyl function corresponding to the quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ of Theorem 3.1. Then $\overline{\operatorname{Im} M(\lambda)} \in \mathfrak{S}_1(\mathcal{G})$ for all $\lambda \in \rho(A)$ and the limit*

$$\overline{\operatorname{Im} M(\lambda + i0)} := \lim_{\varepsilon \to +0} \overline{\operatorname{Im} M(\lambda + i\varepsilon)} \tag{4.1}$$

exists for a.e. $\lambda \in \mathbb{R}$ in $\mathfrak{S}_1(\mathcal{G})$.

Proof. From Proposition 2.2 (i) and the assumption $\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2(\mathcal{G},\mathfrak{H})$ for some $\lambda_0 \in \rho(A)$ it follows that $\overline{\gamma(\lambda)} \in \mathfrak{S}_2(\mathcal{G},\mathfrak{H})$ for all $\lambda \in \rho(A)$. Hence we also have $\gamma(\lambda)^* \in \mathfrak{S}_2(\mathfrak{H},\mathcal{G})$ and therefore Proposition 2.2 (v) yields

$$\overline{\operatorname{Im} M(\lambda)} = \operatorname{Im}(\lambda)\,\gamma(\lambda)^*\overline{\gamma(\lambda)} \in \mathfrak{S}_1(\mathcal{G}), \qquad \lambda \in \rho(A).$$

In particular, it follows that the limit in (4.1) exists for a.e. $\lambda \in \mathbb{R}$ in $\mathfrak{S}_1(\mathcal{G})$; cf. [18, 19, 38] or [28, Theorem 2.2]. □

Lemma 4.2. *Let M be the Weyl function corresponding to the quasi boundary triple $\Pi = \{\mathcal{G},\Gamma_0,\Gamma_1\}$ in Theorem 3.1. For all $\varphi \in \operatorname{ran}\Gamma_0$ and a.e. $\lambda \in \mathbb{R}$ the limit*

$$M(\lambda \pm i0)\varphi := \lim_{\varepsilon\to+0} M(\lambda \pm i\varepsilon)\varphi \tag{4.2}$$

exists and the operator $M(\lambda \pm i0)$ with $\operatorname{dom} M(\lambda \pm i0) = \operatorname{ran}\Gamma_0$ is closable. Moreover, for a.e. $\lambda \in \mathbb{R}$ the closure $\overline{M(\lambda + i0)}$ is boundedly invertible and

$$\big(\overline{M(\lambda + i0)}\big)^{-1} = \lim_{\varepsilon\to 0+} \overline{M(\lambda + i\varepsilon)^{-1}} = \lim_{\varepsilon\to+0}\big(\overline{M(\lambda + i\varepsilon)}\big)^{-1} \tag{4.3}$$

holds in the operator norm for a.e. $\lambda \in \mathbb{R}$.

Proof. In order to see that the limit in (4.2) exists and defines a closable operator in $\mathcal{G}$ we recall that $M(\lambda)$, $\lambda \in \rho(A)$, admits the representation

$$M(\lambda)\varphi = \operatorname{Re} M(i)\varphi + L(\lambda)\varphi$$

for $\varphi \in \operatorname{ran}\Gamma_0$, see Proposition 2.2 (v). Since $\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2(\mathcal{G},\mathfrak{H})$ by assumption we also have $\overline{\gamma(i)} \in \mathfrak{S}_2(\mathcal{G},\mathfrak{H})$ by Proposition 2.2 (i). Hence [9, Proposition 3.14] yields that the limits $L(\lambda \pm i0)$ of $L(\lambda \pm i\varepsilon)$ exist as $\varepsilon \to +0$ with respect to the Hilbert-Schmidt norm for a.e. $\lambda \in \mathbb{R}$. In particular, one has $L(\lambda \pm i0) \in \mathfrak{S}_2(\mathcal{G})$ for a.e. $\lambda \in \mathbb{R}$. Hence definition (4.2) makes sense and yields the representation

$$M(\lambda \pm i0)\varphi = \operatorname{Re} M(i)\varphi + L(\lambda \pm i0)\varphi$$

for all $\varphi \in \operatorname{dom} M(\lambda \pm i0) := \operatorname{ran}\Gamma_0$ and a.e. $\lambda \in \mathbb{R}$; thus there is a Borel set $\Lambda \subset \mathbb{R}$ of Lebesgue measure zero such that for each $\lambda \in \mathbb{R}\setminus\Lambda$ the limit operator $M(\lambda \pm i0)$ is well defined. The operators $M(\lambda \pm i0)$ are closable for a.e. $\lambda \in \mathbb{R}$ and the closures $\overline{M(\lambda \pm i0)}$ are given by

$$\overline{M(\lambda \pm i0)}\varphi = \overline{\operatorname{Re} M(i)}\varphi + L(\lambda \pm i0)\varphi \tag{4.4}$$

for all $\varphi \in \operatorname{dom}\overline{M(\lambda \pm i0)} = \operatorname{dom}\overline{\operatorname{Re} M(i)}$ and a.e. $\lambda \in \mathbb{R}$.

