Functional model for extensions of symmetric operators and applications to scattering theory

Kirill D. Cherednichenko
Department of Mathematical Sciences
University of Bath
Claverton Down, Bath BA2 7AY, U.K.
K.Cherednichenko@bath.ac.uk

Alexander V. Kiselev
Institute of Physics and Mathematics
Dragomanov National Pedagogical University
9 Pyrohova St, Kyiv, 01601, Ukraine
alexander.v.kiselev@gmail.com

Luis O. Silva
Departamento de Física Matemática
Instituto de Investigaciones en Matemáticas Aplicadas y en Sistemas
Universidad Nacional Autónoma de México
C.P. 04510, México D.F.
silva@iimas.unam.mx

To the memory of Professor Boris Pavlov

Abstract

This work deals with the functional model for extensions of symmetric operators and its applications to the theory of wave scattering. In terms of Boris Pavlov's spectral form of this model, we find explicit formulae for the action of the unitary group of exponentials corresponding to almost solvable extensions of a given closed symmetric operator with equal deficiency indices. On the basis of these formulae, we are able to derive a new representation for the scattering matrix for pairs of such extensions. We use this representation to *explicitly* recover the coupling constants in the inverse scattering problem for a finite non-compact quantum graph with δ-type vertex conditions.

Mathematics Subject Classification (2010): 47A45 34L25 81Q35

Keywords: Functional model; Extensions of symmetric operators; Boundary triples; Inverse scattering problems

1. Introduction

Over the last eighty years or so, the subject of the mathematical analysis of waves interacting with obstacles and structures ("scattering theory") has served as one of the most impressive examples of bridging abstract mathematics and physics applications, which in turn motivated the development of new mathematical techniques. The pioneering works of von Neumann [62], [63] and his contemporaries during 1930–1950, on the mathematical foundations of quantum mechanics, fuelled the interest of mathematical analysts to formulating and addressing the problems of direct and inverse wave scattering in a rigorous way.

The foundations of the modern mathematical scattering theory were laid by Kato, Rosenblum and Friedrichs [27, 64, 65, 20] and subsequently by Birman and Kreĭn [5], Birman [4], Kato and Kuroda [28] and Pearson [54]. For a detailed exposition of this subject, see [55, 71]. A parallel approach, which provides a connection to the theory of dissipative operators, was developed by Lax and Phillips [41], who analysed the direct scattering problem for a wide class of linear operators in the Hilbert space, including those associated with the multi-dimensional acoustic problem outside an obstacle, using the language of group theory (and, indeed, thereby developing the semigroup methods in operator theory). The associated techniques were also termed "resonance scattering" by Lax and Phillips.

By virtue of the underlying dissipative framework, the above activity set the stage for the applications of non-selfadjoint techniques, in particular for the functional model for contractions and dissipative operators by Szökefalvi-Nagy and Foiaş [61], which has shown the special rôle in it of the characteristic function of Livšic [44] and allowed Pavlov [53] to construct a spectral form of the functional model for dissipative operators. The connection between this work and the concepts of scattering theory was uncovered by the famous theorem of Adamyan and Arov [1]. Further, Naboko [48] advanced the research initiated by Pavlov, Adamyan and Arov in two directions. Firstly, he generalised Pavlov's construction to the case of non-dissipative operators, and secondly, he bridged the gap back to the mathematical scattering theory. In particular, he provided explicit formulae for the wave operators and scattering matrices of a pair of (in general, non-selfadjoint) operators in the functional model setting. It is remarkable that in this work of Naboko the difference between the so-called stationary and non-stationary scattering approaches disappears.

Our first aim in the present work is to extend the approach of Naboko [48], which was formulated for additive perturbations of self-adjoint operators, to the case of extensions of symmetric operators. In pursuing this, we will use a version of the functional model of Pavlov and Naboko as developed by Ryzhov [58]. The work [58] stopped short of proving the crucial, from the scattering point of view, theorem on "smooth" vectors and therefore was not able to extend Naboko's results on the scattering theory to the setting of (in general, non-selfadjoint) extensions of symmetric operators.

Our second aim is, on the basis of the above construction, to provide an explicit solution to an open problem of inverse scattering on a finite non-compact quantum graph, that is, to the problem of determining matching conditions at the graph vertices. The uniqueness part of this problem has been treated in a preprint by Kostrykin and Schrader [33]. There is also substantial literature on scattering for vector Schrödinger operators on a half-line with matrix potentials, which corresponds to the particular case of a star-graph. Among the latest works on this subject we point out [68], [69], see also references therein, in which scattering is treated in the case of most general matching conditions at the vertex.

The mentioned problem on quantum graphs is a natural generalisation of the now extensively-studied problem of inverse scattering on the infinite and semi-infinite line, which was solved using the classical integral-operator techniques by Borg [7, 8], Levinson [42], Krein [36, 37, 38], Gel'fand and Levitan [21], Marchenko [45], Faddeev [18, 19], Deift and Trubowitz [11]. This body of work has also included the solution to the inverse spectral problem, *i.e.* the problem of determining the potential in the Schrödinger equation from the spectral data. The inverse scattering problem in these works is reduced to the analysis of the inverse problem based on the Weyl-Titchmarsh m-coefficient, and our analysis below benefits from a reduction of the same kind.

In the general operator-theoretic context, the m-coefficient is generalised to both the classical Dirichlet-to-Neumann map (in the PDE setting), and to the so-called M-operator, which takes the form of the generalised Weyl-Titchmarsh M-matrix in the case of quantum graphs and, more generally, symmetric operators with finite deficiency indices. This has been exploited extensively in the study of operators, self-adjoint non-selfadjoint alike, through the works of Krein's school in Ukraine on the theory of boundary triples and the associated M-operators (Gorbachuk and Gorbachuk [23], Kochubei [30, 31], Derkach [12] and others) and of the students of Pavlov in St. Petersburg on the derivation and analysis of functional models for various classes of non-selfadjoint operators and of the associated formulae for wave operators (see *e.g.* [48]). In our view, the theory of boundary triples is conveniently tailored to the study of quantum graphs, when it can also be viewed as a version of the celebrated Birman-Kreĭn-Višik theory [3, 35, 67].

Quantum graphs, *i.e.* metric graphs with ordinary differential operators acting on the edges subject to some "coupling" conditions at the graph vertices, see *e.g.* [2] are known to combine certain one-dimensional and multidimensional features. Assuming that the graph topology and the lengths of the edges are known, for the operator of second differentiation on all graph edges and δ-type conditions at all graph vertices (see Section 8 for precise definitions), in the present paper we determine the coupling constants at all vertices of a finite graph from the knowledge of its scattering matrix. Our approach to the above problem uses as a starting point the strategy of the work [58] mentioned above, which derived the functional model for dissipative restrictions of "maximal" operators, *i.e.* the adjoints of symmetric densely-defined operators with equal deficiency indices. The functional-model approach allows us to obtain a new formula for the wave operator for any pair of such restrictions, in terms of the M-operator for an appropriate boundary triple on the graph. This formula, in turn, implies an expression for the scattering operator and its spectral representation ("scattering matrix"). The obtained formula is given explicitly in terms of the coupling constants at the graph vertices, which allows us to carry out the inverse procedure of recovering these constants from the knowledge of the scattering matrix. Our approach is a development of the idea of Ershova *et al.* [14, 15, 16], who studied the inverse spectral problem and the inverse topology problem for quantum graphs using boundary triples and M-operators.

The paper is organised as follows. In Section 2 we recall the key points of the theory of boundary triples for extensions of symmetric operators with equal deficiency indices and introduce the associated M-operators, following mainly [13] and [58]. In Section

3 we derive formulae for the resolvents of the family of extensions $A_\varkappa$ parametrised by operators $\varkappa$ in the boundary space, in terms of the so-called characteristic function of a fixed element of the family. These formulae are then employed in Section 4 to derive the functional model for the above family of extensions. The material of Sections 3 and 4 closely follows the approach of [58]. In Section 5 we characterise the absolutely continuous subspace of $A_\varkappa$ as the closure of the set of "smooth" vectors in the model Hilbert space introduced in Section 4. On the basis of this characterisation, in Section 6 we define the wave operators for a pair from the family $\{A_\varkappa\}$ and demonstrate their completeness property. This, in combination with the functional model, allows us to obtain formulae for the scattering operator of the pair. In Section 7 we describe a convenient representation of the scattering operator, namely the "scattering matrix", which is explicitly written in terms of the M-operator, analogous to the classical notion of the scattering matrix. All material up to this point is applicable to a general class of operators subject to the assumptions discussed in Sections 2 and 5. In Section 8 we recall the concept of a quantum graph and discuss the implications of the preceding theory for the associated scattering operator for the pair $(A_\varkappa, A_0)$, where $\varkappa$ is the parametrising operator as before, now written in terms of the "coupling" constants at the graph vertices and $A_0 = A_\varkappa|_{\varkappa=0}$ is the "unperturbed" operator with Kirchhoff vertex conditions. Finally, in Section 9 we solve the inverse scattering problem for a graph with δ-type couplings at the vertices, using the formulae for the scattering matrix in terms of the M-matrix of the graph.

2. Extension theory and boundary triples

Let $\mathcal{H}$ be a separable Hilbert space and denote by $\langle\cdot,\cdot\rangle$ the inner product in this space (which we consider to be antilinear in the second argument).

Let A be a closed symmetric operator densely defined in $\mathcal{H}$, *i.e.* $A \subset A^*$, with domain $\operatorname{dom}(A) \subset \mathcal{H}$. For such operators, the lower and upper half-planes are points of regular type and the deficiency indices $n_+(A), n_-(A)$ are defined as follows:

$$n_\pm(A) := \dim(\mathcal{H} \ominus \operatorname{ran}(A - zI)) = \dim(\ker(A^* - \overline{z}I))\,, \quad z \in \mathbb{C}_\pm\,.$$

If $A = A^*$ then A is referred to as self-adjoint.

Definition 1. A closed operator L is said to be *completely non-selfadjoint* if there is no subspace reducing L such that the part of L in this subspace is self-adjoint. A completely non-selfadjoint symmetric operator is often referred to as *simple*.

For a closed symmetric operator to be simple it suffices that it has no invariant subspace in which the operator is self-adjoint [6, Thm. 4.6.1].

As shown in [39, Sec. 1.3](see also [24, Thm. 1.2.1]), the maximal invariant subspace for the closed symmetric operator A in which it is self-adjoint is

$$\bigcap_{z\in\mathbb{C}\setminus\mathbb{R}} \operatorname{ran}(A - zI)\,.$$

Thus, a necessary and sufficient condition for the closed symmetric operator A to be completely non-selfadjoint (or simple) is that

$$\bigcap_{z\in\mathbb{C}\setminus\mathbb{R}} \operatorname{ran}(A - zI) = \{0\}\,. \tag{2.1}$$

In this work we consider extensions of a given closed symmetric operator A with equal deficiency indices, *i. e.* $n_-(A) = n_+(A)$, and use the theory of boundary triples. In order to deal with the family of extensions $\{A_\varkappa\}$ of the symmetric operator A (where the parameter $\varkappa$ is itself an operator, see notation immediately following Proposition 2.2), we first construct a functional model of its particular dissipative extension. This is done following the Pavlov-Naboko procedure, which in turn stems from Sz.-Nagy-Foiaş functional model. This allows us to obtain a simple model for the whole family $\{A_\varkappa\}$, in particular yielding a possibility to apply it to the scattering theory for certain pairs of operators in $\{A_\varkappa\}$, including both the cases when these operators are self-adjoint and non-selfadjoint.

Taking into account the importance of dissipative operators in our work, we briefly recall that a densely defined operator L in $\mathcal{H}$ is called dissipative if

$$\operatorname{Im}\langle Lf, f\rangle \geq 0 \qquad \forall f \in \operatorname{dom}(L). \tag{2.2}$$

For a dissipative operator L, the lower half-plane is contained in the set of points of regular type, *i.e.*

$$\mathbb{C}_- \subset \{z \in \mathbb{C} : \exists C > 0 \;\; \forall f \in \operatorname{dom}(L) \quad \|(L - zI)f\| \geq C\,\|f\|\}\,.$$

A dissipative operator L is called maximal if $\mathbb{C}_-$ is actually contained in its resolvent set $\rho(L) := \{z \in \mathbb{C} : (L - zI)^{-1} \in \mathcal{B}(\mathcal{H})\}$. ($\mathcal{B}(\mathcal{H})$ denotes the space of bounded operators defined on the whole Hilbert space $\mathcal{H}$). Clearly, a maximal dissipative operator is closed.

We next describe the boundary triple approach to the extension theory of symmetric operators with equal deficiency indices. It has proven to be particularly useful in the study of self-adjoint extensions of differential operators of second order.

Definition 2. For a closed symmetric operator A with equal deficiency indices, consider the linear mappings

$$\Gamma_1 : \operatorname{dom}(A^*) \to \mathcal{K}, \qquad \Gamma_0 : \operatorname{dom}(A^*) \to \mathcal{K}\,,$$

where $\mathcal{K}$ is an auxiliary separable Hilbert space, such that

$$(1) \quad \langle A^*f, g\rangle_{\mathcal{H}} - \langle f, A^*g\rangle_{\mathcal{H}} = \langle \Gamma_1 f, \Gamma_0 g\rangle_{\mathcal{K}} - \langle \Gamma_0 f, \Gamma_1 g\rangle_{\mathcal{K}}\,; \tag{2.3}$$

$$(2) \quad \text{The mapping } \operatorname{dom}(A^*) \ni f \mapsto \begin{pmatrix}\Gamma_1 f\\ \Gamma_0 f\end{pmatrix} \in \mathcal{K}\oplus\mathcal{K} \text{ is surjective.}$$

Then the triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$ is said to be a *boundary triple* for A^*.

Remark 1. There exist boundary triples for A^* whenever A has equal deficiency indices (the case of infinite indices is not excluded).

In this work we consider *proper extensions* of A, *i.e.* extensions of A that are restrictions of A^*. For a closed linear relation B on $\mathcal{K}$, *i.e.* a subspace of $\mathcal{K}\oplus\mathcal{K}$, let A_B be the restriction of A^* such that, for a specific choice of the triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$ one has

$$\operatorname{dom}(A_B) = \left\{ f \in \operatorname{dom}(A^*) : \begin{pmatrix} \Gamma_1 f \\ \Gamma_0 f \end{pmatrix} \in B \right\} . \tag{2.4}$$

Clearly, A_B is a proper extension of A (see [59, Sec. 14]).

In this paper we treat those proper extensions A_B of A that arise from linear relations B that are graphs of bounded operators defined on the whole space $\mathcal{K}$. In this case we identify the relation B and the corresponding bounded operator, *i. e.,* $B \in \mathcal{B}(\mathcal{K})$. The extensions A_B for which there exists a triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$ and $B \in \mathcal{B}(\mathcal{K})$ are called *almost solvable* with respect to the triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$. In this case, (2.4) implies that

$$f \in \operatorname{dom}(A_B) \iff \Gamma_1 f = B \Gamma_0 f . \tag{2.5}$$

Remark 2. Most of what is said henceforth remains valid not only for almost solvable extensions but for more general extensions given by relations, which we shall pursue elsewhere.

The following assertions, written in slightly different terms, can be found in [30, Thm. 2] and [25, Chap. 3 Sec. 1.4] (see also [29, Thm. 2.3], [58, Thm. 1.1], and [59, Sec. 14] for a closer formulation). We compile them in the next proposition for easy reference.

Proposition 2.1. *Let A be a closed symmetric operator with equal deficiency indices and let $(\mathcal{K}, \Gamma_1, \Gamma_0)$ be a the boundary triple for A^*. Assume that A_B is an almost solvable extension. Then the following statements hold:*

1. *$f \in \operatorname{dom}(A)$ if and only if $\Gamma_1 f = \Gamma_0 f = 0$.*

2. *A_B is maximal, i. e., $\rho(A_B) \neq \emptyset$.*

3. *$A_B^* = A_{B^*}$.*

4. *A_B is dissipative if and only if B is dissipative.*

5. *A_B is self-adjoint if and only if B is self-adjoint.*

Definition 3. The function $M : \mathbb{C}_- \cup \mathbb{C}_+ \to \mathcal{B}(\mathcal{H})$ such that

$$M(z)\Gamma_0 f = \Gamma_1 f \qquad \forall f \in \ker(A^* - zI)$$

is *the Weyl function of the boundary triple* $(\mathcal{K}, \Gamma_1, \Gamma_0)$ for A^*.

The Weyl function defined above has the following properties [13].