It will be shown next that the closures in (4.4) are boundedly invertible for a.e. $\lambda \in \mathbb{R}$ and that (4.3) holds in the operator norm for a.e. $\lambda \in \mathbb{R}$. Let us observe first that $\overline{M(\lambda)}$ is boundedly invertible for all $\lambda \in \rho(A)\setminus\mathcal{D}$, where $\mathcal{D}$ is a discrete subset of $\rho(A)$. In fact, since by our assumption there is some $\lambda_1 \in \rho(A)$ such that $\overline{M(\lambda_1)}$ is boundedly invertible it follows from Proposition 2.2 (v) that

$$\begin{aligned}\overline{M(\lambda)} &= \overline{M(\lambda_1)} + (\lambda - \overline{\lambda}_1)\gamma(\overline{\lambda}_1)^*\overline{\gamma(\lambda)}\\ &= \overline{M(\lambda_1)}\big[I - (\overline{\lambda}_1 - \lambda)\overline{M(\lambda_1)}^{\,-1}\gamma(\overline{\lambda}_1)^*\overline{\gamma(\lambda)}\,\big]\end{aligned}$$

holds for all $\lambda \in \rho(A)$. Furthermore, the operator-valued function

$$\lambda \mapsto (\overline{\lambda}_1 - \lambda)\overline{M(\lambda_1)}^{-1}\gamma(\overline{\lambda}_1)^*\overline{\gamma(\lambda)}$$

is holomorphic on $\rho(A)$ by Proposition 2.2 (i) and hence the analytic Fredholm theorem (see, e.g. [44, Theorem VI.14]) implies that

$$\overline{M(\lambda)}^{-1} = \bigl[I - (\overline{\lambda}_1 - \lambda)\overline{M(\lambda_1)}^{-1}\gamma(\overline{\lambda}_1)^*\overline{\gamma(\lambda)}\bigr]^{-1}\overline{M(\lambda_1)}^{-1}$$

is a bounded operator for all $\lambda \in \rho(A) \setminus \mathcal{D}$, where $\mathcal{D}$ is a discrete subset of $\rho(A)$.

Observe that the transposed triple $\Pi^\top = \{\mathcal{G}, \Gamma_1, -\Gamma_0\}$ is also a quasi boundary triple. The corresponding γ-field $\gamma^\top$ and Weyl function $M^\top$ are given by

$$\lambda \mapsto \gamma^\top(\lambda) = \gamma(\lambda)M(\lambda)^{-1} \quad \text{and} \quad \lambda \mapsto M^\top(\lambda) = -M(\lambda)^{-1},$$

for $\lambda \in \rho(A) \cap \rho(B)$, respectively. Hence $\overline{M^\top(\lambda)}$ is boundedly invertible for any $\lambda \in \rho(A) \cap \rho(B)$ and

$$\overline{M(\lambda)}\,\overline{M^\top(\lambda)} = \overline{M^\top(\lambda)}\,\overline{M(\lambda)} = -I, \quad \lambda \in \rho(A) \cap \rho(B).$$

Since $M^\top$ is the Weyl function of $\Pi^\top = \{\mathcal{G}, \Gamma_1, -\Gamma_0\}$ Proposition 2.2 (v) yields the representation

$$M^\top(\lambda)\varphi = \operatorname{Re} M^\top(i)\varphi + \gamma^\top(i)^*\bigl(\lambda + (\lambda^2+1)(B-\lambda)^{-1}\bigr)\gamma^\top(i)\varphi$$

for $\varphi \in \operatorname{ran}\Gamma_1$, and hence

$$K(\lambda) := \overline{M^\top(\lambda)} = \overline{\operatorname{Re} M^\top(i)} + L^\top(\lambda), \qquad \lambda \in \rho(A) \cap \rho(B),$$

where

$$L^\top(\lambda) := \gamma^\top(i)^*\bigl(\lambda + (\lambda^2+1)(B-\lambda)^{-1}\bigr)\overline{\gamma^\top(i)}.$$

Our assumptions in Theorem 3.1 yield $\overline{\gamma^\top(i)} = \overline{\gamma(i)}\,\overline{M(i)}^{-1} \in \mathfrak{S}_2(\mathcal{G}, \mathfrak{H})$ and $\gamma^\top(i)^* \in \mathfrak{S}_2(\mathfrak{H}, \mathcal{G})$, and therefore we conclude from [9, Proposition 3.14] that the limits $K(\lambda + i0)$ of $K(\lambda + i\varepsilon)$ as $\varepsilon \to +0$ exist for a.e. $\lambda \in \mathbb{R}$ in the operator norm. Hence we get

$$K(\lambda + i0)\overline{M(\lambda + i0)} = \overline{M(\lambda + i0)}K(\lambda + i0) = -I$$

for a.e. $\lambda \in \mathbb{R}$ and it follows that the operator $\overline{M(\lambda + i0)}$ is boundedly invertible for a.e. $\lambda \in \mathbb{R}$. □

The remaining part of the proof of Theorem 3.1 is similar to the proof of [15, Theorem 3.8] and [17, Theorem 3.1]. The idea is mainly based on Theorem 4.3 below, which follows from [9, Theorem 18.4]; cf. [17, Theorem A.2]. Some of the arguments require special care when working in the more general context of quasi boundary triples since the values of the γ-field and Weyl function are not closed operators in general; we provide the full details whenever necessary. In the following we shall denote by $\mathcal{L}(\mathcal{G})$ the space of bounded and everywhere defined operators in $\mathcal{G}$.