Proposition 2.2. *Let M be a Weyl function of the boundary triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$ for A^*. Then the following statements hold:*

1. *$M : \mathbb{C} \setminus \mathbb{R} \to \mathcal{B}(\mathcal{K})$.*

2. *M is a $\mathcal{B}(\mathcal{K})$-valued double-sided $\mathcal{R}$-function [26], that is,*

$$M(z)^* = M(\overline{z}) \quad \textit{and} \quad \operatorname{Im}(z)\operatorname{Im}(M(z)) > 0 \quad \textit{for } z \in \mathbb{C} \setminus \mathbb{R} .$$

3. *The spectrum of A_B coincides with the set of points $z_0 \in \mathbb{C}$ such that $(M - B)^{-1}$ does not admit analytic continuation into z_0.*

Let us lay out the notation for some of the main objects in this paper. In the auxiliary Hilbert space $\mathcal{K}$, choose a bounded nonnegative self-adjoint operator α so that the operator

$$B_\varkappa := \frac{\alpha\varkappa\alpha}{2} \tag{2.6}$$

belongs to $\mathcal{B}(\mathcal{K})$, where $\varkappa$ is a bounded operator in $E := \operatorname{clos}(\operatorname{ran}(\alpha)) \subset \mathcal{K}$. In what follows, we deal with almost solvable extensions of a given symmetric operator A that are generated by $B_\varkappa$ via (2.5). It is always assumed that the deficiency indices of A are equal and that some boundary triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$ for A^* is fixed. In order to streamline the formulae, we write

$$A_\varkappa := A_{B_\varkappa}. \tag{2.7}$$

Here $\varkappa$ should be understood as a parameter for a family of almost solvable extensions of A. Note that if $\varkappa$ is self-adjoint then so is $B_\varkappa$ and, hence by Proposition 2.1(5), $A_\varkappa$ is self-adjoint. Note also that $A_{\mathrm{i}I}$ is maximal dissipative, again by Proposition 2.1.

Definition 4. The characteristic function of the operator $A_{\mathrm{i}I}$ is the operator-valued function S on $\mathbb{C}_+$ given by

$$S(z) := I\upharpoonright_E + \mathrm{i}\alpha\big(B_{\mathrm{i}I}^* - M(z)\big)^{-1}\alpha\upharpoonright_E, \qquad z \in \mathbb{C}_+. \tag{2.8}$$

In the general setting, the characteristic function is defined as in [58, Def. 1.7]. Our definition is justified by [58, Eq. 1.16].

Remark 3. The function S is analytic in $\mathbb{C}_+$ and, for each $z \in \mathbb{C}_+$, the mapping $S(z) : E \to E$ is a contraction. Therefore, S has nontangential limits almost everywhere on the real line in the strong topology [61], which we will henceforth denote by $S(k)$, $k \in \mathbb{R}$.

Remark 4. When $\alpha = \sqrt{2}I$, an straightforward calculation yields that $S(z)$ is the Cayley transform of $M(z)$, *i.e.*

$$S(z) = (M(z) - \mathrm{i}I)(M(z) + \mathrm{i}I)^{-1}.$$

3. Formulae for the resolvents of almost solvable extensions

In this section we establish some useful relations between the resolvents of the operators $A_\varkappa$ for any $\varkappa \in \mathcal{B}(E)$ and the resolvents of the maximal dissipative operator $A_{\mathrm{i}I}$ and its adjoint. These relations are instrumental for the construction of the functional model in the next section.

Notation 1. We abbreviate

$$\Theta_\varkappa(z) := I - \mathrm{i}\alpha(B_{\mathrm{i}I} - M(z))^{-1}\alpha\chi_\varkappa^+, \qquad z \in \mathbb{C}_-, \tag{3.1}$$

$$\widehat{\Theta}_\varkappa(z) := I + \mathrm{i}\alpha(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^-, \qquad z \in \mathbb{C}_+, \tag{3.2}$$

where

$$\chi_\varkappa^\pm := \frac{I \pm \mathrm{i}\varkappa}{2}, \tag{3.3}$$

and for simplicity we have written I instead of $I\restriction_E$. We use this convention throughout the text.

It follows from Definition 4 and Proposition 2.2(2) that the operator-valued functions $\Theta_\varkappa(z)$ and $\widehat{\Theta}_\varkappa(z)$ can be expressed in terms of the characteristic function S, as follows:

$$\Theta_\varkappa(z) = I + (S^*(\overline{z}) - I)\chi_\varkappa^+ \qquad \forall\, z \in \mathbb{C}_- \,, \tag{3.4}$$

$$\widehat{\Theta}_\varkappa(z) = I + (S(z) - I)\chi_\varkappa^- \qquad \forall\, z \in \mathbb{C}_+ \,. \tag{3.5}$$

The formulae in the next lemma are analogous to [58, Eqs. 2.18 and 2.22].

Lemma 3.1. *The following identities hold:*

(i) $\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1} = \Theta_\varkappa(z)\alpha\Gamma_0(A_\varkappa - zI)^{-1} \qquad \forall\, z \in \mathbb{C}_- \cap \rho(A_\varkappa)$*;*

(ii) $\alpha\Gamma_0(A_\varkappa - zI)^{-1} = \Theta_\varkappa(z)^{-1}\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1} \qquad \forall\, z \in \mathbb{C}_- \cap \rho(A_\varkappa)$*;*

(iii) $\alpha\Gamma_0(A_{\mathrm{i}I}^* - zI)^{-1} = \widehat{\Theta}_\varkappa(z)\alpha\Gamma_0(A_\varkappa - zI)^{-1} \qquad \forall\, z \in \mathbb{C}_+ \cap \rho(A_\varkappa)$*;*

(iv) $\alpha\Gamma_0(A_\varkappa - zI)^{-1} = \widehat{\Theta}_\varkappa(z)^{-1}\alpha\Gamma_0(A_{\mathrm{i}I}^* - zI)^{-1} \qquad \forall\, z \in \mathbb{C}_+ \cap \rho(A_\varkappa)\,.$

Proof. We start by proving (i). To this end, suppose that $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$ so $(A_{\mathrm{i}I} - zI)^{-1}$ and $(A_\varkappa - zI)^{-1}$ are defined on the whole space $\mathcal{H}$. Fix an arbitrary $h \in \mathcal{H}$ and define

$$\varphi := (A_{\mathrm{i}I} - zI)^{-1}h, \qquad g := (A_\varkappa - zI)^{-1}h\,. \tag{3.6}$$

Clearly, the vector

$$f := \varphi - g = \left((A_{\mathrm{i}I} - zI)^{-1} - (A_\varkappa - zI)^{-1}\right)h$$

is in $\ker(A^* - zI)$ since A^* is an extension of both operators $A_{\mathrm{i}I}$ and $A_\varkappa$. According to (2.5), it follows from $\varphi \in \mathrm{dom}(A_{\mathrm{i}I})$ and $g \in \mathrm{dom}(A_\varkappa)$ that $\Gamma_1\varphi = B_{\mathrm{i}I}\Gamma_0\varphi$ and $\Gamma_1 g = B_\varkappa\Gamma_0 g$. Thus, one has

$$\begin{aligned}
0 &= \Gamma_1(f+g) - B_{\mathrm{i}I}\Gamma_0(f+g)\\
&= \Gamma_1 f - B_{\mathrm{i}I}\Gamma_0 f + \Gamma_1 g - B_{\mathrm{i}I}\Gamma_0 g\\
&= M(z)\Gamma_0 f - B_{\mathrm{i}I}\Gamma_0 f + B_\varkappa\Gamma_0 g - B_{\mathrm{i}I}\Gamma_0 g\,,
\end{aligned}$$

where in the last equality we also use the fact that $f \in \ker(A^* - zI)$, together with Definition 3. Hence one has

$$\Gamma_0 f = (B_{\mathrm{i}I} - M(z))^{-1}(B_\varkappa - B_{\mathrm{i}I})\Gamma_0 g\,,$$

which, in turn, implies that

$$\Gamma_0\varphi = \Gamma_0 f + \Gamma_0 g = \left[I + (B_{\mathrm{i}I} - M(z))^{-1}(B_\varkappa - B_{\mathrm{i}I})\right]\Gamma_0 g. \tag{3.7}$$

Taking into account (3.6), using the fact that $B_\varkappa - B_{\mathrm{i}I} = -\mathrm{i}\alpha\chi_\varkappa^+\alpha$ and applying the operator α to both sides of (3.7), we obtain

$$\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1}h = \left[I - \mathrm{i}\alpha(B_{\mathrm{i}I} - M(z))^{-1}\alpha\chi_\varkappa^+\right]\alpha\Gamma_0(A_\varkappa - zI)^{-1}h,$$

which is the identity (i), in view of the definition (3.4).

Similar computations with the pairs $A_\varkappa, B_\varkappa$ and $A_{\mathrm{i}I}, B_{\mathrm{i}I}$ interchanged lead to

$$\alpha\Gamma_0(A_\varkappa - zI)^{-1}h = \left[I + \mathrm{i}\alpha(B_\varkappa - M(z))^{-1}\alpha\chi_\varkappa^+\right]\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1}h, \tag{3.8}$$

for $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$. Now, (ii) follows from (3.8) using the identity

$$\Theta_\varkappa(z)^{-1} = I + \mathrm{i}\alpha\big(B_\varkappa - M(z)\big)^{-1}\alpha\chi_\varkappa^+ \qquad \forall\, z \in \mathbb{C}_- \cap \rho(A_\varkappa)\,, \tag{3.9}$$

which is validated by multiplying together the right-hand sides of (3.9) and (3.1) and employing a version of the second resolvent identity (*cf.* [70, Thm. 5.13]):

$$(B_\varkappa - M(z))^{-1} - (B_{\mathrm{i}I} - M(z))^{-1} = (B_\varkappa - M(z))^{-1}(B_{\mathrm{i}I} - B_\varkappa)(B_{\mathrm{i}I} - M(z))^{-1}$$

which holds for all $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$.

We next proceed to the proof of (iii) and (iv). Fix an arbitrary $z \in \mathbb{C}_+ \cap \rho(A_\varkappa)$ and an arbitrary $h \in \mathcal{H}$ and define

$$\varphi := (A_{\mathrm{i}I}^* - zI)^{-1}h\,, \qquad g := (A_\varkappa - zI)^{-1}h\,, \tag{3.10}$$

then $f := \varphi - g$ is in $\ker(A^* - zI)$. Since $\varphi \in \operatorname{dom}(A_{\mathrm{i}I}^*)$, one has that

$$\begin{aligned} 0 &= \Gamma_1(f+g) - B_{\mathrm{i}I}^*\Gamma_0(f+g) \\ &= M(z)\Gamma_0 f + \Gamma_1 g - B_{\mathrm{i}I}^*\Gamma_0 f - B_{\mathrm{i}I}\Gamma_0 g\,, \end{aligned}$$

where in the second equality we use the fact that $f \in \ker(A^* - zI)$. On the other hand, in view of the inclusion $g \in \operatorname{dom}(A_\varkappa)$, the formula (2.5) allows us to replace the second term in the last expression by $B_\varkappa\Gamma_0 g$, which yields

$$0 = (M(z) - B_{\mathrm{i}I}^*)\Gamma_0 f + (B_\varkappa - B_{\mathrm{i}I}^*)\Gamma_0 g\,. \tag{3.11}$$

Since $B_\varkappa - B_{\mathrm{i}I}^* = \mathrm{i}\alpha\chi_\varkappa^-\alpha$, the equality (3.11) is rewritten as

$$\Gamma_0 f = \mathrm{i}(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^-\alpha\Gamma_0 g\,,$$

which in turn implies that

$$\Gamma_0\varphi = \left[I + \mathrm{i}(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^-\alpha\right]\Gamma_0 g\,.$$

Applying the operator α to both sides of the last equation and using (3.10), we obtain

$$\alpha\Gamma_0(A_{\mathrm{i}I}^* - zI)^{-1}h = \left[I + \mathrm{i}\alpha(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^-\right]\alpha\Gamma_0(A_\varkappa - zI)^{-1}h,$$

which is (iii), in view of the definition (3.5).

Finally, we interchange the operators $A_{\mathrm{i}I}^*$ and $A_\varkappa$ in (3.10) and repeat the computations, correspondingly interchanging $B_{\mathrm{i}I}$ and $B_\varkappa$. This yields the identity

$$\alpha\Gamma_0(A_\varkappa^* - zI)^{-1}h = \left[I - \mathrm{i}\alpha(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^-\right]\alpha\Gamma_0(A_{\mathrm{i}I}^* - zI)^{-1}h, \tag{3.12}$$

for all $z \in \mathbb{C}_+ \cap \rho(A_\varkappa)$. In a similar way to (3.9), we verify that

$$\widehat{\Theta}_\varkappa(z)^{-1} = I - \mathrm{i}\alpha(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^- \qquad \forall\, z \in \mathbb{C}_+ \cap \rho(A_\varkappa)$$

and hence establish (iv). □

4. Functional model and theorems about smooth vectors

Following [48], we introduce a Hilbert space serving as a functional model for the family of operators $A_\varkappa$. This functional model was constructed for completely non-selfadjoint maximal dissipative operators in [53, 51, 52] and further developed in [48]. Next we recall some related necessary information. In what follows, in various formulae, we use the subscript "±" to indicate two different versions of the same formula in which the subscripts "+" and "−" are taken individually.

A function f analytic on $\mathbb{C}_\pm$ and taking values in $\mathcal{K}$ is said to be in the Hardy class $H^2_\pm(E)$ if and only if

$$\sup_{y>0} \int_{\mathbb{R}} \|f(x \pm \mathrm{i}y)\|_{\mathrm{e}}^2\, dx < +\infty$$

(*cf.* [56, Sec. 4.8]). Whenever $f \in H^2_\pm(E)$, the left-hand side of the above inequality defines $\|f\|^2_{H^2_\pm(E)}$. We use the notation H^2_+ and H^2_- for the usual Hardy spaces of $\mathbb{C}$-valued functions.

Any element in the Hardy spaces $H^2_\pm(E)$ can be associated with its boundary values in the topology of $\mathcal{K}$, which exist almost everywhere on the real line. The spaces of boundary functions of $H^2_\pm(E)$ are denoted by $\hat{H}^2_\pm(E)$ and they are subspaces of $L^2(\mathbb{R}, E)$ [56, Sec. 4.8, Thm. B]). By the Paley-Wiener theorem [56, Sec. 4.8, Thm. E]), one verifies that these subspaces are the orthogonal complements of each other (*i.e.*, $L^2(\mathbb{R}, E) = \hat{H}^2_+(E) \oplus \hat{H}^2_-(E)$).

Following the argument of [48, Thm. 1], it is shown in [58, Lem. 2.4] that

$$\alpha\Gamma_0(A_{\mathrm{i}I} - \cdot I)^{-1}h \in H^2_-(E) \quad \text{and} \quad \alpha\Gamma_0(A^*_{\mathrm{i}I} - \cdot I)^{-1}h \in H^2_+(E)\,. \tag{4.1}$$

As mentioned in Remark 3, the characteristic function S given in Definition 4 has nontangential limits almost everywhere on the real line in the strong topology. Thus, for a two-component vector function $\binom{\widetilde{g}}{g}$ taking values in $E \oplus E$, one can consider the integral

$$\int_{\mathbb{R}} \left\langle \begin{pmatrix} I & S^*(s) \\ S(s) & I \end{pmatrix} \begin{pmatrix} \widetilde{g}(s) \\ g(s) \end{pmatrix}, \begin{pmatrix} \widetilde{g}(s) \\ g(s) \end{pmatrix} \right\rangle_{E\oplus E} ds, \tag{4.2}$$

which is always nonnegative, also due to the contractive properties of S. The space

$$\mathfrak{H} := L^2\left(E \oplus E; \begin{pmatrix} I & S^* \\ S & I \end{pmatrix}\right) \tag{4.3}$$

is the completion of the linear set of two-component vector functions $\binom{\widetilde{g}}{g} : \mathbb{R} \to E \oplus E$ in the norm (4.2), factored with respect to vectors of zero norm. Naturally, not every element of the set can be identified with a pair $\binom{\widetilde{g}}{g}$ of two independent functions. Still, in what follows we keep the notation $\binom{\widetilde{g}}{g}$ for the elements of this space.

Another consequence of the contractive properties of the characteristic function S is that for $\widetilde{g}, g \in L^2(\mathbb{R}, E)$ one has

$$\left\| \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \right\|_{\mathfrak{H}} \geq \begin{cases} \|\widetilde{g} + S^* g\|_{L^2(\mathbb{R},E)} \,, \\ \|S\widetilde{g} + g\|_{L^2(\mathbb{R},E)} \,. \end{cases}$$

Thus, for every Cauchy sequence $\{\binom{\widetilde{g}_n}{g_n}\}_{n=1}^{\infty}$, with respect to the $\mathfrak{H}$-topology, such that $\widetilde{g}_n, g_n \in L^2(\mathbb{R}, E)$ for all $n \in \mathbb{N}$, the limits of $\widetilde{g}_n + S^* g_n$ and $S\widetilde{g}_n + g_n$ exists in $L^2(\mathbb{R}, E)$, so that the objects $\widetilde{g} + S^* g$ and $S\widetilde{g} + g$ can always be treated as $L^2(\mathbb{R}, E)$ functions.

Consider the orthogonal subspaces of $\mathfrak{H}$

$$D_- := \begin{pmatrix} 0 \\ \hat{H}^2_-(E) \end{pmatrix} , \quad D_+ := \begin{pmatrix} \hat{H}^2_+(E) \\ 0 \end{pmatrix} . \tag{4.4}$$

We define the space

$$K := \mathfrak{H} \ominus (D_- \oplus D_+),$$

which is characterised as follows (see *e.g.* [51, 52]):

$$K = \left\{ \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} : \widetilde{g} + S^* g \in \hat{H}^2_-(E) \,, S\widetilde{g} + g \in \hat{H}^2_+(E) \right\} . \tag{4.5}$$

The orthogonal projection P_K onto the subspace K is given by (see *e.g.* [47])

$$P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \begin{pmatrix} \widetilde{g} - P_+(\widetilde{g} + S^* g) \\ g - P_-(S\,\widetilde{g} + g) \end{pmatrix} , \tag{4.6}$$

where $P_\pm$ are the orthogonal Riesz projections in $L^2(E)$ onto $\hat{H}^2_\pm(E)$.

On the other hand, a completely non-selfadjoint dissipative operator admits [61] a self-adjoint dilation. According to [58], this dilation for the operator $A_{\mathrm{i}I}$ can be constructed following Pavlov's procedure [51, 53, 52], i. e., the dilation $\mathcal{A} = \mathcal{A}^*$ is defined in the Hilbert space

$$\mathcal{H} = L^2(\mathbb{R}_-, E) \oplus \mathcal{H} \oplus L^2(\mathbb{R}_+, E) \tag{4.7}$$

where $\mathcal{H}$ is the original Hilbert space, see Section 2, so that

$$P_{\mathcal{H}}(\mathcal{A} - zI)^{-1} \restriction_{\mathcal{H}} = (A_{\mathrm{i}I} - zI)^{-1} \,, \qquad z \in \mathbb{C}_-$$

and therefore

$$P_{\mathcal{H}}(\mathcal{A} - zI)^{-1} \restriction_{\mathcal{H}} = (A^*_{\mathrm{i}I} - zI)^{-1} \,, \qquad z \in \mathbb{C}_+ \,.$$

As in the case of additive non-selfadjoint perturbation [48], Ryzhov was able to establish in [58, Thm. 2.3] that $\mathfrak{H}$ serves as the functional model for the dilation $\mathcal{A}$, i. e., there exists an isometry Φ from $\mathcal{H}$ onto $\mathfrak{H}$ such that $\mathcal{A}$ is transformed into the operator of multiplication by the independent variable in $\mathfrak{H}$; more precisely,

$$\Phi(\mathcal{A} - zI)^{-1} = (\cdot - z)^{-1}\Phi \,. \tag{4.8}$$

Furthermore, under this isometry the space $\mathcal{H}$ is mapped onto K:

$$\Phi\mathcal{H} = K\,.$$

The next theorem generalises [58, Thm. 2.5], and its form is similar to [48, Thm. 3], which treats the case of additive perturbartions. Its proof blends together the arguments of [58] and [48] taking advantage of the similarity between the formulae (3.1)–(3.5) and those of [48, Section 2]. The proof is given in the Appendix for the sake of completeness.

Theorem 4.1. *(i) If $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$ and $\binom{\widetilde{g}}{g} \in K$, then*

$$\Phi(A_\varkappa - zI)^{-1}\Phi^* \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \frac{1}{\cdot - z} \begin{pmatrix} \widetilde{g} \\ g - \chi_\varkappa^+ \Theta_\varkappa^{-1}(z)(\widetilde{g} + S^* g)(z) \end{pmatrix}. \tag{4.9}$$

(ii) If $z \in \mathbb{C}_+ \cap \rho(A_\varkappa)$ and $\binom{\widetilde{g}}{g} \in K$, then

$$\Phi(A_\varkappa - zI)^{-1}\Phi^* \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \frac{1}{\cdot - z} \begin{pmatrix} \widetilde{g} - \chi_\varkappa^- \widehat{\Theta}_\varkappa^{-1}(z)(S\widetilde{g} + g)(z) \\ g \end{pmatrix}. \tag{4.10}$$

Here, $(\widetilde{g}+S^*g)(z)$ and $(S\widetilde{g}+g)(z)$ denote the values at z of the analytic continuations of the functions $\widetilde{g}+S^*g \in \hat{H}^2_-(E)$ and $S\widetilde{g}+g \in \hat{H}^2_+(E)$ into the lower half-plane and upper half-plane.

Following the ideas of Naboko, in the functional model space $\mathfrak{H}$ consider two subspaces $\mathcal{N}_\pm^\varkappa$ defined as follows:

$$\mathcal{N}_\pm^\varkappa := \left\{ \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} : P_\pm \left(\chi_\varkappa^+(\widetilde{g} + S^* g) + \chi_\varkappa^-(S\widetilde{g} + g) \right) = 0 \right\}. \tag{4.11}$$

These subspaces have a characterisation in terms of the resolvent of the operator $A_\varkappa$, whose proof, which we provide for completeness in the Appendix, follows the approach of [48, Thm. 4].

Theorem 4.2. *The following characterisation holds:*

$$\mathcal{N}_\pm^\varkappa = \left\{ \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \frac{1}{\cdot - z} \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \text{ for all } z \in \mathbb{C}_\pm \right\}. \tag{4.12}$$

Consider the counterparts of $\mathcal{N}_\pm^\varkappa$ in the original Hilbert space $\mathcal{H}$:

$$\widetilde{N}_\pm^\varkappa := \Phi^* P_K \mathcal{N}_\pm^\varkappa\,, \tag{4.13}$$

which are linear sets albeit not necessarily subspaces. In a way similar to [48], we introduce the set

$$\widetilde{N}_\mathrm{e}^\varkappa := \widetilde{N}_+^\varkappa \cap \widetilde{N}_-^\varkappa$$

of so-called smooth vectors and its closure $N_\mathrm{e}^\varkappa := \operatorname{clos}(\widetilde{N}_\mathrm{e}^\varkappa)$. These prove to be suitable for the model description of the absolutely continuous subspace and, therefore, for the construction of the wave operators. In Section 5 we prove that $N_\mathrm{e}^\varkappa$ coincides with the absolutely continuous subspace of the operator $A_\varkappa$, in the case when $A_\varkappa = A_\varkappa^*$ and under the additional assumption that $\ker(\alpha) = \{0\}$. The reason for the choice of the term "smooth vector" stems from the statement of Theorem 4.2 together with (4.13).

The next assertion is an alternative non-model characterisation of the linear sets $\widetilde{N}_\pm^\varkappa$. The proof is found in the Appendix.

Theorem 4.3. *The sets $\widetilde{N}_\pm^\varkappa$ are as follows:*

$$\widetilde{N}_\pm^\varkappa = \left\{u \in \mathcal{H} : \chi_\varkappa^\mp \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_\pm^2(E)\right\}. \tag{4.14}$$

Corollary 4.4. *The right-hand side of (4.14) coincides with $\{u \in \mathcal{H} : \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_\pm^2(E)\}$ and therefore equivalently one has*

$$\widetilde{N}_\pm^\varkappa = \{u \in \mathcal{H} : \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_\pm^2(E)\}. \tag{4.15}$$

Proof. Indeed, if $\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_+^2(E)$ then clearly $\chi_\varkappa^-\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_+^2(E)$. Conversely, we write

$$S(z)\chi_\varkappa^-\alpha\Gamma_0(A_\varkappa - zI)^{-1}u = (S(z)\chi_\varkappa^- + \chi_\varkappa^+)\alpha\Gamma_0(A_\varkappa - zI)^{-1}u - \chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \tag{4.16}$$

$$= \widehat{\Theta}_\varkappa(z)\alpha\Gamma_0(A_\varkappa - zI)^{-1}u - \chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \tag{4.17}$$

$$= \alpha\Gamma_0(A_{iI}^* - zI)^{-1}u - \chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u, \tag{4.18}$$

where $S(z)\chi_\varkappa^- + \chi_\varkappa^+ = (S(z) - I)\chi_\varkappa^- + I = \widehat{\Theta}_\varkappa(z)$, see (3.5), and in (4.17)–(4.18) we use the part (iii) of Lemma 3.1.

Further, as we noted in (4.1), one has $\alpha\Gamma_0(A_{iI}^* - zI)^{-1}u \in H_+^2(E)$, and since S is an analytic contraction in $\mathbb{C}_+$ the function $S(z)\chi_\varkappa^-\alpha\Gamma_0(A_\varkappa - zI)^{-1}u$, $z \in \mathbb{C}_+$, is an element of $H_+^2(E)$ as long as $\chi_\varkappa^-\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_+^2(E)$. Recalling (4.16), (4.18), we conclude that $\chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_+^2(E)$ and therefore

$$\chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u + \chi_\varkappa^-\alpha\Gamma_0(A_\varkappa - zI)^{-1}u = \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_+^2(E),$$

as required.

The equality

$$\left\{u \in \mathcal{H} : \chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_-^2(E)\right\} = \left\{u \in \mathcal{H} : \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_-^2(E)\right\}$$

is shown in a similar way. $\square$

Remark 5. The above corollary together with Theorem 5.5 motivates extending the notion of the absolutely continuous subspace $\mathcal{H}_{\rm ac}(A_\varkappa)$ to the case of non-selfadjoint extensions $A_\varkappa$ of a symmetric operator A, by identifying it with the set $N_{\rm e}^\varkappa$. This generalisation follows in the footsteps of the corresponding definition by Naboko [48] in the case of additive perturbations. In particular, an argument similar to [48, Corollary 1] shows that for the functional model image of $\tilde{N}_{\rm e}^\varkappa$ the following representation holds:

$$\Phi\widetilde{N}_{\rm e}^\varkappa = \left\{\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \quad \forall\, z \in \mathbb{C}_- \cup \mathbb{C}_+\right\}. \tag{4.19}$$

(Note that the inclusion of the right-hand side of (4.19) into $\Phi\widetilde{N}_{\mathrm{e}}^{\varkappa}$ follows immediately from Theorem 4.2.) Further, we arrive at equivalent description:

$$\Phi\widetilde{N}_{\mathrm{e}}^{\varkappa}=\left\{P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}:\chi_{\varkappa}^{+}(\widetilde{g}+S^*g)+\chi_{\varkappa}^{-}(S\widetilde{g}+g)=0\right\}. \tag{4.20}$$

5. The relationship between the set of smooth vectors and the absolutely continuous subspace in the self-adjoint setting

The argument of this section is similar to that of [48], subject to appropriate modifications in order to account for the fact that we deal with extensions of symmetric operators rather than additive perturbations. The same strategy seems to be applicable in the "mixed" case that incorporates both extensions and perturbations, which has recently been studied in [10].

The following proposition is found in [48, Lemma 5]. For reader's convenience, we provide its proof in the Appendix.

Proposition 5.1. *If the Borel transform of a Borel measure μ*

$$\int_{\mathbb{R}}\frac{d\mu(s)}{s-z}$$

is either an element of H_+^2 when $z\in\mathbb{C}_+$ or an element of H_-^2 when $z\in\mathbb{C}_-$, then μ is absolutely continuous with respect to the Lebesgue measure.

Lemma 5.2. *Assume that $\varkappa=\varkappa^*$, $\ker(\alpha)=\{0\}$ and let P_S be the orthogonal projection onto the singular subspace of $A_{\varkappa}$. Then following inclusion holds:*

$$P_S\widetilde{N}_{\mathrm{e}}^{\varkappa}\subset\bigcap_{z\in\mathbb{C}\setminus\mathbb{R}}\operatorname{ran}(A-zI).$$

Proof. We first demonstrate the validity of the claim for $\varkappa=0$.

We decompose the smooth vector u into its projections onto the absolutely continuous and singular subspaces of A_0, that is, $u=u_{\mathrm{ac}}+u_s$, where $u_{\mathrm{ac}}\in\mathcal{H}_{\mathrm{ac}}(A_0)$ and $u_s\in\mathcal{H}_s(A_0)$, so $u_{\mathrm{ac}}\perp u_s$ and $u_s\in P_S\widetilde{N}_{\mathrm{e}}^{\varkappa}$.

Consider an arbitrary $w\in\mathcal{K}$ and note that, due to the surjectivity of Γ_1, there exists a vector $v\in\operatorname{dom}(A^*)$ such that $\alpha w=\Gamma_1 v$, and therefore

$$\begin{aligned}\left\langle\Gamma_0(A_0-zI)^{-1}u,\alpha w\right\rangle_{\mathcal{K}}&=\left\langle\Gamma_0(A_0-zI)^{-1}u,\Gamma_1 v\right\rangle_{\mathcal{K}} &(5.1)\\ &=\left\langle\Gamma_0(A_0-zI)^{-1}u,\Gamma_1 v\right\rangle_{\mathcal{K}}-\left\langle\Gamma_1(A_0-zI)^{-1}u,\Gamma_0 v\right\rangle_{\mathcal{K}} &(5.2)\\ &=\left\langle(A_0-zI)^{-1}u,A^*v\right\rangle_{\mathcal{H}}-\left\langle A^*(A_0-zI)^{-1}u,v\right\rangle_{\mathcal{H}} &(5.3)\\ &=\int_{\mathbb{R}}\frac{1}{t-z}d\mu_{u,A^*v}(t)-\int_{\mathbb{R}}\frac{t}{t-z}d\mu_{u,v}(t)=\int_{\mathbb{R}}\frac{1}{t-z}d\hat{\mu}(t). &(5.4)\end{aligned}$$

Here

$$\mu_{u,A^*v}(\delta):=\langle E_{A_0}(\delta)u,A^*v\rangle_{\mathcal{H}},\qquad\mu_{u,v}(\delta):=\langle E_{A_0}(\delta)u,v\rangle_{\mathcal{H}}\qquad\forall\,\text{Borel }\delta\subset\mathbb{R},$$

where E_{A_0} is the spectral resolution of the identity for the operator A_0, and $\hat{\mu}(t) := \mu_{u,A^*v}(t) - t\mu_{u,v}(t)$. Furthermore, the measure $\hat{\mu}$ admits the decomposition into its absolutely continuous and singular parts with respect to the Lebesgue measure. Its singular part is equal to $\mu_{u_s,A^*v}(t) - t\mu_{u_s,v}(t) =: \hat{\mu}_s(t)$, see *e.g.* [6]. The equality (5.1)–(5.2) is due to the observation that Γ_1 vanishes on $\mathrm{dom}(A_0)$, and the equality (5.2)–(5.3) is a consequence of the "Green formula" (2.3) and the fact that $A \subset A_0$.

At the same time, it follows from Corollary 4.4 that the scalar analytic function $\left\langle \Gamma_0(A_0 - zI)^{-1}u, \alpha w \right\rangle_{\mathcal{K}}$ is an element of H^2_+ and also of H^2_-. Therefore, by Lemma 5.1 we infer from (5.1)–(5.4) that the measure $\hat{\mu}$ is absolutely continuous, which implies that its singular part $\hat{\mu}_s$ is the zero measure.

Finally, we invoke (5.1)–(5.4) once again, having replaced u by u_s and $\hat{\mu}$ by $\hat{\mu}_s$, and conclude that

$$\left\langle \Gamma_0(A_0 - zI)^{-1}u_s, \alpha w \right\rangle_{\mathcal{K}} = 0 \qquad \forall\, z \in \mathbb{C} \setminus \mathbb{R}. \tag{5.5}$$

Now, by virtue of the facts that $w \in \mathcal{K}$ in (5.5) is arbitrary and $\ker(\alpha) = \{0\}$, it follows that $\Gamma_0(A_0 - zI)^{-1}u_s = 0$, and since $(A_0 - zI)^{-1}u_s \in \mathrm{dom}(A_0)$ and therefore $\Gamma_1(A_0 - zI)^{-1}u_s = 0$ automatically, we obtain $(A_0 - zI)^{-1}u_s \in \mathrm{dom}(A)$. Finally, since $A_0 \supset A$, we conclude that $u_s \in \mathrm{ran}(A - zI)$ for all $z \in \mathbb{C} \setminus \mathbb{R}$, as claimed.