Theorem 4.3. *Assume that the self-adjoint operators A and B satisfy the trace class condition* (3.1) *and suppose that the resolvent difference admits the factorization*

$$(B-i)^{-1}-(A-i)^{-1}=\phi(A)CGC^*=QC^*,$$

where $C\in\mathfrak{S}_2(\mathcal{G},\mathfrak{H})$, let $\phi:\mathbb{R}\to\mathbb{R}$ be a bounded continuous function and $Q=\phi(A)CG$. Assume that

$$\mathfrak{H}^{ac}(A)=\operatorname{clsp}\left\{E_A^{ac}(\delta)[\operatorname{ran}C]:\delta\in\mathcal{B}(\mathbb{R})\right\} \tag{4.5}$$

holds and let $D(\lambda)=\frac{d}{d\lambda}C^*E_A((-\infty,\lambda))C$ and $\mathcal{G}_\lambda=\overline{\operatorname{ran}D(\lambda)}$ for a.e. $\lambda\in\mathbb{R}$. Then $L^2(\mathbb{R},d\lambda,\mathcal{G}_\lambda)$ is a spectral representation of A^{ac} and the scattering matrix of the scattering system $\{A,B\}$ is given by

$$S_{AB}(\lambda)=I_{\mathcal{G}_\lambda}+2\pi i(1+\lambda^2)^2\sqrt{D(\lambda)}Z(\lambda)\sqrt{D(\lambda)}$$

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

$$Z(\lambda)=\frac{1}{\lambda+i}Q^*Q+\frac{1}{(\lambda+i)^2}\phi(\lambda)G+\lim_{\varepsilon\to+0}Q^*\big(B-(\lambda+i\varepsilon)\big)^{-1}Q$$

and the limit of the last term on the right hand side exists in the Hilbert-Schmidt norm.

Proof of Theorem 3.1. (i) Since $\overline{\gamma(\lambda_0)}\in\mathfrak{S}_2(\mathcal{G},\mathfrak{H})$ for some $\lambda_0\in\rho(A)$ and $M(\lambda_1)^{-1}$ is bounded for some $\lambda_1\in\rho(A)\cap\rho(B)$ it follows from the statements in [13, Proposition 3.5] that $\overline{\gamma(\lambda)}\in\mathfrak{S}_2(\mathcal{G},\mathfrak{H})$ for all $\lambda\in\rho(A)$ and $M(\lambda)^{-1}$ is bounded for all $\lambda\in\rho(A)\cap\rho(B)$; cf. the proofs of Lemma 4.1 and Lemma 4.2. Then we also have $\gamma(\overline{\lambda})^*\in\mathfrak{S}_2(\mathfrak{H},\mathcal{G})$ for all $\lambda\in\rho(A)$ and hence the resolvent difference

$$(B-\lambda)^{-1}-(A-\lambda)^{-1}=-\gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*=-\overline{\gamma(\lambda)}\,\overline{M(\lambda)^{-1}}\gamma(\overline{\lambda})^*$$

is a trace class operator for all $\lambda\in\rho(A)\cap\rho(B)$.

(ii) This statement follows from Lemma 4.2.

(iii) This item is proved in two separate steps. In the first step we find a preliminary form of the scattering matrix making use of Theorem 4.3. In the second step we then obtain the final form of the scattering matrix.

Step 1. Expressing the resolvent difference at $\lambda=i$ in the same way as in the proof of (i) and using $\gamma(i)=(A+i)(A-i)^{-1}\gamma(-i)$ we obtain

$$\begin{aligned}(B-i)^{-1}-(A-i)^{-1}&=-\overline{\gamma(i)}\,\overline{M(i)^{-1}}\gamma(-i)^*\\&=-(A+i)(A-i)^{-1}\overline{\gamma(-i)}\,\overline{M(i)^{-1}}\gamma(-i)^*\\&=\phi(A)CGC^*,\end{aligned}$$

where we have chosen

$$\phi(t)=\frac{t+i}{t-i},\quad t\in\mathbb{R},\qquad C=\overline{\gamma(-i)}\quad\text{and}\quad G=-\overline{M(i)^{-1}}.$$

It follows in exactly the same way as in [17, Proof of Theorem 3.1] that the condition (4.5) in Theorem 4.3 holds. Now we compute the $\mathcal{L}(\mathcal{G})$-valued function

$$\lambda \mapsto D(\lambda) = \frac{d}{d\lambda} C^* E_A((-\infty,\lambda))C$$

and its square root $\lambda \mapsto \sqrt{D(\lambda)}$ for a.e. $\lambda \in \mathbb{R}$. First of all we have

$$\begin{aligned} D(\lambda) &= \lim_{\varepsilon\to 0+} \frac{1}{2\pi i} C^*\big((A-\lambda-i\varepsilon)^{-1} - (A-\lambda+i\varepsilon)^{-1}\big)C \\ &= \lim_{\varepsilon\to 0+} \frac{\varepsilon}{\pi} C^*\big((A-\lambda-i\varepsilon)^{-1}(A-\lambda+i\varepsilon)^{-1}\big)C. \end{aligned}$$

On the other hand

$$\operatorname{Im} M(\lambda+i\varepsilon) = \varepsilon\gamma(\lambda+i\varepsilon)^*\gamma(\lambda+i\varepsilon)$$

together with $\gamma(\lambda+i\varepsilon) = (A+i)(A-\lambda-i\varepsilon)^{-1}\gamma(-i)$ shows

$$\operatorname{Im} M(\lambda+i\varepsilon) = \varepsilon\gamma(-i)^*(I_{\mathfrak{H}}+A^2)\big(A-\lambda+i\varepsilon\big)^{-1}\big(A-\lambda-i\varepsilon\big)^{-1}\gamma(-i)$$

and hence we conclude

$$\overline{\operatorname{Im} M(\lambda+i\varepsilon)} = \varepsilon C^*(I_{\mathfrak{H}}+A^2)\big(A-\lambda+i\varepsilon\big)^{-1}\big(A-\lambda-i\varepsilon\big)^{-1}C.$$