In order to treat the case of an arbitrary $\varkappa \in \mathcal{B}(\mathcal{K})$ such that $\varkappa = \varkappa^*$, we define "shifted" boundary operators $\widehat{\Gamma}_0 := \Gamma_0$, $\widehat{\Gamma}_1 := \Gamma_1 - B_\varkappa \Gamma_0$. Notice that (*cf.* (2.5))

$$\mathrm{dom}(A_\varkappa) = \{u \in \mathcal{H} : \Gamma_1 u = B_\varkappa \Gamma_0 u\} = \{u \in \mathcal{H} : \widehat{\Gamma}_1 u = 0\},$$

i.e. the operator $A_\varkappa$ plays the rôle of the operator A_0 in the triple $(\mathcal{K}, \widehat{\Gamma}_0, \widehat{\Gamma}_1)$. Further, note that the change of the triple results in a change of the operator that needs to play the rôle of A_{iI}, the dissipative extension used to construct the functional model, which in terms of the "old" triple $(\mathcal{K}, \Gamma_0, \Gamma_1)$ should be the extension A_B with $B = \alpha(i + \varkappa)\alpha/2$. Repeating the above argument in this new functional model and bearing in mind that the characterisation of $\widetilde{N}_{\mathrm{e}}^{\varkappa}$ in Corollary 4.4 holds for all $\varkappa$, yields the stated result. □

An immediate consequence of this result and the criterion of complete non-selfadjointness (2.1) is the following assertion.

Corollary 5.3. *Let $\varkappa$ and α be as in the preceding lemma. If A is completely non-selfadjoint, then*

$$\widetilde{N}_{\mathrm{e}}^{\varkappa} \subset \mathcal{H}_{\mathrm{ac}}(A_\varkappa)\,.$$

We now proceed to the proof of the opposite inclusion.

Lemma 5.4 (Modified Rosenblum lemma, *cf.* [57])**.** *Let β be a self-adjoint operator in a Hilbert space $\mathcal{H}_1$. Suppose that the operator T, defined on* $\mathrm{dom}(\beta)$ *and taking values in a Hilbert space $\mathcal{H}_2$, is such that $T(\beta - z_0 I)^{-1}$ is a Hilbert-Schmidt operator for some $z_0 \in \rho(\beta)$. Then there exists a set $\mathcal{D}$, dense in $\mathcal{H}_{\mathrm{ac}}(\beta)$, such that*

$$\int_{\mathbb{R}} \|T \exp(-i\beta t)u\|^2 \, dt < \infty$$

for all $u \in \mathcal{D}$.

Proof. Let $x \in \mathbb{R}$ and $\epsilon > 0$. By Hilbert's first identity

$$T(\beta - (x + \mathrm{i}\epsilon)I)^{-1} = ((x + \mathrm{i}\epsilon) - z_0)T(\beta - z_0 I)^{-1}(\beta - (x + \mathrm{i}\epsilon)I)^{-1} + T(\beta - z_0 I)^{-1}$$

Consider the first term on the right-hand side of this last equation. By [49], for every f in $\mathcal{H}_1$ the limit

$$\lim_{\epsilon \to 0} T(\beta - z_0 I)^{-1}(\beta - (x + \mathrm{i}\epsilon)I)^{-1} f$$

exists for almost all $x \in \mathbb{R}$ (the convergence set actually depends on f). It follows that the limit

$$\lim_{\epsilon \to 0} T\left((\beta - (x + \mathrm{i}\epsilon)I)^{-1} - (\beta - (x - \mathrm{i}\epsilon)I)^{-1}\right) f =: F(x)$$

exists for all $f \in \mathcal{H}_1$ and almost all $x \in \mathbb{R}$.

Now, define the set

$$\mathcal{X}(n) := \left\{x \in \mathbb{R} : |x| < n, \|F(x)\| < n\right\}$$

If E_β denotes the spectral measure of the operator β, then the set

$$\mathcal{D} := \bigcup_{n \in \mathbb{N}} E_\beta\big(\mathcal{X}(n)\big)\mathcal{H}_{\mathrm{ac}}(\beta)$$

is dense in $\mathcal{H}_{\mathrm{ac}}(\beta)$. Consider an orthonormal basis $\{\phi_k\}$ in $\mathcal{H}_2$ and an arbitrary element $f \in \mathcal{D}$, then, for all k,

$$\begin{aligned}\langle T \exp(-i\beta t) f, \phi_k\rangle &= \int_{\mathcal{X}(n)} e^{-\mathrm{i}xt} \frac{d}{dx} \langle E_\beta(x) f, T^* \phi_k\rangle \, dx \\ &= \int_{\mathcal{X}(n)} e^{-\mathrm{i}xt} \langle F(x), T^* \phi_k\rangle \, dx \,,\end{aligned}$$

where in the last equality we have used the fact that by the spectral theorem

$$\lim_{\epsilon \to 0} \left\langle \left((\beta - (x + \mathrm{i}\epsilon)I)^{-1} - (\beta - (x - \mathrm{i}\epsilon)I)^{-1}\right) f, \phi\right\rangle = \frac{d}{dx} \langle E_\beta(x) f, \phi\rangle$$

for all $f \in \mathcal{H}_{\mathrm{ac}}(\beta)$ and for all $\phi \in \mathcal{H}_1$.

By the Parseval identity one has

$$\int_{\mathbb{R}} |\langle T \exp(-i\beta t) f, \phi_k\rangle|^2 \, dt = 2\pi \int_{\mathcal{X}(n)} |\langle F(x), \phi_k\rangle|^2 \, dx$$

for all k, which immediately implies that

$$\int_{\mathbb{R}} \|T \exp(-i\beta t) u\|^2 \, dt = 2\pi \int_{\mathcal{X}(n)} \|F(x)\|^2 \, dx \le 4\pi n^3 < +\infty \,.$$

$\square$

Combining the above statements yields the following result.

Theorem 5.5. *Assume that* $\varkappa = \varkappa^*$, $\ker(\alpha) = \{0\}$ *and let* $\alpha\Gamma_0(A_\varkappa - zI)^{-1}$ *be a Hilbert-Schmidt operator for at least one point* $z \in \rho(A_\varkappa)$. *If* A *is completely non-selfadjoint, then*

$$N_{\mathrm{e}}^{\varkappa} = \mathcal{H}_{\mathrm{ac}}(A_\varkappa)\,.$$

Proof. By applying the Fourier transform to the functions $\mathbb{1}_\pm(t)\alpha\Gamma_0 e^{iA_\varkappa t}e^{\mp\epsilon t}u$, $t \in \mathbb{R}$, where $\mathbb{1}_\pm$ is the characteristic function of $\mathbb{R}_\pm$ and $\epsilon > 0$ is arbitrarily small, one obtains

$$\left\|\alpha\Gamma_0(A_\varkappa - zI)^{-1}u\right\|^2_{H^2_-} + \left\|\alpha\Gamma_0(A_\varkappa - zI)^{-1}u\right\|^2_{H^2_+} = 2\pi\int_{\mathbb{R}}\left\|\alpha\Gamma_0\exp(iA_\varkappa t)u\right\|^2 dt$$

which by Lemma 5.4 is finite for all u in a dense subset of $\mathcal{H}_{\mathrm{ac}}(A_\varkappa)$. Hence, in view of Corollary 4.4 and performing closure, one has $\mathcal{H}_{\mathrm{ac}}(A_\varkappa) \subset N_{\mathrm{e}}^{\varkappa}$. Taking into account Corollary 5.3 completes the proof. □

Remark 6. Alternative conditions, which are less restrictive in general, that guarantee the validity of the assertion of Theorem 5.5 can be obtained along the lines of [50].

6. Wave and scattering operators

The results of the preceding sections allow us to calculate the wave operators for any pair $A_{\varkappa_1}, A_{\varkappa_2}$, where $A_{\varkappa_1}$ and $A_{\varkappa_2}$ are operators in the class introduced in Section 2, under the additional assumption that the operator α (see (2.6)) has a trivial kernel. For simplicity, and bearing in mind the application of the abstract construction to the problem described in Sections 8 and 9, in what follows we set $\varkappa_2 = 0$ and write $\varkappa$ instead of $\varkappa_1$. Note that A_0 is a self-adjoint operator, which is convenient for presentation purposes.

We begin by establishing the model representation for the function $\exp(iA_\varkappa t)$, $t \in \mathbb{R}$, of the operator $A_\varkappa$, evaluated on the set of smooth vectors $\widetilde{N}_{\mathrm{e}}^{\varkappa}$.

Proposition 6.1. *([48, Prop. 2]) For all* $t \in \mathbb{R}$ *and all* $\binom{\widetilde{g}}{g}$ *such that* $\Phi^* P_K\binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{\varkappa}$ *one has*

$$\Phi\exp(iA_\varkappa t)\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\exp(ikt)\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}.$$

Proof. We use the definition

$$\exp(iA_\varkappa t) := \operatorname*{s-lim}_{n\to+\infty}\left(I - \frac{iA_\varkappa t}{n}\right)^{-n}, \quad t \in \mathbb{R},$$

giving in general an unbounded operator (see [27]). Due to Theorem 4.2, if $\binom{\widetilde{g}}{g} \in \mathcal{N}_+^{\varkappa} \cap \mathcal{N}_-^{\varkappa}$, *i.e.* $\Phi^* P_K\binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{\varkappa}$, then

$$\left(I - \frac{iA_\varkappa t}{n}\right)^{-n}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \Phi^* P_K\left(1 - \frac{ikt}{n}\right)^{-n}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}, \quad t \in \mathbb{R}.$$

Thus, to complete the proof it remains to show that

$$\left\|\left(\exp(ikt) - \left(1 - \frac{ikt}{n}\right)^{-n}\right)\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}\right\| \xrightarrow[n\to\infty]{} 0, \quad t \in \mathbb{R},$$

which follows directly from Lebesgue's dominated convergence theorem. □

Proposition 6.2. *([48, Section 4]) If* $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{\varkappa}$ *and* $\Phi^* P_K \binom{\widehat{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{0}$ *(with the same element*[1] g*), then*

$$\left\| \exp(-iA_{\varkappa}t)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} - \exp(-iA_0 t)\Phi^* P_K \begin{pmatrix} \widehat{g} \\ g \end{pmatrix} \right\| \xrightarrow[t\to-\infty]{} 0.$$

Proof. Clearly, $\widetilde{g} - \widehat{g} \in L^2(E)$ since $\binom{\widetilde{g}-\widehat{g}}{0} \in \mathfrak{H}$. Therefore, for all $t \in \mathbb{R}$, we obtain

$$\begin{aligned}
\left\| \exp(-iA_{\varkappa}t)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} - \exp(-iA_0 t)\Phi^* P_K \begin{pmatrix} \widehat{g} \\ g \end{pmatrix} \right\| &= \left\| P_K e^{-it\cdot} \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} - P_K e^{-it\cdot} \begin{pmatrix} \widehat{g} \\ g \end{pmatrix} \right\| \\
&= \left\| P_K \begin{pmatrix} e^{-it\cdot}(\widetilde{g} - \widehat{g}) \\ 0 \end{pmatrix} \right\| \\
&= \left\| P_K \begin{pmatrix} P_- e^{-it\cdot}(\widetilde{g} - \widehat{g}) \\ 0 \end{pmatrix} \right\| \\
&\leq \left\| P_- e^{-it\cdot}(\widetilde{g} - \widehat{g}) \right\|_{L^2(E)} .
\end{aligned}$$

The third equality above follows from the observation that, for all $\binom{\check{g}}{0} \in \mathfrak{H}$, one has

$$P_K \begin{pmatrix} \check{g} \\ 0 \end{pmatrix} - P_K \begin{pmatrix} P_- \check{g} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ P_- S P_+ \check{g} \end{pmatrix} = 0\,,$$

since $S(z)$, $z \in \mathbb{C}_+$, is an analytic contraction in the upper half-plane, while in the inequality we use the fact that

$$\left\| P_K \begin{pmatrix} \check{g} \\ 0 \end{pmatrix} \right\|^2 = \int_{\mathbb{R}} \left(\|P_- \check{g}(s)\|^2 - \|P_- S(s)\check{g}(s)\|^2 \right) ds\,.$$

Finally, since $\exp(-it\cdot) \in H_+^\infty$ for $t \geq 0$ yields the convergence (see *e.g.* [32])

$$\left\| P_- e^{-it\cdot}(\widetilde{g} - \widehat{g}) \right\|_{L^2(E)}^2 = \int_{-\infty}^{t} \|\mathcal{F}(\widetilde{g} - \widehat{g})(\tau)\|_{\mathrm{e}}^2 \, d\tau \xrightarrow[t\to-\infty]{} 0\,,$$

where $\mathcal{F}(\widetilde{g} - \widehat{g})$ stands for the Fourier transform of the function $\widetilde{g} - \widehat{g}$. □

It follows from Proposition 6.2 that whenever $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{\varkappa}$ and $\Phi^* P_K \binom{\widehat{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{0}$ (with the same second component g), formally one has

$$\begin{aligned}
\lim_{t\to-\infty} e^{iA_0 t} e^{-iA_{\varkappa} t} \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} &= \Phi^* P_K \begin{pmatrix} \widehat{g} \\ g \end{pmatrix} \\
&= \Phi^* P_K \begin{pmatrix} -(I+S)^{-1}(I+S^*)g \\ g \end{pmatrix},
\end{aligned}$$

[1]Despite the fact that $\binom{\widetilde{g}}{g} \in \mathfrak{H}$ is nothing but a symbol, still $\widetilde{g}$ and g can be identified with vectors in certain $L^2(E)$ spaces with operators "weights", see details below in Section 7. Further, we recall that even then for $\binom{\widetilde{g}}{g} \in \mathfrak{H}$, the components $\widetilde{g}$ and g are not, in general, *independent* of each other.

where in the last equality we use the inclusion $\Phi^* P_K\binom{\widehat{g}}{g} \in \widetilde{N}_{\mathrm{e}}^0$, which by Remark 5 (*cf.* (4.20)), yields $\widehat{g}+S^*g+S\widehat{g}+g=0$. In view of the classical definition of the wave operator of a pair of self-adjoint operators, see *e.g.* [27],

$$W_\pm(A_0, A_\varkappa) := \operatorname*{s-lim}_{t\to\pm\infty} e^{iA_0t}e^{-iA_\varkappa t}P_{\mathrm{ac}}^\varkappa,$$

where $P_{\mathrm{ac}}^\varkappa$ is the projection onto the absolutely continuous subspace of $A^\varkappa$, we obtain that, at least formally, for $\Phi^* P_K\binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^\varkappa$ one has

$$W_-(A_0, A_\varkappa)\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \Phi^* P_K\begin{pmatrix}-(I+S)^{-1}(I+S^*)g\\ g\end{pmatrix}. \tag{6.1}$$

By an argument similar to that of Proposition 6.2 (*i.e.* considering the case $t\to+\infty$), one also obtains

$$W_+(A_0, A_\varkappa)\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \lim_{t\to+\infty} e^{iA_0t}e^{-iA_\varkappa t}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \Phi^* P_K\begin{pmatrix}\widetilde{g}\\ -(I+S^*)^{-1}(I+S)\widetilde{g}\end{pmatrix} \tag{6.2}$$

again for $\Phi^* P_K\binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^\varkappa$.

Further, the definition of the wave operators $W_\pm(A_\varkappa, A_0)$

$$\left\| e^{-iA_\varkappa t}W_\pm(A_\varkappa, A_0)\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} - e^{-iA_0t}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}\right\| \xrightarrow[t\to\pm\infty]{} 0$$

yields, for all $\Phi^* P_K\binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^0$,

$$W_-(A_\varkappa, A_0)\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \Phi^* P_K\begin{pmatrix}-(I+\chi_\varkappa^-(S-I))^{-1}(I+\chi_\varkappa^+(S^*-I))g\\ g\end{pmatrix} \tag{6.3}$$

and

$$W_+(A_\varkappa, A_0)\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \Phi^* P_K\begin{pmatrix}\widetilde{g}\\ -(I+\chi_\varkappa^+(S^*-I))^{-1}(I+\chi_\varkappa^-(S-I))\widetilde{g}\end{pmatrix}, \tag{6.4}$$

where we have used the fact that $\Phi^* P_K\binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^\varkappa$ and the corresponding criterion provided by Remark 5, *cf.* (4.20).

In order to rigorously justify the above formal argument, *i.e.* in order to prove the existence and completeness of the wave operators, one needs to first show that the right-hand sides of the formulae (6.1)–(6.4) make sense on dense subsets of the corresponding absolutely continuous subspaces. Noting that (6.1)–(6.4) have the form identical to the expressions for wave operators derived in [48, Section 4], [50], the remaining part of this justification is a modification of the argument of [50], as follows.