This implies

$$\overline{\operatorname{Im} M(\lambda+i0)} = \lim_{\varepsilon\to 0+} \overline{\operatorname{Im} M(\lambda+i\varepsilon)} = \pi(1+\lambda^2)D(\lambda)$$

for a.e. $\lambda \in \mathbb{R}$ and, in particular, $\operatorname{ran}(\overline{\operatorname{Im} M(\lambda+i0)}) = \operatorname{ran} D(\lambda)$ for a.e. $\lambda \in \mathbb{R}$ and hence

$$\mathcal{G}_\lambda = \overline{\operatorname{ran}\big(\overline{\operatorname{Im} M(\lambda+i0)}\big)} = \overline{\operatorname{ran} D(\lambda)} \quad \text{for a.e. } \lambda \in \mathbb{R}.$$

Therefore, Theorem 4.3 yields that $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda)$ is a spectral representation of A^{ac} and the scattering matrix $\{S_{AB}(\lambda)\}_{\lambda\in\mathbb{R}}$ is given by

$$\begin{aligned} S_{AB}(\lambda) &= I_{\mathcal{G}_\lambda} + 2\pi i(1+\lambda^2)^2\sqrt{D(\lambda)}Z(\lambda)\sqrt{D(\lambda)} \\ &= I_{\mathcal{G}_\lambda} + 2i(1+\lambda^2)\sqrt{\overline{\operatorname{Im} M(\lambda+i0)}}Z(\lambda)\sqrt{\overline{\operatorname{Im} M(\lambda+i0)}} \end{aligned} \tag{4.6}$$

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

$$Z(\lambda) = \frac{1}{\lambda+i}Q^*Q + \frac{1}{(\lambda+i)^2}\phi(\lambda)G + \lim_{\varepsilon\to 0+} Q^*\big(B-(\lambda+i\varepsilon)\big)^{-1}Q \tag{4.7}$$

and $Q = \phi(A)CG$ is given by

$$Q = -(A+i)(A-i)^{-1}\overline{\gamma(-i)}\,\overline{M(i)^{-1}} = -\overline{\gamma(i)}\,\overline{M(i)^{-1}} \in \mathfrak{S}_2(\mathcal{G},\mathfrak{H}).$$

Step 2. In this step we compute the explicit form

$$Z(\lambda) = -\frac{1}{1+\lambda^2}\overline{M(\lambda+i0)^{-1}} \tag{4.8}$$

for a.e. $\lambda \in \mathbb{R}$ of $Z(\lambda)$ in (4.7). From this and (4.6) the asserted form of the scattering matrix follows immediately.

Observe that by Proposition 2.4 we have

$$\begin{aligned}\Gamma_0(B-\lambda)^{-1} &= \Gamma_0(A-\lambda)^{-1} - \Gamma_0\gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^* \\ &= -M(\lambda)^{-1}\gamma(\overline{\lambda})^* \\ &= -\overline{M(\lambda)^{-1}}\gamma(\overline{\lambda})^*\end{aligned}$$

for $\lambda \in \rho(A)\cap\rho(B)$ and hence

$$\begin{aligned}\Gamma_0(B+i)^{-1} &= -\overline{M(-i)^{-1}}\gamma(i)^* \\ &= \big(-\overline{\gamma(i)}(M(-i)^{-1})^*\big)^* \\ &= \big(-\overline{\gamma(i)}\,\overline{M(i)^{-1}}\big)^* \\ &= Q^*,\end{aligned}$$

where we have used $(M(-i)^{-1})^* = (M(-i)^*)^{-1} = \overline{M(i)^{-1}}$. This yields

$$\begin{aligned}Q^*(B-\lambda)^{-1}Q &= \Gamma_0(B+i)^{-1}(B-\lambda)^{-1}Q \\ &= \Gamma_0\big(Q^*(B-\overline{\lambda})^{-1}(B-i)^{-1}\big)^* \\ &= \Gamma_0\big(\Gamma_0(B+i)^{-1}(B-\overline{\lambda})^{-1}(B-i)^{-1}\big)^*.\end{aligned}\tag{4.9}$$

Since

$$\begin{aligned}(B+i)^{-1}(B-\overline{\lambda})^{-1}(B-i)^{-1} = \frac{-1}{1+\overline{\lambda}^2}&\big((B+i)^{-1}-(B-\overline{\lambda})^{-1}\big) \\ &+ \frac{1}{2i(\overline{\lambda}-i)}\big((B+i)^{-1}-(B-i)^{-1}\big)\end{aligned}$$

it follows from Proposition 2.4 that

$$\begin{aligned}&\Gamma_0(B+i)^{-1}(B-\overline{\lambda})^{-1}(B-i)^{-1} \\ &\qquad = \frac{1}{1+\overline{\lambda}^2}\big(M(-i)^{-1}\gamma(i)^* - M(\overline{\lambda})^{-1}\gamma(\lambda)^*\big) \\ &\qquad\quad - \frac{1}{2i(\overline{\lambda}-i)}\big(M(-i)^{-1}\gamma(i)^* - M(i)^{-1}\gamma(-i)^*\big).\end{aligned}$$

Taking into account $(M(\overline{\mu})^{-1})^* = \overline{M(\mu)^{-1}}$ for $\mu \in \rho(A)\cap\rho(B)$ we obtain for the adjoint

$$\begin{aligned}&\big(\Gamma_0(B+i)^{-1}(B-\overline{\lambda})^{-1}(B-i)^{-1}\big)^* \\ &\qquad = \frac{1}{1+\lambda^2}\big(\overline{\gamma(i)}\,\overline{M(i)^{-1}} - \overline{\gamma(\lambda)}\,\overline{M(\lambda)^{-1}}\big) \\ &\qquad\quad + \frac{1}{2i(\lambda+i)}\big(\overline{\gamma(i)}\,\overline{M(i)^{-1}} - \overline{\gamma(-i)}\,\overline{M(-i)^{-1}}\big)\end{aligned}$$

and for $\varphi \in \operatorname{ran}\Gamma_1 = \operatorname{dom} M(\mu)^{-1}$, $\mu \in \rho(A) \cap \rho(B)$, we then conclude from (4.9)

$$\begin{aligned}
Q^*(B-\lambda)^{-1}Q\varphi &= \Gamma_0\bigl(\Gamma_0(B+i)^{-1}(B-\overline{\lambda})^{-1}(B-i)^{-1}\bigr)^*\varphi \\
&= \frac{1}{1+\lambda^2}\Gamma_0\bigl(\gamma(i)M(i)^{-1} - \gamma(\lambda)M(\lambda)^{-1}\bigr)\varphi \\
&\qquad + \frac{1}{2i(\lambda+i)}\Gamma_0\bigl(\gamma(i)M(i)^{-1} - \gamma(-i)M(-i)^{-1}\bigr)\varphi \\
&= \frac{1}{1+\lambda^2}\bigl(M(i)^{-1} - M(\lambda)^{-1}\bigr)\varphi \\
&\qquad + \frac{1}{2i(\lambda+i)}\bigl(M(i)^{-1} - M(-i)^{-1}\bigr)\varphi
\end{aligned}$$

which extends by continuity from the dense set $\operatorname{ran}\Gamma_1$ onto $\mathcal{G}$ and takes the form

$$\begin{aligned}
Q^*(B-\lambda)^{-1}Q = \frac{1}{1+\lambda^2}&\bigl(\,\overline{M(i)^{-1}} - \overline{M(\lambda)^{-1}}\,\bigr) \\
&+ \frac{1}{2i(\lambda+i)}\bigl(\,\overline{M(i)^{-1}} - \overline{M(-i)^{-1}}\,\bigr).
\end{aligned}$$

This leads to

$$\begin{aligned}
\lim_{\varepsilon\to 0+} Q^*\bigl(B-(\lambda+i\varepsilon)\bigr)^{-1}Q = \frac{1}{1+\lambda^2}&\bigl(\,\overline{M(i)^{-1}} - \overline{M(\lambda+i0)^{-1}}\,\bigr) \\
&+ \frac{1}{2i(\lambda+i)}\bigl(\,\overline{M(i)^{-1}} - \overline{M(-i)^{-1}}\,\bigr)
\end{aligned}$$

for a.e. $\lambda \in \mathbb{R}$. Note also that by Lemma 4.2 the limit $\overline{M(\lambda+i0)^{-1}}$ exists for a.e. $\lambda \in \mathbb{R}$ in the operator norm.

Moreover, for $\varphi \in \operatorname{ran}\Gamma_1 = \operatorname{dom} M(\mu)^{-1}$, $\mu \in \rho(A) \cap \rho(B)$, we have

$$\begin{aligned}
Q^*Q\varphi &= \bigl(\overline{\gamma(i)}\,\overline{M(i)^{-1}}\bigr)^*\overline{\gamma(i)}\,\overline{M(i)^{-1}}\varphi \\
&= \overline{M(-i)^{-1}}\gamma(i)^*\gamma(i)M(i)^{-1}\varphi \\
&= \frac{1}{2i}M(-i)^{-1}\bigl(M(i) - M(-i)\bigr)M(i)^{-1}\varphi \\
&= \frac{1}{2i}\bigl(M(-i)^{-1} - M(i)^{-1}\bigr)\varphi.
\end{aligned}$$

Hence we obtain for $\varphi \in \operatorname{ran}\Gamma_1$ and a.e. $\lambda \in \mathbb{R}$ that

$$\begin{aligned} Z(\lambda)\varphi &= \frac{1}{\lambda+i}Q^*Q\varphi + \frac{1}{(\lambda+i)^2}\phi(\lambda)G\varphi + Q^*\big(B-(\lambda+i0)\big)^{-1}Q\varphi \\ &= \frac{1}{2i(\lambda+i)}\big(M(-i)^{-1}-M(i)^{-1}\big)\varphi - \frac{1}{1+\lambda^2}M(i)^{-1}\varphi \\ &\quad + \frac{1}{1+\lambda^2}\big(M(i)^{-1}-\overline{M(\lambda+i0)^{-1}}\big)\varphi \\ &\qquad\qquad + \frac{1}{2i(\lambda+i)}\big(M(i)^{-1}-M(-i)^{-1}\big)\varphi \\ &= -\frac{1}{1+\lambda^2}\overline{M(\lambda+i0)^{-1}}\varphi \end{aligned}$$

and since $\overline{M(\lambda+i0)^{-1}} \in \mathcal{L}(\mathcal{G})$ we conclude (4.8). This completes the proof of Theorem 3.1. □

5. An example

In this section we discuss a scattering system consisting of the one-dimensional Schrödinger operators $\{A, B\}$, where

$$Af = -f'', \quad Bf = -f'' + Vf, \qquad \operatorname{dom} A = \operatorname{dom} B = H^2(\mathbb{R}). \tag{5.1}$$