Let $S(z)-I$ be of the class $\mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$, *i.e.* a compact analytic operator function in the upper half-plane up to the real line. Then so is $(S(z)-I)/2$, which is also uniformly bounded in the upper half-plane along with $S(z)$. We next use the result of [50, Theorem 3] about the non-tangential boundedness of operators of the form $(I+T(z))^{-1}$ for $T(z)$ compact up to the real line. We infer that, provided $(I+(S(z_0)-I)/2)^{-1}$ exists for some $z_0\in\mathbb{C}_+$ (and hence, see [9], everywhere in $\mathbb{C}_+$ except for a countable set of points accumulating only to the real line), one has non-tangential boundedness of $(I + (S(z) - I)/2)^{-1}$, and therefore also of $(I + S(z))^{-1}$, for almost all points of the real line.

On the other hand, the latter inverse can be computed in $\mathbb{C}_+$:

$$\big(I + S(z)\big)^{-1} = \frac{1}{2}\big(I + i\alpha M(z)^{-1}\alpha/2\big). \tag{6.5}$$

Indeed, one has

$$\begin{aligned}&\big(I + i\alpha M(z)^{-1}\alpha/2\big)(I + S(z))\\ &\quad = 2I + i\alpha M(z)^{-1}\alpha + i\alpha\big(B_{iI}^* - M(z)\big)^{-1}\alpha - i\alpha M(z)^{-1}B_{iI}^*\big(B_{iI}^* - M(z)\big)^{-1}\alpha = 2I\end{aligned}$$

and the second similar identity for the multiplication in the reverse order proves the claim.

It follows from (6.5) and the analytic properties of $M(z)$ that the inverse $(I+S(z))^{-1}$ exists everywhere in the upper half-plane. Thus, Theorem 3 of [50] is indeed applicable, which yields that $(I + S(z))^{-1}$ is $\mathbb{R}$-a.e. nontangentially bounded and, by the operator generalisation of the Calderon theorem (see [60]), which was extended to the operator context in [50, Theorem 1], it admits measurable non-tangential limits in the strong operator topology almost everywhere on $\mathbb{R}$. As it is easily seen, these limits must then coincide with $(I + S(k))^{-1}$ for almost all $k \in \mathbb{R}$.

The same argument obviously applies to $(I + S^*(\bar{z}))^{-1}$ for $z \in \mathbb{C}_-$, where the invertibility follows from the identity

$$\big(I + S^*(\bar{z})\big)^{-1} = \frac{1}{2}\big(I - i\alpha M(z)^{-1}\alpha/2\big) \tag{6.6}$$

obtained exactly as (6.5), by taking into account analytic properties of $M(z)$.

Finally, the identities

$$(I + \chi_\varkappa^-(S(z) - I))^{-1} = I - i\chi_\varkappa^-\alpha(B_\varkappa - M(z))^{-1}\alpha \tag{6.7}$$

for $z \in \mathbb{C}_+$ and

$$(I + \chi_\varkappa^+(S^*(\bar{z}) - I))^{-1} = I + i\chi_\varkappa^+\alpha(B_\varkappa - M(z))^{-1}\alpha \tag{6.8}$$

for $z \in \mathbb{C}_-$ are used, again by an application of Theorem 3 of [50], to ascertain the existence of bounded $(I + \chi_\varkappa^-(S(k) - I))^{-1}$ and $(I + \chi_\varkappa^+(S^*(k) - I))^{-1}$ almost everywhere on $\mathbb{R}$, provided that the operator $A_\varkappa$ has at least one regular point in each half-plane of the complex plane, see Proposition 2.2. Under the assumptions on S specified above, this latter condition immediately implies that the non-real spectrum of $A_\varkappa$ is countable and accumulates to $\mathbb{R}$ only. (Nevertheless, it could still accumulate to all points of the real line simultaneously.)

The presented argument allows one to verify the correctness of the formulae (6.1)–(6.4) for the wave operators. Indeed, for the first of them one considers $\mathbb{1}_n(k)$, the indicator of the set $\{k \in \mathbb{R} : \|(I + S(k))^{-1}\| \le n\}$. Clearly, $\mathbb{1}_n(k) \to 1$ as $n \to \infty$ for almost all $k \in \mathbb{R}$.

Next, suppose that $P_K(\tilde{g}, g) \in \tilde{N}_{\mathrm{e}}^{\varkappa}$. Then $P_K \mathbb{1}_n(\tilde{g}, g)$ is also a smooth vector and

$$\begin{pmatrix} -(I+S)^{-1}\mathbb{1}_n(I+S^*)g \\ \mathbb{1}_n g \end{pmatrix} \in \mathfrak{H}.$$

Indeed, for any $(\tilde{g}, g) \in \mathfrak{H}$ one has

$$\begin{pmatrix} -\mathbb{1}_n(1+S)^{-1}(1+S^*)g \\ \mathbb{1}_n g \end{pmatrix} - \begin{pmatrix} \mathbb{1}_n \tilde{g} \\ \mathbb{1}_n g \end{pmatrix} \\ = \begin{pmatrix} -\mathbb{1}_n(1+S)^{-1}[(\tilde{g}+S^*g)+(S\tilde{g}+g)] \\ 0 \end{pmatrix} \in \begin{pmatrix} L^2(E) \\ 0 \end{pmatrix} \in \mathfrak{H},$$

whereas the inclusion in the set of smooth vectors follows directly from Remark 5. It follows, by the Lebesgue dominated convergence theorem, that the set of vectors $P_K \mathbb{1}_n(\tilde{g}, g)$ is dense in $N_{\mathrm{e}}^{\varkappa}$. The remaining three wave operators are treated in a similar way. Finally, the density of the range of the four wave operators follows from the density of their domains, by a standard inversion argument, see *e.g.* [71].

We have thus proved the following theorem.

Theorem 6.3. *Let A be a closed, symmetric, completely nonselfadjoint operator with equal deficiency indices and consider its extension $A_\varkappa$, as described in Section 2, under the assumptions that* $\ker(\alpha) = \{0\}$ *(see (2.6)) and that $A_\varkappa$ has at least one regular point in $\mathbb{C}_+$ and in $\mathbb{C}_-$. If $S-I \in \mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$, then the wave operators $W_\pm(A_0, A_\varkappa)$ and $W_\pm(A_\varkappa, A_0)$ exist on dense sets in $N_{\mathrm{e}}^{\varkappa}$ and $\mathcal{H}_{\mathrm{ac}}(A_0)$, respectively, and are given by the formulae (6.1)–(6.4). The ranges of $W_\pm(A_0, A_\varkappa)$ and $W_\pm(A_\varkappa, A_0)$ are dense in $\mathcal{H}_{\mathrm{ac}}(A_0)$ and $N_{\mathrm{e}}^{\varkappa}$, respectively.*[2]

Remark 7. 1. The identities (6.5)–(6.6) can be used to replace the condition $S(z) - I \in \mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$ by the following equivalent condition: $\alpha M(z)^{-1}\alpha$ is nontangentially bounded almost everywhere on the real line, and $\alpha M(z)^{-1}\alpha \in \mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$ for $\Im z \geq 0$. In order to do so, one notes that $(I+T)^{-1} - I = -(I+T)^{-1}T \in \mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$ as long as $T \in \mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$ and $(I+T)^{-1}$ is bounded.

2. The latter condition is satisfied [22], as long as the scalar function $\|\alpha M(z)^{-1}\alpha\|_{\mathfrak{S}_p}$ is nontangentially bounded almost everywhere on the real line for some $p < \infty$, where $\mathfrak{S}_p$, $p \in (0, \infty]$ are the standard Schatten – von Neumann classes of compact operators.

3. An alternative sufficient condition is the condition $\alpha \in \mathfrak{S}_2$ (and therefore $B_\varkappa \in \mathfrak{S}_1$), or, more generally, $\alpha M(z)^{-1}\alpha \in \mathfrak{S}_1$, see [49] for details.

4. Following from the analysis above, the existence and completeness of the wave operators for the par $A_\varkappa$, A_0 is closely linked to the condition of α having a "relative Hilbert-Schmidt property" with respect to $M(z)$. Recalling that $B_\varkappa = \alpha\varkappa\alpha/2$, this is not always feasible to expect. Nevertheless, by appropriately modifying the boundary triple, the situation can often be rectified. For example, if $C_\varkappa = C_0 + \alpha\varkappa\alpha/2$, where C_0 and $\varkappa$ are bounded and $\alpha \in \mathfrak{S}_2$, replaces the operator $B_\varkappa$ in (2.6), then one "shifts" the boundary triple (*cf.* the proof of Lemma 5.2): $\widehat{\Gamma}_0 = \Gamma_0$, $\widehat{\Gamma}_1 = \Gamma_1 - C_0\Gamma_0$. One thus obtains that in the new triple $(\mathcal{K}, \widehat{\Gamma}_0, \widehat{\Gamma}_1)$ the operator $A_\varkappa$ coincides with the extension corresponding to the

[2] In the case when $A_\varkappa$ is self-adjoint, or, in general, the named wave operators are bounded, the claims of the theorem are equivalent (by the classical Banach-Steinhaus theorem) to the statement of the existence and completeness of the wave operators for the pair $A_0, A_\varkappa$. Sufficient conditions of boundedness of these wave operators are contained in *e.g.* [48, Section 4], [50] and references therein.

boundary operator $B_\varkappa = \alpha\varkappa\alpha/2$, whereas the Weyl-Titchmarsh function $M(z)$ undergoes a shift to the function $M(z) - C_0$. The proof of Theorem 6.1 remains intact, while Part 3 of this remark yields that the condition $\alpha(M(z) - C_0)^{-1}\alpha \in \mathfrak{S}_1$ guarantees the existence and completeness of the wave operators for the pair A_{C_0}, $A_{C_\varkappa}$. The fact that the operator A_0 here is replaced by the operator A_{C_0} reflects the standard argument that the complete scattering theory for a pair of operators requires that the operators forming this pair are "close enough" to each other.

Finally, the scattering operator Σ for the pair $A_\varkappa$, A_0 is defined by

$$\Sigma = W_+^{-1}(A_\varkappa, A_0)W_-(A_\varkappa, A_0).$$

The above formulae for the wave operators lead (*cf.* [48]) to the following formula for the action of Σ in the model representation:

$$\Phi\Sigma\Phi^* P_K \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} = P_K \begin{pmatrix} -(I + \chi_\varkappa^-(S - I))^{-1}(I + \chi_\varkappa^+(S^* - I))g \\ (I + S^*)^{-1}(I + S)(I + \chi_\varkappa^-(S - I))^{-1}(I + \chi_\varkappa^+(S^* - I))g \end{pmatrix}, \tag{6.9}$$

whenever $\Phi^* P_K \binom{\tilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^0$. In fact, as explained above, this representation holds on a dense linear set in $\widetilde{N}_{\mathrm{e}}^0$ within the conditions of Theorem 6.3, which guarantees that all the objects on the right-hand side of the formula (6.9) are correctly defined.

7. Spectral representation for the absolutely continuous part of the operator A_0

The identity

$$\left\| P_K \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} \right\|_{\mathcal{H}}^2 = \langle (I - S^*S)\tilde{g}, \tilde{g} \rangle$$

which is derived in the same way as in [48, Section 7] for all $P_K\binom{\tilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^0$ and is equivalent to the condition $(\tilde{g} + S^*g) + (S\tilde{g} + g) = 0$, see (4.20), allows us to consider the isometry $F : \Phi\widetilde{N}_{\mathrm{e}}^0 \mapsto L^2(E; I - S^*S)$ defined by the formula

$$FP_K \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} = \tilde{g}. \tag{7.1}$$

Here $L^2(E; I - S^*S)$ is the Hilbert space of $\mathcal{K}$-valued functions on $\mathbb{R}$ square summable with the matrix "weight" $I - S^*S$, *cf.* (4.3). Similarly, the formula

$$F_* P_K \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} = g$$

defines an isometry F_* from $\Phi\widetilde{N}_{\mathrm{e}}^0$ to $L^2(E; I - SS^*)$.

Lemma 7.1. *Suppose that the assumptions of Theorem 6.3 hold. Then the ranges of the operators F and F_* are dense in the spaces $L^2(E; I - S^*S)$ and $L^2(E; I - SS^*)$, respectively.*

Proof. Indeed, for all $\tilde{g} \in L^2(E; I - S^*S)$ and $g = -S\tilde{g}$ one has $(\tilde{g}, g) \in \mathcal{H}$ with $\|(\tilde{g}, g)\|_{\mathcal{H}} = \|\tilde{g}\|_{L^2(E; I - S^*S)}$. By repeating the proof of Theorem 6.3, the operator $I + S^*$ is boundedly invertible almost everywhere on $\mathbb{R}$.

Further, consider $\mathbb{1}_n(k)$, the indicator of the set $\{k \in \mathbb{R} : \|(I + S^*(k))^{-1}\| \le n\}$. For $\tilde{g} \in L^2(E; I - S^*S)$ and, as above, $g = -S\tilde{g}$, one has $\mathbb{1}_n(\tilde{g}, -(I + S^*)^{-1}(I + S)\tilde{g}) \in \mathcal{H}$, since

$$\mathbb{1}_n\begin{pmatrix}\tilde{g}\\ -(I + S^*)^{-1}(I + S)\tilde{g}\end{pmatrix} - \mathbb{1}_n\begin{pmatrix}\tilde{g}\\ g\end{pmatrix}$$
$$= \begin{pmatrix}0\\ -\mathbb{1}_n(I + S^*)^{-1}\big[(S\tilde{g} + g) + (\tilde{g} + S^*g)\big]\end{pmatrix} \in \begin{pmatrix}0\\ L^2(E)\end{pmatrix}.$$

Finally, the set $\{\mathbb{1}_n\tilde{g}\}$ is dense in $L^2(E; I - S^*S)$ by the Lebesgue dominated convergence theorem, whereas $P_K\mathbb{1}_n(\tilde{g}, -(I + S^*)^{-1}(I + S)\tilde{g}) \in \widetilde{N}_{\mathrm{e}}^0$ by direct calculation. $\square$

Corollary 7.2. *The operator F, respectively F_*, admits an extension to the unitary mapping between ΦN_{e}^0 and $L^2(E; I - S^*S)$, respectively $L^2(E; I - SS^*)$.*

It follows that the operator $(A_0 - z)^{-1}$ (see notation (2.7)) considered on $\widetilde{N}_{\mathrm{e}}^0$ acts as the multiplication by $(k - z)^{-1}$, $k \in \mathbb{R}$, both in $L^2(E; I - S^*S)$ and $L^2(E; I - SS^*)$. In particular, if one considers the absolutely continuous "part" of the operator A_0, namely the operator $A_0^{(\mathrm{e})} := A_0|_{N_{\mathrm{e}}^0}$, then $F\Phi A_0^{(\mathrm{e})}\Phi^*F^*$ and $F_*\Phi A_0^{(\mathrm{e})}\Phi^*F_*^*$ are the operators of multiplication by the independent variable in the spaces $L^2(E; I - S^*S)$ and $L^2(E; I - SS^*)$, respectively.

In order to obtain a spectral representation from the above result, it is necessary to diagonalise the weights in the definitions of the above L^2-spaces. This diagonalisation is straightforward when $\alpha = \sqrt{2}I$. (This choice of α satisfies the conditions of Theorem 6.3 *e.g.* when the boundary space $\mathcal{K}$ is finite-dimensional, which is the case we deal with in the application discussed in Sections 8, 9. The corresponding diagonalisation in the general setting will be treated elsewhere.) In this particular case one has

$$S = (M - iI)(M + iI)^{-1}, \tag{7.2}$$

and consequently

$$I - S^*S = -2i(M^* - iI)^{-1}(M - M^*)(M + iI)^{-1} \tag{7.3}$$

and

$$I - SS^* = 2i(M + iI)^{-1}(M^* - M)(M^* - iI)^{-1}.$$

Introducing the unitary transformations

$$G : L^2(E; I - S^*S) \mapsto L^2(E; -2i(M - M^*)), \tag{7.4}$$

$$G_* : L^2(E; I - SS^*) \mapsto L^2(E; -2i(M - M^*)) \tag{7.5}$$

by the formulae $g \mapsto (M + iI)^{-1}g$ and $g \mapsto (M^* - iI)^{-1}g$ respectively, one arrives at the fact that $GF\Phi A_0^{(\mathrm{e})}\Phi^*F^*G^*$ and $G_*F_*\Phi A_0^{(\mathrm{e})}\Phi^*F_*^*G_*^*$ are the operators of multiplication by the independent variable in the space $L^2(E; -2i(M - M^*))$. We show next that this amounts to the spectral representation in particular in the case of (non-compact) quantum graphs.