Our aim is to show in a particularly simple situation how quasi boundary triples for the adjoints of non-densely defined symmetric operators appear and can be applied to obtain a formula for the scattering matrix via Theorem 3.1. To avoid technical difficulties we will assume that the real-valued potential V in (5.1) satisfies the condition

$$V \in L^\infty(\mathbb{R}). \tag{5.2}$$

It is well known that the operators A and B in (5.1) are self-adjoint in $L^2(\mathbb{R})$. Later, in Lemma 5.2, it will also be assumed that $V \in L^1(\mathbb{R})$. In the present situation the symmetric operator $S = A \cap B$ has the form

$$Sf = -f'' = -f'' + Vf, \qquad \operatorname{dom} S = \big\{f \in H^2(\mathbb{R}) : Vf = 0\big\}, \tag{5.3}$$

and, in general, S is not densely defined. In particular, it may happen that $\operatorname{dom} S = \{0\}$. In the following we use the factorization

$$V = \sqrt{|V|}\,\operatorname{sgn}(V)\sqrt{|V|} = D^*UD, \tag{5.4}$$

where

$$D : L^2(\mathbb{R}) \to \mathcal{G}, \qquad f \mapsto \sqrt{|V|}f,$$

$\mathcal{G} := \overline{\operatorname{ran}\sqrt{|V|}}$, and $U : \mathcal{G} \to \mathcal{G}$, $\varphi \mapsto \operatorname{sgn}(V)\varphi$. Observe that $\operatorname{ran} D$ is dense in $\mathcal{G}$ and that U is a unitary operator in $\mathcal{G}$. In the next proposition we shall construct a suitable quasi boundary triple for the adjoint relation S^*. For our purposes it is convenient to introduce the linear relation

$$T = \big\{\{f, -f'' + Vh\} : f, h \in H^2(\mathbb{R})\big\}$$

in $L^2(\mathbb{R})\times L^2(\mathbb{R})$. It is not difficult to see that $T = A \widehat{+} B$ holds. We emphasize that the quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ below is not a generalized boundary triple in the sense of [23, Definition 6.1] whenever $\operatorname{ran} D$ is not closed.

Proposition 5.1. *Let A, B and S, T be as above. Then $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$, where*

$$\mathcal{G} = \overline{\operatorname{ran}\sqrt{|V|}}, \qquad \Gamma_0 \widehat{f} = Dh \quad \text{and} \quad \Gamma_1 \widehat{f} = UDh - UDf,$$

$\widehat{f} = \{f, -f'' + Vh\} \in T$, is a quasi boundary triple for $\overline{T} = S^*$ such that $A = \ker\Gamma_0$ and $B = \ker\Gamma_1$. The corresponding γ-field and Weyl function are given by

$$\gamma(\lambda)\varphi = -(A-\lambda)^{-1}D^*\varphi, \quad \varphi \in \operatorname{ran}\Gamma_0,$$

and

$$M(\lambda)\varphi = U\varphi + UD(A-\lambda)^{-1}D^*U\varphi, \quad \varphi \in \operatorname{ran}\Gamma_0.$$

Proof. Consider two elements $\widehat{f} = \{f, -f'' + Vh\}$, $\widehat{g} = \{g, -g'' + Vk\} \in T$ and note that $(-f'', g)_{L^2(\mathbb{R})} - (f, -g'')_{L^2(\mathbb{R})} = 0$ as $f, g \in H^2(\mathbb{R}) = \operatorname{dom} A$ and A is a self-adjoint operator. A straightforward computation shows

$$\begin{aligned}
&\big(-f'' + Vh, g\big)_{L^2(\mathbb{R})} - \big(f, -g'' + Vk\big)_{L^2(\mathbb{R})}\\
&\quad= (Vh, g)_{L^2(\mathbb{R})} - (f, Vk)_{L^2(\mathbb{R})}\\
&\quad= (h, Vg)_{L^2(\mathbb{R})} - (Vf, k)_{L^2(\iota)} + (Vh, k)_{L^2(\mathbb{R})} - (h, Vk)_{L^2(\mathbb{R})}\\
&\quad= \big(Vh - Vf, k\big)_{L^2(\mathbb{R})} - \big(h, Vk - Vg\big)_{L^2(\mathbb{R})}\\
&\quad= \big(UDh - UDf, Dk\big)_{\mathcal{G}} - \big(Dh, UDk - UDg\big)_{\mathcal{G}}\\
&\quad= (\Gamma_1\widehat{f}, \Gamma_0\widehat{g})_{\mathcal{G}} - (\Gamma_0\widehat{f}, \Gamma_1\widehat{g})_{\mathcal{G}}
\end{aligned}$$

and hence the abstract Green's identity in Definition 2.1 is satisfied. Next we check that $\operatorname{ran}(\Gamma_0, \Gamma_1)^\top$ is dense in $\mathcal{G}\times\mathcal{G}$. Assume that for some $\zeta, \xi \in \mathcal{G}$ we have

$$0 = (\zeta, \Gamma_0\widehat{f})_{\mathcal{G}} + (\xi, \Gamma_1\widehat{f})_{\mathcal{G}} = (\zeta, Dh)_{\mathcal{G}} + (\xi, UDh - UDf)_{\mathcal{G}} \tag{5.5}$$

for all $\widehat{f} = \{f, -f'' + Vh\} \in T$. In particular, if $h = 0$ then

$$0 = (\xi, UDf)_{\mathcal{G}} = (D^*U^*\xi, f)_{L^2(\mathbb{R})}$$

for all $f \in H^2(\mathbb{R})$. Hence $D^*U^*\xi = 0$ and $\ker D^* = (\operatorname{ran} D)^\perp = \{0\}$ yields $U^*\xi = 0$. But U is unitary and thus we conclude $\xi = 0$. Now (5.5) reduces to $0 = (\zeta, Dh)_{\mathcal{G}} = (D^*\zeta, h)_{L^2(\mathbb{R})}$ for all $h \in H^2(\mathbb{R})$. As above $\ker D^* = \{0\}$ implies $\zeta = 0$. We have shown that $\operatorname{ran}(\Gamma_0, \Gamma_1)^\top$ is dense in $\mathcal{G}\times\mathcal{G}$.