8. Quantum graphs and their scattering matrices

We remark, that the result of the previous section only pertains to the absolutely continuous part of the self-adjoint operator A_0, unlike *e.g.* the passage to the classical von Neumann direct integral, under which the whole of the self-adjoint operator gets mapped to the multiplication operator in a weighted L^2-space (see *e.g.* [6, Chapter 7]). Nevertheless, our consideration proves to be useful in scattering theory, since it yields an explicit expression for the scattering matrix $\widehat{\Sigma}$ for the pair $A_\varkappa$, A_0, which is the image of the scattering operator Σ in the spectral representation of the operator A_0 described in the previous section. Namely, we prove the following statement.

Theorem 8.1. *In the case $\alpha = \sqrt{2}I$ (and hence $E = \mathcal{K}$) the following formula holds:*

$$\widehat{\Sigma} = GF\Sigma(GF)^* = (M-\varkappa)^{-1}(M^*-\varkappa)(M^*)^{-1}M, \tag{8.1}$$

where the right-hand side represents the operator of multiplication by the corresponding function.

Proof. Using the definition (7.1) of the isometry F along with the relationship (4.20) between $\tilde{g}$ and g whenever $P_K\binom{\tilde{g}}{g} \in \Phi\widetilde{N}_{\rm e}^{\varkappa}$ with $\varkappa = 0$, we obtain from (6.9):

$$F\Sigma F^* = \bigl(I + \chi_\varkappa^-(S-I)\bigr)^{-1}\bigl(I + \chi_\varkappa^+(S^*-I)\bigr)(I+S^*)^{-1}(I+S), \tag{8.2}$$

where the right-hand side represents the operator of multiplication by the corresponding function.

Furthermore, substituting the expression (7.2) for S in terms of M implies that $F\Sigma F^*$ is the operator of multiplication by

$$(M+iI)(M-\varkappa)^{-1}(M^*-\varkappa)(M^*)^{-1}M(M+iI)$$

in the space $L^2(E; I - S^*S)$. Using (7.3), we now obtain the following identity for all $f, g \in L^2(E; I - S^*S)$:

$$\langle F\Sigma F^* f, g\rangle_{L^2(E;I-S^*S)} = \bigl\langle (I - S^*S)(M+iI)(M-\varkappa)^{-1}(M^*-\varkappa)(M^*)^{-1}M(M+iI)f, g\bigr\rangle$$

$$= \bigl\langle -2i(M^*-iI)^{-1}(M-M^*)(M+iI)^{-1}(M+iI)(M-\varkappa)^{-1}(M^*-\varkappa)(M^*)^{-1}M(M+iI)f, g\bigr\rangle$$

$$= \bigl\langle -2i(M-M^*)(M-\varkappa)^{-1}(M^*-\varkappa)(M^*)^{-1}M(M+iI)f, (M+iI)g\bigr\rangle,$$

which is equivalent to (8.1), in view of the definition of the operator G. □

In applications to quantum graphs it may turn out that the operator weight $-2i(M - M^*)$ (see (7.4), (7.5)) is degenerate: more precisely, $M(s) - M(s)^* = 2i\sqrt{s}P_{\rm e}$, $s \in \mathbb{R}$, where $P_{\rm e}$ is the orthogonal projection onto the subspace of $\mathcal{K}$ corresponding to the set of "external" vertices of the graph, *i.e.* those vertices to which semi-infinite edges are attached. Next, we describe the notation pertaining to the quantum graph setting.

In what follows, we denote by $\mathbb{G} = \mathbb{G}(\mathcal{E}, \sigma)$ a finite metric graph, *i.e.* a collection of a finite non-empty set $\mathcal{E}$ of compact or semi-infinite intervals $e_j = [x_{2j-1}, x_{2j}]$ (for semi-infinite intervals we set $x_{2j} = +\infty$), $j = 1, 2, \dots, n$, which we refer to as *edges*, and of a partition σ of the set of endpoints $\mathcal{V} := \{x_k : 1 \le k \le 2n,\ x_k < +\infty\}$ into

N equivalence classes V_m, $m = 1, 2, \ldots, N$, which we call *vertices*: $\mathcal{V} = \bigcup_{m=1}^{N} V_m$. The degree, or valence, $\deg(V_m)$ of the vertex V_m is defined as the number of elements in V_m, *i.e.* $\mathrm{card}(V_m)$. Further, we partition the set $\mathcal{V}$ into the two non-overlapping sets of *internal* $\mathcal{V}^{(\mathrm{i})}$ and *external* $\mathcal{V}^{(\mathrm{e})}$ vertices, where a vertex V is classed as internal if it is incident to no non-compact edge and external otherwise. Similarly, we partition the set of edges $\mathcal{E} = \mathcal{E}^{(\mathrm{i})} \cup \mathcal{E}^{(\mathrm{e})}$, into the collection of compact ($\mathcal{E}^{(\mathrm{i})}$) and non-compact ($\mathcal{E}^{(\mathrm{e})}$) edges. We assume for simplicity that the number of non-compact edges incident to any graph vertex is not greater than one.

For a finite metric graph $\mathbb{G}$, we consider the Hilbert spaces $L^2(\mathbb{G}) := \bigoplus_{j=1}^{n} L^2(e_j)$ and $W^{2,2}(\mathbb{G}) := \bigoplus_{j=1}^{n} W^{2,2}(e_j)$. (Notice that these spaces do not feel the graph connectivity, as each of them is the same for different graphs with the same number of edges of the same lengths.) Further, for a function $f \in W^{2,2}(\mathbb{G})$, we define the normal derivative at each vertex along each of the adjacent edges, as follows:

$$\partial_n f(x_j) := \begin{cases} f'(x_j), & \text{if } x_j \text{ is the left endpoint of the edge,} \\ -f'(x_j), & \text{if } x_j \text{ is the right endpoint of the edge.} \end{cases} \tag{8.3}$$

In the case of semi-infinite edges we only apply this definition at the left endpoint of the edge.

Definition 5. For $f \in W^{2,2}(\mathbb{G})$ and $a_m \in \mathbb{C}$ (below referred to as the "coupling constant"), the condition of continuity of the function f through the vertex V_m (*i.e.* $f(x_j) = f(x_k)$ if $x_j, x_k \in V_m$) together with the condition

$$\sum_{x_j \in V_m} \partial_n f(x_j) = a_m f(V_m)$$

is called the δ-type matching at the vertex V_m.

Remark 8. Note that the δ-type matching condition in a particular case when $a_m = 0$ reduces to the standard Kirchhoff matching condition at the vertex V_m, see *e.g.* [2].

Definition 6. The graph Laplacian A_a, $a := (a_1, ..., a_N)$, on a graph $\mathbb{G}$ with δ-type matching conditions is the operator of minus second derivative $-d^2/dx^2$ in the Hilbert space $L^2(\mathbb{G})$ on the domain of functions that belong to the Sobolev space $W^{2,2}(\mathbb{G})$ and satisfy the δ-type matching conditions at every vertex V_m, $m = 1, 2, \ldots, N$. The Schrödinger operator on the same graph is defined likewise on the same domain in the case of summable edge potentials (*cf.* [14]).

If all coupling constants a_m, $m = 1, \ldots, N$, are real, it is shown that the operator A_a is a proper self-adjoint extension (see (2.5)) of a closed symmetric operator A in $L^2(\mathbb{G})$ [17, 34]. Note that, without loss of generality, each edge e_j of the graph $\mathbb{G}$ can be considered to be an interval $[0, l_j]$, where $l_j := x_{2j} - x_{2j-1}$, $j = 1, \ldots, n$ is the length of the corresponding edge. Throughout the present paper we will therefore only consider this situation.

In [14], the following result is obtained for the case of finite *compact* metric graphs.

Proposition 8.2 ([14]). *Let $\mathbb{G}$ be a finite compact metric graph with δ-type coupling at all vertices. There exists a closed densely defined symmetric operator A and a boundary triple such that the operator A_a is an almost solvable extension of A, for which the parametrising* *matrix B (see (2.5)) is given by $B = \operatorname{diag}\{a_1, \dots, a_N\}$, whereas the Weyl function is an $N \times N$ matrix with elements*

$$m_{jk}(z) = \begin{cases} -\sqrt{z}\left(\sum\limits_{e_p \in E_k} \cot \sqrt{z} l_p - 2 \sum\limits_{e_p \in L_k} \tan \dfrac{\sqrt{z} l_p}{2}\right), & j = k, \\ \sqrt{z} \sum\limits_{e_p \in C_{jk}} \dfrac{1}{\sin \sqrt{z} l_p}, & j \neq k;\ V_j, V_k \text{ adjacent}, \\ 0, & j \neq k;\ V_j, V_k \text{ non-adjacent}. \end{cases} \tag{8.4}$$

Here the branch of the square root is chosen so that $\Im\sqrt{z} \geq 0$, l_p is the length of the edge e_p, E_k is the set of non-loop graph edges incident to the vertex V_k, L_k is the set of loops at the vertex V_k, and C_{jk} is the set of graph edges connecting vertices V_j and V_k.

It is easily seen that the rationale of [14] is applicable to the situation of non-compact metric graphs. Indeed, denote by $\mathbb{G}^{(\mathrm{i})}$ the compact part of the graph $\mathbb{G}$, *i.e.* the graph $\mathbb{G}$ with all the non-compact edges removed. Proposition 8.2 yields an expression for the Weyl function $M^{(\mathrm{i})}$ pertaining to the graph $\mathbb{G}^{(\mathrm{i})}$. A simple calculation then implies the following representation for the M-matrix pertaining to the original graph $\mathbb{G}$.

Lemma 8.3. *The matrix functions M, $M^{(\mathrm{i})}$ described above are related by the formula*

$$M(z) = M^{(\mathrm{i})}(z) + i\sqrt{z} P_{\mathrm{e}}, \qquad z \in \mathbb{C}_+, \tag{8.5}$$

where P_{e} is the orthogonal projection in the boundary space $\mathcal{K}$ onto the set of external vertices $V_{\mathbb{G}}^{(\mathrm{e})}$, i.e. the matrix P_{e} such that $(P_{\mathrm{e}})_{ij} = 1$ if $i = j$, $V_i \in V_{\mathbb{G}}^{(\mathrm{e})}$, and $(P_{\mathrm{e}})_{ij} = 0$ otherwise.

Proof. Note first that Weyl function of the graph $\mathbb{G}$ for the triple described in Proposition 8.2 coincides with the sum of the matrices $M_j(z)$, $j = 1, 2, \dots, n$, that are obtained by the formulae

$$\Gamma_1 f = M_j(z) \Gamma_0 f, \qquad f \in \ker(A^* - zI), \qquad f \equiv 0 \text{ on } \mathbb{G} \setminus e_j.$$

In order words, the matrix functions M_j describe the Dirichlet-to-Neumann mappings for the data supported on each individual edge e_j, $j = 1, 2, \dots, n$, where A is as in Proposition 8.2.

Furthermore, functions $f \in \ker(A^* - zI)$ that vanish on all edges of the graph $\mathbb{G}$ but one non-compact edge e_∞, satisfy

$$-f''(x) = z f(x), \quad x \in [0, +\infty), \qquad f \in W^{2,2}(0, +\infty), \tag{8.6}$$

where we identify e_∞ and the semi-infinite line $[0, +\infty)$, as well as f and its restriction to e_∞. Next, all non-trivial solutions to (8.6) have the form

$$f(x) = f(0) \exp(i\sqrt{z} x), \quad x \in [0, +\infty), \qquad f(0) \neq 0,$$

for which the value of the co-derivative (8.3) at $x = 0$ is clearly given by $\partial_n f(0) = i\sqrt{z} f(0)$. Therefore, the corresponding (additive) contribution to the M-matrix, see Definition 3, is given by the matrix all of whose elements except the diagonal element corresponding to the vertex from which e_∞ emanates are zero, while the only non-zero element equals

$(f(0))^{-1}\partial_n f(0) = i\sqrt{z}$. Repeating this argument for all non-compact edges of $\mathbb{G}$ and using the additivity property for the M-matrix discussed above yields the claim. $\square$

The formula (8.5) leads to $M(s) - M^*(s) = 2i\sqrt{s}P_{\rm e}$ a.e. $s \in \mathbb{R}$, and the expression (8.1) for $\widehat{\Sigma}$ leads to the classical scattering matrix $\widehat{\Sigma}_{\rm e}(k)$ of the pair of operators A_0 (which is the Laplacian on the graph $\mathbb{G}$ with standard Kirchhoff matching at all the vertices) and $A_\varkappa$, where $\varkappa = B = \operatorname{diag}\{a_1, \dots, a_N\}$:

$$\widehat{\Sigma}_{\rm e}(s) = P_{\rm e}(M(s) - \varkappa)^{-1}(M(s)^* - \varkappa)(M(s)^*)^{-1}M(s)P_{\rm e}, \qquad s \in \mathbb{R},$$

which acts as the operator of multiplication in the space $L^2(P_{\rm e}\mathcal{K}; 4\sqrt{s}ds)$.

Remark 9. The concrete choice of boundary triple in accordance with Proposition 8.2 leads to the fact that the "unperturbed" operator A_0 is fixed as the Laplacian on the graph with Kirchhoff matching conditions at the vertices. On the other hand, in applications it may be more convenient to consider a formulation where the operator A_0 corresponds to some other matching conditions, which would motivate another choice of the triple. This is readily facilitated by the analysis carried out in the preceding sections. In particular, we point out that the formula (8.2) is written in a triple-independent way.

Furthermore, Part 4 of Remark 7 suggests one particular way of "shifting" the unperturbed operator A_0. Another feasible choice for the unperturbed operator would be the operator of Dirichlet decoupling on the graph $\mathbb{G}$. This possibility can attained by passing to the new triple: $\widehat{\Gamma}_1 = \Gamma_0$, $\widehat{\Gamma}_0 = -\Gamma_1$.

In the remaining part of the paper we will consider the first choice above, postponing the discussion of other possibilities to future work.

We reiterate that the analysis above pertains not only to the cases when the coupling constants are real, leading to self-adjoint operators A_a, but also to the case of non-selfadjoint extensions, *cf.* Theorem 6.3.

In what follows we often drop the argument $s \in \mathbb{R}$ of the Weyl function M and the scattering matrices $\widehat{\Sigma}$, $\widehat{\Sigma}_{\rm e}$. Since

$$(M - \varkappa)^{-1}(M^* - \varkappa) = I + (M - \varkappa)^{-1}(M^* - M) = I - 2i\sqrt{s}(M - \varkappa)^{-1}P_{\rm e} \tag{8.7}$$

and

$$(M^*)^{-1}M = I + 2i\sqrt{s}(M^*)^{-1}P_{\rm e},$$

a factorisation of $\widehat{\Sigma}_{\rm e}$ into a product of $\varkappa-$dependent and $\varkappa-$independent factors (*cf.* (8.1)) still holds in this case in $P_{\rm e}\mathcal{K}$, namely

$$\widehat{\Sigma}_{\rm e} = \bigl[P_{\rm e}(M - \varkappa)^{-1}(M^* - \varkappa)P_{\rm e}\bigr]\bigl[P_{\rm e}(M^*)^{-1}MP_{\rm e}\bigr]. \tag{8.8}$$

The reason why the explicit expression (8.1) for $\widehat{\Sigma}$ in the higher-dimensional space $\mathcal{K}$ is useful in applications is that, compared to the lower-dimensional setting of $\widehat{\Sigma}_{\rm e}$, the matrices M and $\varkappa$ are decoupled (*cf.* $P_{\rm e}(M - \varkappa)^{-1}(M^* - \varkappa)P_{\rm e}$ just above, where the pieces of information contained in M and $\varkappa$ are mixed together after matrix multiplication and sandwiching between two projectors) and the named two matrices admit an explicit, easily analysed, form.

9. Inverse scattering problem for graphs with δ-coupling

We will now exploit the above approach in the analysis of the inverse scattering problem for Laplace operators on finite metric graphs, whereby the scattering matrix $\widehat{\Sigma}_{\rm e}(s)$, defined by (8.8), is assumed to be known for almost all positive "energies" $s \in \mathbb{R}$, along with the graph $\mathbb{G}$ itself. The data to be determined is the set of coupling constants $\{a_j\}_{j=1}^N$. For simplicity, in what follows we treat the inverse problem for graphs with real coupling constants, which corresponds to self-adjoint operators, leaving the non-selfadjont situation to be addressed elsewhere.

First, given $\widehat{\Sigma}_{\rm e}(s)$ for almost all $s > 0$, we reconstruct the meromorphic matrix-function $P_{\rm e}(M^{(\rm i)}(z) - \varkappa)^{-1} P_{\rm e}$ for all complex z, excluding the poles. This is an explicit calculation based on the second resolvent identity (see *e.g.* [70, Thm. 5.13]). Namely, almost everywhere on the positive half-line one has

$$
\begin{aligned}
(M - \varkappa)^{-1} &= (M^{(\rm i)} - \varkappa)^{-1} - (M - \varkappa)^{-1}(M - M^{(\rm i)})(M^{(\rm i)} - \varkappa)^{-1} \\
&= \bigl[I - (M - \varkappa)^{-1}(M - M^{(\rm i)})\bigr](M^{(\rm i)} - \varkappa)^{-1},
\end{aligned}
$$

and hence

$$
P_{\rm e}(M - \varkappa)^{-1}P_{\rm e} = \bigl[P_{\rm e} - i\sqrt{s}P_{\rm e}(M - \varkappa)^{-1}P_{\rm e}\bigr]P_{\rm e}(M^{(\rm i)} - \varkappa)^{-1}P_{\rm e}. \tag{9.1}
$$

Further, the first factor on the right-hand side of (9.1) is invertible for almost all $s > 0$. Indeed, we note first that $\widehat{\Sigma}_{\rm e}^{\varkappa} := P_{\rm e}(M(s) - \varkappa)^{-1}(M(s)^* - \varkappa)$ is unitary in $P_{\rm e}\,\mathcal{K}$ for almost all $s > 0$, since

$$
\begin{aligned}
&(M - \varkappa)(M^* - \varkappa)^{-1}(M - M^*)(M - \varkappa)^{-1}(M^* - \varkappa) \\
&\quad = (M - \varkappa)(M^* - \varkappa)^{-1}\bigl[(M - \varkappa) - (M^* - \varkappa)\bigr](M - \varkappa)^{-1}(M^* - \varkappa) \\
&\quad = (M - \varkappa) - (M^* - \varkappa) = M - M^*
\end{aligned}
$$

and $M - M^* = 2i\sqrt{s}P_{\rm e}$. Now, since

$$
P_{\rm e} - i\sqrt{s}P_{\rm e}(M - \varkappa)^{-1}P_{\rm e} = \bigl(I + \widehat{\Sigma}_{\rm e}^{\varkappa}\bigr)/2
$$

it suffices to show that -1 is not an eigenvalue of $\widehat{\Sigma}_{\rm e}^{\varkappa}(s)$ for almost all $s > 0$. Assume the opposite, *i.e.* for some $s > 0$ one has

$$
(M(s)^* - \varkappa)^{-1}u_s = -(M(s) - \varkappa)^{-1}u_s, \qquad u_s \in P_{\rm e}\,\mathcal{K} \setminus \{0\}.
$$

A straightforward calculation then yields

$$
(M(s)^* - \varkappa)^{-1}(M^{(\rm i)}(s) - \varkappa)(M(s) - \varkappa)^{-1}u_s = 0,
$$

from where

$$
(M(s) - \varkappa)^{-1}u_s \in \ker\bigl(M^{(\rm i)}(s) - \varkappa\bigr).
$$

The latter kernel is non-trivial only at the points s which belong to the (discrete) spectrum of the Laplacian on the compact part $\mathbb{G}^{(\rm i)}$ of the graph $\mathbb{G}$. It follows that $(M(s) - \varkappa)^{-1}u_s$

is zero for almost all $s > 0$, which is a contradiction with $u_s \neq 0$.

Note that, for a given graph $\mathbb{G}$, the expression $P_{\rm e}(M-\varkappa)^{-1}P_{\rm e}$ is found by combining (8.7) and (8.8):

$$P_{\rm e}(M-\varkappa)^{-1}P_{\rm e} = \frac{1}{2i\sqrt{s}}\bigl(P_{\rm e} - \widehat{\Sigma}_{\rm e}[P_{\rm e}(M^*)^{-1}MP_{\rm e}]^{-1}\bigr), \tag{9.2}$$

where we treat both $[P_{\rm e}(M^*)^{-1}MP_{\rm e}]^{-1}$ and, as before, $\widehat{\Sigma}_{\rm e}$ as operators in $P_{\rm e}\mathcal{K}$.

It follows from (9.1) and (9.2) that for given M, $\widehat{\Sigma}_{\rm e}$ the expression $P_{\rm e}(M^{(\rm i)}-\varkappa)^{-1}P_{\rm e}$ is determined uniquely for almost all $s > 0$:

$$\begin{aligned} P_{\rm e}(M^{(\rm i)}-\varkappa)^{-1}P_{\rm e} &= \bigl[P_{\rm e} - i\sqrt{s}P_{\rm e}(M-\varkappa)^{-1}P_{\rm e}\bigr]^{-1}P_{\rm e}(M-\varkappa)^{-1}P_{\rm e} \\ &= \frac{1}{i\sqrt{s}}\bigl(P_{\rm e}+\widehat{\Sigma}_{\rm e}[P_{\rm e}(M^*)^{-1}MP_{\rm e}]^{-1}\bigr)^{-1}\bigl(P_{\rm e}-\widehat{\Sigma}_{\rm e}[P_{\rm e}(M^*)^{-1}MP_{\rm e}]^{-1}\bigr) \\ &= \frac{1}{i\sqrt{s}}\Bigl(2\bigl(P_{\rm e}+\widehat{\Sigma}_{\rm e}[P_{\rm e}(M^*)^{-1}MP_{\rm e}]^{-1}\bigr)^{-1} - I\Bigr)P_{\rm e}. \end{aligned} \tag{9.3}$$

In particular, due to the property of analytic continuation, the expression $P_{\rm e}(M^{(\rm i)}-\varkappa)^{-1}P_{\rm e}$ is determined uniquely in the whole of $\mathbb{C}$ with the exception of a countable set of poles, which coincides with the set of eigenvalues of the self-adjoint Laplacian $A_\varkappa^{(\rm i)}$ on the compact part $\mathbb{G}^{(\rm i)}$ of the graph $\mathbb{G}$ with matching conditions at the graph vertices given by the matrix $\varkappa$, *cf.* Proposition 8.2.

Definition 7. Given a partition $\mathcal{V}_1 \cup \mathcal{V}_2$ of the set of graph vertices, for $z \in \mathbb{C}$ consider the linear set $U(z)$ of functions that satisfy the differential equation $-u_z'' = zu_z$ on each edge, subject to the conditions of continuity at all vertices of the graph and the δ-type matching conditions at the vertices in the set $\mathcal{V}_2$. For each function $f \in U(z)$, consider the vectors

$$\Gamma_1^{\mathcal{V}_1}u_z := \Bigl\{\sum_{x_j\in V_m}\partial_n f(x_j)\Bigr\}_{V_m\in\mathcal{V}_1}, \qquad \Gamma_0^{\mathcal{V}_1}u_z := \bigl\{f(V_m)\bigr\}_{V_m\in\mathcal{V}_1}.$$

The *Delta-to-Dirichlet map* of the set $\mathcal{V}_1$ maps the vector $(\Gamma_1^{\mathcal{V}_1}-\varkappa^{\mathcal{V}_1}\Gamma_0^{\mathcal{V}_1})u_z$ to $\Gamma_0^{\mathcal{V}_1}u_z$, where $\varkappa^{\mathcal{V}_1} := \operatorname{diag}\{a_m : \ V_m \in \mathcal{V}_1\}$. (Note that the function $u_z \in U(z)$ is determined uniquely by $(\Gamma_1^{\mathcal{V}_1}-\varkappa^{\mathcal{V}_1}\Gamma_0^{\mathcal{V}_1})u_z$ for all $z \in \mathbb{C}$ except a countable set of real points accumulating to infinity).

Remark 10. The above definition is a natural generalisation of the corresponding definitions of Dirichlet-to-Neumann and Neumann-to-Dirichlet maps pertaining to the graph boundary, considered in *e.g.* [2], [40].

We argue that the matrix $P_{\rm e}(M^{(\rm i)}-\varkappa)^{-1}P_{\rm e}$ is the Delta-to-Dirichlet map for the set $\mathcal{V}^{(\rm e)}$. Indeed, assuming $\phi := \Gamma_1u_z - \varkappa\Gamma_0u_z$ and $\phi = P_{\rm e}\phi$, where the latter condition ensures the correct δ-type matching on the set $\mathcal{V}^{(\rm i)}$, one has $P_{\rm e}\phi = (M^{(\rm i)}-\varkappa)\Gamma_0u_z$ and hence $\Gamma_0u_z = (M^{(\rm i)}-\varkappa)^{-1}P_{\rm e}\phi$. Applying $P_{\rm e}$ to the last identity yields the claim, in accordance with Definition 7.

We have thus proved the following theorem.

Theorem 9.1. *The Delta-to-Dirichlet map for the vertices $\mathcal{V}^{(\rm e)}$ is determined uniquely by the scattering matrix $\widehat{\Sigma}_{\rm e}(s)$, $s \in \mathbb{R}$, via the formula (9.3).*

The following definition, required for the formulation of the next theorem, is a generalisation of the procedure of graph contraction well studied in the algebraic graph theory, see *e.g.* [66].

Definition 8 (Contraction procedure for graphs and associated graph Laplacians)**.** For a given graph $\mathbb{G}$ vertices V and W connected by an edge e are "glued" together to form a new vertex (VW) of the contracted graph $\widetilde{\mathbb{G}}$ while simultaneously the edge e is removed, whereas the rest of the graph remains unchanged. We do allow the situation of multiple edges, when V and W are connected in $\mathbb{G}$ by more than one edge, in which case all such edges but the edge e become loops of their respective lengths attached to the vertex (VW). The corresponding graph Laplacian A_a defined on $\mathbb{G}$ is contracted to the graph Laplacian $\tilde{A}_{\tilde{a}}$ by the application of the following rule pertaining to the coupling constants: a coupling constant at any unaffected vertex remains the same, whereas the coupling constant at the new vertex (VW) is set to be the sum of the coupling constants at V and W. Here it is always assumed that all graph Laplacians are described by Definition 6.

The matrix $\varkappa$ of the coupling constants is now determined as part of an iterative procedure based on the following result.

Theorem 9.2. *Suppose that the edge lengths of the graph $\mathbb{G}^{(\mathrm{i})}$ are rationally independent. The element*[3] $(1,1)$ *of the Delta-to-Dirichlet map described above yields the element* $(1,1)$ *of the "contracted" graph $\widetilde{\mathbb{G}}^{(\mathrm{i})}$ obtained from the graph $\mathbb{G}^{(\mathrm{i})}$ by removing a non-loop edge e emanating from V_1. The procedure of passing from the graph $\mathbb{G}^{(\mathrm{i})}$ to the contracted graph $\widetilde{\mathbb{G}}^{(\mathrm{i})}$ is given in Definition 8.*

Proof. Due to the assumption that the edge lengths of the graph $\mathbb{G}^{(\mathrm{i})}$ are rationally independent, the element (1,1), which we denote by f_1, is given explicitly as a function of $\sqrt{z}$ *and* all the edge lengths l_j, $j = 1, 2, \dots, n$, in particular, of the length of the edge e, which we assume to be l_1 without loss of generality. This is an immediate consequence of the explicit form of the matrix $M^{(\mathrm{i})}$. Again without loss of generality, we also assume that the edge e connects the vertices V_1 and V_2.

Further, consider the expression $\lim_{l_1\to 0} f_1(\sqrt{z}; l_1, \dots, l_n; a)$. On the one hand, this limit is known from the mentioned explicit expression for f_1. On the other hand, f_1 is the ratio of the determinant $\mathcal{D}^{(1)}(\sqrt{z}; l_1, \dots, l_n; a)$ of the principal minor of the matrix $M^{(\mathrm{i})}(z) - \varkappa$ obtained by removing its first row and and first column and the determinant of $M^{(\mathrm{i})}(z) - \varkappa$ itself:

$$f_1(\sqrt{z}; l_1, \dots, l_n; a) = \frac{\mathcal{D}^{(1)}(\sqrt{z}; l_1, \dots, l_n; a)}{\det\bigl(M^{(\mathrm{i})}(z) - \varkappa\bigr)}$$

Next, we multiply by $-l_1$ both the numerator and denominator of this ratio, and pass to the limit in each of them separately:

$$\lim_{l_1\to 0} f_1(\sqrt{z}; l_1, \dots, l_n; a) = \frac{\lim\limits_{l_1\to 0}(-l_1)\mathcal{D}^{(1)}(\sqrt{z}; l_1, \dots, l_n; a)}{\lim\limits_{l_1\to 0}(-l_1)\det\bigl(M^{(\mathrm{i})}(z) - \varkappa\bigr)} \tag{9.4}$$

[3] By renumbering if necessary, this does not lead to loss of generality.

The numerator of (9.4) is easily computed as the determinant $\mathcal{D}^{(2)}(z; l_1, \dots, l_n; a)$ of the minor of $M^{(\mathrm{i})}(z) - \varkappa$ obtained by removing its first two rows and first two columns.

As for the denominator of (9.4), we add to the second row of the matrix $M^{(\mathrm{i})}(z) - \varkappa$ its first row multiplied by $\cos(\sqrt{z} l_1)$, which leaves the determinant unchanged. This operation, due to the identity

$$-\cot(\sqrt{z} l_1) \cos(\sqrt{z} l_1) + \frac{1}{\sin(\sqrt{z} l_1)} = \sin(\sqrt{z} l_1),$$

cancels out the singularity of all matrix elements of the second row at the point $l_1 = 0$. We introduce the factor $-l_1$ (*cf.* 9.4) into the first row and pass to the limit as $l_1 \to 0$. Clearly, all rows but the first are regular at $l_1 = 0$ and hence converge to their limits as $l_1 \to 0$. Finally, we add to the second column of the limit its first column, which again does not affect the determinant, and note that the first row of the resulting matrix has one non-zero element, namely the $(1,1)$ entry. This procedure reduces the denominator in (9.4) to the determinant of a matrix of the size reduced by one. As in [15], it is checked that this determinant is nothing but $\det(\widetilde{M}^{(\mathrm{i})} - \widetilde{\varkappa})$, where $\widetilde{M}^{(\mathrm{i})}$ and $\widetilde{\varkappa}$ are the Weyl matrix and the (diagonal) matrix of coupling constants pertaining to the contracted graph $\widetilde{\mathbb{G}}^{(\mathrm{i})}$. This immediately implies that the ratio obtained as a result of the above procedure coincides with the entry (1,1) of the matrix $(\widetilde{M}^{(\mathrm{i})} - \widetilde{\varkappa})^{-1}$, *i.e.*

$$\lim_{l_1 \to 0} f_1(\sqrt{z}; l_1, \dots, l_n; a) = f_1^{(1)}(\sqrt{z}; l_2, \dots, l_n; \tilde{a}), \tag{9.5}$$

where $f_1^{(1)}$ is the element (1,1) of the Delta-to-Dirichlet map of the contracted graph $\widetilde{\mathbb{G}}^{(\mathrm{i})}$, and $\tilde{a}$ is given by Definition 8. □

The main result of this section is the theorem below, which is a corollary of Theorems 9.1 and 9.2. We assume without loss of generality that $V_1 \in \mathcal{V}^{(\mathrm{e})}$ and denote by $f_1(\sqrt{z})$ the (1,1)-entry of the Delta-to-Dirichlet map for the set $\mathcal{V}^{(\mathrm{e})}$. We set the following notation. Fix a spanning tree $\mathbb{T}$ (see *e.g.* [66]) of the graph $\mathbb{G}^{(\mathrm{i})}$. We let the vertex V_1 to be the root of $\mathbb{T}$ and assume, again without loss of generality, that the number of edges in the path γ_m connecting V_m and the root is a non-decreasing function of m. Denote by $N^{(m)}$ the number of vertices in the path γ_m, and by $\{l_k^{(m)}\}$, $k = 1, \dots, N^{(m)} - 1$, the associated sequence of lengths of the edges in γ_m, ordered along the path from the root V_1 to V_m. Note that each of the lengths $l_k^{(m)}$ is clearly one of the edge lengths l_j of the compact part of the original graph $\mathbb{G}$.

Theorem 9.3. *Assume that the graph $\mathbb{G}$ is connected and the lengths of its compact edges are rationally independent. Given the scattering matrix $\widehat{\Sigma}_{\mathrm{e}}(s)$, $s \in \mathbb{R}$, the Delta-to-Dirichlet map for the set $\mathcal{V}^{(\mathrm{e})}$ and the matrix of coupling constants $\varkappa$ are determined constructively in a unique way. Namely, the following formulae hold for $l = 1, 2, \dots, N$ and determine a_m, $m = 1, \dots, N$:*

$$\sum_{m: V_m \in \gamma_l} a_m = \lim_{\tau \to +\infty} \left\{ -\tau \Big(\sum_{V_m \in \gamma_l} \deg(V_m) - 2(N^{(l)} - 1) \Big) - \frac{1}{f_1^{(l)}(i\tau)} \right\},$$

where

$$f_1^{(l)}(\sqrt{z}) := \lim_{l^{(l)}_{N^{(l)}-1}\to 0} \dots \lim_{l_2^{(l)}\to 0} \lim_{l_1^{(l)}\to 0} f_1(\sqrt{z}), \tag{9.6}$$

where in the case $l = 1$ no limits are taken in (9.6).