Furthermore, if $\widehat{f} \in \ker\Gamma_0$ then $Dh = 0$ for all $h \in H^2(\mathbb{R})$, and hence $Vh = 0$ for all $h \in H^2(\mathbb{R})$ by (5.4). Therefore

$$\ker\Gamma_0 = \big\{\{f, -f''\} : f \in H^2(\mathbb{R})\big\} = A$$

and it follows that $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for $\overline{T} = S^*$. Moreover, if $\widehat{f} \in \ker\Gamma_1$ then $Dh = Df$ and hence $Vh = Vf$ by (5.4). This implies

$$\ker\Gamma_1 = \big\{\{f, -f'' + Vf\} : f \in H^2(\mathbb{R})\big\} = B.$$

It remains to verify the assertions on the form of the γ-field and Weyl function corresponding to the quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$. Note first that in the present situation for $\lambda \in \rho(A)$ we have

$$\widehat{\mathcal{N}}_\lambda(T) = \bigl\{\{f_\lambda, \lambda f_\lambda\} : f_\lambda = -(A-\lambda)^{-1}Vh,\, h \in H^2(\mathbb{R})\bigr\}.$$

As

$$\lambda f_\lambda = -\lambda(A-\lambda)^{-1}Vh = -A(A-\lambda)^{-1}Vh + Vh = Af_\lambda + Vh$$

it follows that the elements $\widehat{f}_\lambda \in \widehat{\mathcal{N}}_\lambda(T)$ have the form

$$\widehat{f}_\lambda = \bigl\{f_\lambda, -f_\lambda'' + Vh\bigr\}, \quad f_\lambda = -(A-\lambda)^{-1}Vh.$$

Using (5.4) we find

$$\widehat{f}_\lambda = \bigl\{f_\lambda, -f_\lambda'' + D^*UDh\bigr\}, \quad f_\lambda = -(A-\lambda)^{-1}D^*UDh. \tag{5.6}$$

Setting $\varphi = Dh \in \operatorname{ran}\Gamma_0$, $h \in H^2(\mathbb{R})$, we get

$$\widehat{f}_\lambda = \bigl\{f_\lambda, -f_\lambda'' + D^*U\varphi\bigr\}, \quad f_\lambda = -(A-\lambda)^{-1}D^*U\varphi.$$

By definition one has $\Gamma_0\widehat{f}_\lambda = Dh = \varphi$ which yields

$$\gamma(\lambda)\varphi = f_\lambda = -(A-\lambda)^{-1}D^*U\varphi.$$

Hence the assertion on the γ-field is proven. Furthermore, applying Γ_1 to the same element in (5.6) gives

$$\Gamma_1\widehat{f}_\lambda = UDh - UDf_\lambda = U\varphi + UD(A-\lambda)^{-1}D^*U\varphi$$

which implies the assertion on the Weyl function. □

In the next lemma we shall strengthen the condition (5.2) on V such that the assumptions on γ and M in Theorem 3.1 are satisfied.

Lemma 5.2. *Assume that the real-valued potential V in* (5.1) *satisfies*

$$V \in L^\infty(\mathbb{R}) \cap L^1(\mathbb{R}) \tag{5.7}$$

and let γ and M be the γ-field and Weyl function corresponding to the quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ in Proposition 5.1. *Then*

$$\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2\bigl(\mathcal{G}, L^2(\mathbb{R})\bigr) \tag{5.8}$$

for some $\lambda_0 \in \rho(A)$ and $\overline{M(\lambda_1)}$ is boundedly invertible for some $\lambda_1 \in \rho(A) \cap \rho(B)$.

Proof. The assumption (5.7) yields that $D(A-\overline{\lambda})^{-1}$ is a Hilbert-Schmidt operator for all $\lambda \in \rho(A)$. Hence $(A-\lambda)^{-1}D^*U$ is also a Hilbert-Schmidt operator and (5.8) follows for all $\lambda_0 \in \rho(A)$. Moreover, one has

$$\overline{M(\lambda)} = U + UD(A-\lambda)^{-1}D^*U, \quad \lambda \in \rho(A).$$

For $\mathrm{Im}(\lambda)$ sufficiently large the operator norm $UD(A-\lambda)^{-1}D^*U^*$ becomes small and hence $\overline{M(\lambda_1)}$ is boundedly invertible for some $\lambda_1 \in \rho(A)\cap\rho(B)$. □

Finally, we summarize the conclusion for the scattering matrix of the scattering system $\{A, B\}$. Here it is clear that the resolvent difference of A and B is a trace class operator (see, e.g. [47, Lemma 9.34]) and this also follows from Theorem 3.1. Furthermore, the symmetric operator S in (5.3) is simple and the absolutely continuous part A^{ac} of A coincides with A. Hence by Theorem 3.1 the scattering matrix $\{S_{AB}(\lambda)\}_{\lambda\in\mathbb{R}}$ of the scattering system $\{A, B\}$ admits the representation

$$S_{AB}(\lambda) = I_{\mathcal{G}_\lambda} - 2i\sqrt{\operatorname{Im} M(\lambda + i0)}\left(\overline{M(\lambda + i0)}\right)^{-1}\sqrt{\operatorname{Im} M(\lambda + i0)} \tag{5.9}$$

for a.e. $\lambda \in \mathbb{R}$, and $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda)$, where

$$\mathcal{G}_\lambda := \overline{\operatorname{ran}\big(\overline{\operatorname{Im} M(\lambda + i0)}\big)} \tag{5.10}$$

for a.e. $\lambda \in \mathbb{R}$, is a spectral representation of A. It will turn out next that the limit $\operatorname{Im} M(\lambda + i0)$ is zero for a.e. $\lambda < 0$ and a rank two operator for a.e. $\lambda > 0$ and hence (5.10) simplifies to

$$\mathcal{G}_\lambda = \operatorname{ran}\big(\operatorname{Im} M(\lambda + i0)\big)$$

and for the scattering matrix we get

$$S_{AB}(\lambda) = I_{\mathcal{G}_\lambda} - 2i\sqrt{\operatorname{Im} M(\lambda + i0)}\left(\overline{M(\lambda + i0)}\right)^{-1}\sqrt{\operatorname{Im} M(\lambda + i0)}.$$

In fact, for $\varphi \in H^2(\mathbb{R})$ we first compute $\operatorname{Im} M(\lambda + i0)\varphi$ for $\lambda \in \mathbb{R}$. Observe that for $\lambda \in \mathbb{C}\setminus\mathbb{R}$ we have

$$((A - \lambda)^{-1} f)(x) = \int_{\mathbb{R}} \frac{i}{2\sqrt{\lambda}} e^{i\sqrt{\lambda}|x-y|} f(y)dy, \quad f \in L^2(\mathbb{R}),$$

where the square root $\sqrt{\cdot}$ is defined for all $\lambda \in \mathbb{C}\setminus[0,\infty)$ such that $\operatorname{Im}\sqrt{\lambda} > 0$ and $\sqrt{\lambda} \geq 0$ for $\lambda \in [0,\infty)$. Making use of $\sqrt{\overline{\lambda}} = -\overline{\sqrt{\lambda}}$ for $\lambda \in \mathbb{C}\setminus[0,\infty)$ we find

$$\begin{aligned}(\operatorname{Im} M(\lambda)\varphi)(x) &= \frac{1}{2}\operatorname{sgn}(V(x))\sqrt{|V(x)|}\times \\ &\times \int_{\mathbb{R}}\left[\frac{1}{2\sqrt{\lambda}}e^{i\sqrt{\lambda}|x-y|} + \frac{1}{2\overline{\sqrt{\lambda}}}e^{-i\overline{\sqrt{\lambda}}|x-y|}\right]\sqrt{|V(y)|}\operatorname{sgn}(V(y))\varphi(y)dy\end{aligned}$$

for $\lambda \in \mathbb{C}\setminus\mathbb{R}$ and for $\lambda + i0 = \lambda > 0$ this implies

$$\begin{aligned}&(\operatorname{Im} M(\lambda + i0)\varphi)(x) \\ &= \frac{1}{2\sqrt{\lambda}}\operatorname{sgn}(V(x))\sqrt{|V(x)|}\int_{\mathbb{R}}\cos\big(\sqrt{\lambda}|x-y|\big)\sqrt{|V(y)|}\operatorname{sgn}(V(y))\varphi(y)dy \\ &= \frac{1}{2\sqrt{\lambda}}\operatorname{sgn}(V(x))\sqrt{|V(x)|}\cos(\sqrt{\lambda}x)\int_{\mathbb{R}}\cos(\sqrt{\lambda}y)\sqrt{|V(y)|}\operatorname{sgn}(V(y))\varphi(y)dy \\ &+ \frac{1}{2\sqrt{\lambda}}\operatorname{sgn}(V(x))\sqrt{|V(x)|}\sin(\sqrt{\lambda}x)\int_{\mathbb{R}}\sin(\sqrt{\lambda}y)\sqrt{|V(y)|}\operatorname{sgn}(V(y))\varphi(y)dy;\end{aligned}$$

in particular, $\operatorname{Im} M(\lambda + i0)$ is a rank two operator for $\lambda > 0$ and the spaces $\mathcal{G}_\lambda$, $\lambda > 0$, in the spectral representation $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda)$ of A^{ac} are given by

$$\mathcal{G}_\lambda = \operatorname{span}\left\{\operatorname{sgn}(V)\sqrt{|V|}\cos(\sqrt{\lambda}\cdot), \operatorname{sgn}(V)\sqrt{|V|}\sin(\sqrt{\lambda}\cdot)\right\}.$$

Note that $\operatorname{Im} M(\lambda + i0) = 0$ for a.e. $\lambda < 0$ as $(-\infty, 0) \subset \rho(A)$, and hence $\mathcal{G}_\lambda = \{0\}$ for a.e. $\lambda < 0$.

Remark 5.3. (i) The representation (5.9) of the scattering matrix coincides with the one obtained in quite different manner in [9, Section 18.2.2].

(ii) Proposition 5.1 admits a straight forward generalization to higher dimensions. However, under the assumption (5.7) the condition (5.8) in Lemma 5.2 remains valid only for space dimensions $n = 2, 3$.

(iii) If $\operatorname{ran} D$ is not closed then the quasi boundary triple in Proposition 5.1 is not a generalized boundary triple and hence our extension of [17, Theorem 3.1] for quasi boundary triples is necessary here.

(iv) If for some $C > 0$ the condition

$$|V(x)| \leqslant C\frac{1}{(1+|x|)^{1+\varepsilon}}, \quad \varepsilon > 0,$$

is satisfied for a.e. $x \in \mathbb{R}^n$ it was shown by Kato in [30] (see also [31]) that the wave operators $W_\pm(B, A)$ exist and are complete. In this proof it also turns out that the limit $\overline{M(\lambda + i0)}$ of the function $\overline{M}$ exists for a.e. $\lambda \in \mathbb{R}$ in the operator norm.

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