Proof. We first apply Theorem 9.1 to determine the Delta-to-Dirichlet map for the vertices $\mathcal{V}^{(\mathrm{e})}$. Next, we notice that the knowledge of the (1,1)-element f_1 of the Delta-to-Dirichlet map for the set $\mathcal{V}^{(\mathrm{e})}$, *i.e.* of the matrix $P_{\mathrm{e}}(M^{(\mathrm{i})} - \varkappa)^{-1}P_{\mathrm{e}}$, together with the asymptotic expansion for $M^{(\mathrm{i})}(z)$ as $\sqrt{z} \to +i\infty$, yields the element (1,1) of the matrix $\varkappa$, which is the coupling constant a_1 at the vertex V_1, see Proposition 8.2. Indeed, setting $\sqrt{z} = i\tau$, $\tau \to +\infty$, one has (*cf.* (8.4))

$$\frac{1}{f_1} = i\tau\Bigl(-\sum_{e_p\in E_1} \cot(i\tau l_p) + 2\sum_{e_p\in L_1} \tan\frac{i\tau l_p}{2}\Bigr) - a_1 + o\bigl(\tau^{-K}\bigr) \tag{9.7}$$

$$= -\tau \deg(V_1) - a_1 + o\bigl(\tau^{-K}\bigr), \qquad \tau \to +\infty \tag{9.8}$$

for all $K > 0$, where the first sum in (9.7) is taken over all non-loop edges e_p of $\mathbb{G}^{(\mathrm{i})}$ emanating from the vertex V_1 and the second over all loops e_p attached to V_1. The coupling constant a_1 is then recovered directly from (9.8).

In order to determine the coupling constant a_2, we apply Theorem 9.2. In order to do so we note that the the vertex V_2 is connected to V_1 by the edge of the length $l_1^{(2)}$ and apply the contraction procedure along this edge. In particular, the formula (9.5), together with asymptotics (9.8) re-written for the first diagonal element of the contracted graph, yields the coupling constant pertaining to the vertex $\widetilde{V}_1 := (V_1V_2)$ of the contracted graph, which, by Theorem 9.2, is equal to $a_1 + a_2$:

$$a_1 + a_2 = \lim_{\tau\to+\infty}\biggl\{i\tau\Bigl(-\sum_{e_p\in\widetilde{E}_1} \cot(i\tau l_p) + 2\sum_{e_p\in\widetilde{L}_1} \tan\frac{i\tau l_p}{2}\Bigr) - \frac{1}{f_1^{(1)}}\biggr\}$$

$$= \lim_{\tau\to+\infty}\biggl\{-\tau\bigl(\deg(V_1) + \deg(V_2) - 2\bigr) - \frac{1}{f_1^{(1)}}\biggr\}, \tag{9.9}$$

where $\widetilde{E}_1$ is the set of all non-loop edges of the contracted graph $\widetilde{\mathbb{G}}^{(\mathrm{i})}$ emanating from the vertex $\widetilde{V}_1$, $\widetilde{L}_1$ is the set of loops attached to this same vertex, and $f_1^{(1)}$, explicitly given by (9.5), is the element (1,1) of the Delta-to-Dirichlet map of the contracted graph. Thus we recover the value of the coupling constant a_2, as a result of consequent evaluations of indeterminate forms of two different types: "0/0" (see (9.5)) and "$\infty - \infty$" (see (9.9)).

Since the graph $\mathbb{G}$ is connected, the above procedure is iterated until the only remaining vertex of the contracted graph is V_1, at which point the last coupling constant a_N is determined. The claim of the theorem follows. □

Remark 11. 1. Notice that each step of the above iterative process generates a set of loops, which is treated according to the formula (9.7). Alternatively, these loops can be discarded by an elementary recalculation of the corresponding element of the Delta-to-Dirichlet map in the application of Theorem 9.2.

2. From the proof of Theorem 9.3 it actually follows that the inverse problem of determining matching conditions based on the Delta-to-Dirichlet map pertaining to any subset of graph vertices for any finite and compact graph $\mathbb{G}$ has a unique and constructive solution. As in the theorem, the graph is assumed connected and its edge lengths rationally independent. More than that, for the solution of the named inverse problem it suffices to know any one diagonal element of the Delta-to-Dirichlet map.

Acknowledgements

KDC is grateful for the financial support of the Engineering and Physical Sciences Research Council: Grant EP/L018802/2 "Mathematical foundations of metamaterials: homogenisation, dissipation and operator theory". AVK has been partially supported by a grant of the Ukrainian Ministry for Education and by the RFBR grant 16-01-00443-a. LOS has been partially supported by UNAM-DGAPA-PAPIIT IN105414 and SEP-CONACYT 254062.

Appendix

Proof of Theorem 4.1.

We prove Theorem 4.1(i). The proof of Theorem 4.1(ii) is carried out along the same lines.

For any (v_-, u, v_+) in the space $\mathcal{H}$ given in (4.7), consider the mappings $\mathcal{F}_\pm : \mathcal{H} \to L^2(\mathbb{R}, E)$ introduced in [58, Sec. 2.1] following the corresponding definitions in [48] and given by

$$\mathcal{F}_+(v_-, u, v_+) = -\frac{1}{\sqrt{2\pi}} \lim_{\epsilon \searrow 0} \alpha \Gamma_0 (A_{\mathrm{i}I} - (\cdot - \mathrm{i}\epsilon)I)^{-1} u + S^* \hat{v}_- + \hat{v}_+ \tag{A.10}$$

$$\mathcal{F}_-(v_-, u, v_+) = -\frac{1}{\sqrt{2\pi}} \lim_{\epsilon \searrow 0} \alpha \Gamma_0 (A^*_{\mathrm{i}I} - (\cdot + \mathrm{i}\epsilon)I)^{-1} u + \hat{v}_- + S\hat{v}_+ \,, \tag{A.11}$$

where $\hat{v}_\pm$ are the Fourier transforms of $v_\pm \in L^2(\mathbb{R}_\pm, E)$ extended by zero to $L^2(\mathbb{R}, E)$. Note that the limits exist almost everywhere due to (4.1).

According to [58, Thm. 2.3], if $\binom{\widetilde{g}}{g} = \Phi h$, then

$$\mathcal{F}_+ h = \widetilde{g} + S^* g \,, \qquad \mathcal{F}_- h = S\widetilde{g} + g \,. \tag{A.12}$$

Therefore, for proving Theorem 4.1(i), one should establish the validity of the identities:

$$\mathcal{F}_\pm (A_\varkappa - zI)^{-1} \Phi^{-1} \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \mathcal{F}_\pm \Phi^{-1} P_K \frac{1}{\cdot - z} \begin{pmatrix} \widetilde{g} \\ g - \chi^+_\varkappa \Theta^{-1}_\varkappa (z)(\widetilde{g} + S^* g)(z) \end{pmatrix} \tag{A.13}$$

for $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$. First we compute the left-hand-side of (A.13). It follows from

Lemma 3.1(i), (ii) that, for $z, \lambda \in \mathbb{C}_- \cap \rho(A_\varkappa)$ and $h \in \mathcal{H}$,

$$\begin{aligned}
&\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1}(A_\varkappa - \lambda I)^{-1}h \\
&\qquad = \Theta_\varkappa(z)\alpha\Gamma_0(A_\varkappa - zI)^{-1}(A_\varkappa - \lambda I)^{-1}h \\
&\qquad = \frac{1}{z-\lambda}\Theta_\varkappa(z)\alpha\Gamma_0\left[(A_\varkappa - zI)^{-1} - (A_\varkappa - \lambda I)^{-1}\right]h \\
&\qquad = \frac{1}{z-\lambda}\left[\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1} - \Theta_\varkappa(z)\alpha\Gamma_0(A_\varkappa - \lambda I)^{-1}\right]h \\
&\qquad = \frac{1}{z-\lambda}\left[\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1} - \Theta_\varkappa(z)\Theta_\varkappa^{-1}(\lambda)\alpha\Gamma_0(A_{\mathrm{i}I} - \lambda I)^{-1}\right]h\,.
\end{aligned}$$

Let $z = k - \mathrm{i}\epsilon$ with $k \in \mathbb{R}$, then it follows from the computation above that

$$\begin{aligned}
&\lim_{\epsilon \searrow 0} \alpha\Gamma_0(A_{\mathrm{i}I} - (k - \mathrm{i}\epsilon)I)^{-1}(A_\varkappa - \lambda I)^{-1}h \\
&= \lim_{\epsilon \searrow 0} \frac{1}{(k-\mathrm{i}\epsilon) - \lambda}\left[\alpha\Gamma_0(A_{\mathrm{i}I} - (k-\mathrm{i}\epsilon)I)^{-1} - \Theta_\varkappa(k-\mathrm{i}\epsilon)\Theta_\varkappa^{-1}(\lambda)\alpha\Gamma_0(A_{\mathrm{i}I} - \lambda I)^{-1}\right]h\,.
\end{aligned}$$

Substituting (A.10) into the last equality, one has

$$\mathcal{F}_+(A_\varkappa - \lambda I)^{-1}h = \frac{1}{\cdot - \lambda}\left[\mathcal{F}_+ h - \Theta_\varkappa(\cdot)\Theta_\varkappa^{-1}(\lambda)\mathcal{F}_+ h(\lambda)\right]\,.$$

Hence, in view of (A.12), one concludes

$$\mathcal{F}_+(A_\varkappa - \lambda I)^{-1}\Phi^{-1}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \frac{1}{\cdot - \lambda}\left[\widetilde{g} + S^* g - \Theta_\varkappa(\cdot)\Theta_\varkappa^{-1}(\lambda)(\widetilde{g} + S^* g)(\lambda)\right]\,. \tag{A.14}$$

On the basis of Lemma 3.1(iii), (iv) and reasoning in the same fashion as was done to obtain (A.14), one verifies

$$\mathcal{F}_-(A_\varkappa - \lambda I)^{-1}\Phi^{-1}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \frac{1}{\cdot - \lambda}\left[S\widetilde{g} + g - \widehat{\Theta}_\varkappa(\cdot)\Theta_\varkappa^{-1}(\lambda)(\widetilde{g} + S^* g)(\lambda)\right]\,. \tag{A.15}$$

Let us focus on the right hand side of (A.13). Note that

$$\begin{aligned}
&P_K \frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g - \chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g} + S^* g)(z)\end{pmatrix} \\
&= \begin{pmatrix}\frac{\widetilde{g}}{\cdot - z} - P_+\frac{1}{\cdot - z}[\widetilde{g} + S^* g - S^*\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g} + S^* g)(z)]\\ \frac{1}{\cdot - z}(g - \chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g} + S^* g)(z)) - P_-\frac{1}{\cdot - z}[S\widetilde{g} + g - \chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g} + S^* g)(z)]\end{pmatrix} \\
&= \frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g} - (\widetilde{g} + S^* g)(z) + S^*(\overline{z})\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g} + S^* g)(z)\\ g - \chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g} + S^* g)(z)\end{pmatrix}
\end{aligned} \tag{A.16}$$

where (4.6) is used in the first equality and in the second the fact that if f is a function in $\hat{H}^2_-$, then, for any $z \in \mathbb{C}_-$,

$$P_+\left(\frac{f}{\cdot - z}\right) = P_+\left(\frac{f + f(z) - f(z)}{\cdot - z}\right) = P_+\left(\frac{f(z)}{\cdot - z}\right) = \frac{f(z)}{\cdot - z}\,. \tag{A.17}$$

Now, apply $\mathcal{F}_+\Phi^{-1}$ to (A.16) taking into account (A.12):

$$\begin{aligned}
&\mathcal{F}_+\Phi^{-1}\frac{1}{\cdot - z}\begin{pmatrix} \widetilde{g} - (\widetilde{g} + S^*g)(z) + S^*(\overline{z})\chi^+_\varkappa\Theta^{-1}_\varkappa(z)(\widetilde{g} + S^*g)(z) \\ g - \chi^+_\varkappa\Theta^{-1}_\varkappa(z)(\widetilde{g} + S^*g)(z) \end{pmatrix} \\
&= \frac{1}{\cdot - z}[\widetilde{g} + S^*g - (\widetilde{g} + S^*g)(z) + (S^*(\overline{z}) - S^*)\chi^+_\varkappa\Theta^{-1}_\varkappa(z)(\widetilde{g} + S^*g)(z)] \\
&= \frac{1}{\cdot - z}[\widetilde{g} + S^*g - (\Theta_\varkappa(z) - (S^*(\overline{z}) - S^*)\chi^+_\varkappa)\Theta^{-1}_\varkappa(z)(\widetilde{g} + S^*g)(z)] \\
&= \frac{1}{\cdot - z}[\widetilde{g} + S^*g - \Theta(\cdot)\Theta^{-1}_\varkappa(z)(\widetilde{g} + S^*g)(z)].
\end{aligned}$$

By combining the last equality with (A.14), we have established the first identity in (A.13).

Now, if one applies $\mathcal{F}_-\Phi^{-1}$ to (A.16), then, in view of (A.12), one has

$$\begin{aligned}
&\mathcal{F}_-\Phi^{-1}\frac{1}{\cdot - z}\begin{pmatrix} \widetilde{g} - (\widetilde{g} + S^*g)(z) + S^*(\overline{z})\chi^+_\varkappa\Theta^{-1}_\varkappa(z)(\widetilde{g} + S^*g)(z) \\ g - \chi^+_\varkappa\Theta^{-1}_\varkappa(z)(\widetilde{g} + S^*g)(z) \end{pmatrix} \\
&= \frac{1}{\cdot - z}[S\widetilde{g} + g - S(\widetilde{g} + S^*g)(z) - (I - SS^*(\overline{z}))\chi^+_\varkappa\Theta^{-1}_\varkappa(z)(\widetilde{g} + S^*g)(z)] \\
&= \frac{1}{\cdot - z}[S\widetilde{g} + g - (S\Theta_\varkappa(z) + \chi^+_\varkappa - SS^*(\overline{z})\chi^+_\varkappa)\Theta^{-1}_\varkappa(z)(\widetilde{g} + S^*g)(z)] \\
&= \frac{1}{\cdot - z}[S\widetilde{g} + g - (S\chi^-_\varkappa + \chi^-_\varkappa)\Theta^{-1}_\varkappa(z)(\widetilde{g} + S^*g)(z)] \\
&= \frac{1}{\cdot - z}[S\widetilde{g} + g - \widehat{\Theta}_\varkappa(\cdot)\Theta^{-1}_\varkappa(z)(\widetilde{g} + S^*g)(z)]
\end{aligned}$$

Thus, after comparing this last equality with (A.15), we arrive at the second identity in (A.13).

Proof of Theorem 4.2.

Let us first show that the following inclusion holds

$$\mathcal{N}^\varkappa_\pm \subset \left\{\begin{pmatrix}\widetilde{g} \\ g\end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^*P_K\begin{pmatrix}\widetilde{g} \\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g} \\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_\pm\right\}$$

Consider $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$. By (4.6) and Theorem 4.1, one has

$$\Phi(A_\varkappa - zI)^{-1}\Phi^{-1}P_K\begin{pmatrix}\widetilde{g} \\ g\end{pmatrix} = \Phi(A_\varkappa - zI)^{-1}\Phi^{-1}\begin{pmatrix}\widetilde{g} - P_+(\widetilde{g} + S^*g) \\ g - P_-(S\,\widetilde{g} + g)\end{pmatrix}$$

$$= \frac{P_K}{s - z}\begin{pmatrix} \widetilde{g} - P_+(\widetilde{g} + S^*g) \\ g - P_-(S\widetilde{g} + g) - \chi^+_\varkappa\Theta^{-1}_\varkappa(z)\left[\widetilde{g} - P_+(\widetilde{g} + S^*g) + S^*(g - P_-(S\widetilde{g} + g))\right](z)\end{pmatrix}$$

where

$$[\widetilde{g} - P_+(\widetilde{g} + S^* g) + S^*(g - P_-(S\widetilde{g} + g))]\,(z)$$

is to be understood as the analytic continuation into the lower half-plane of the function

$$\widetilde{g} - P_+(\widetilde{g} + S^* g) + S^*(g - P_-(S\widetilde{g} + g)) \in \hat{H}^2_-(E)\,. \tag{A.18}$$

The fact that (A.18) holds follows from (4.5) and (4.6). Now, one rewrites the expression for this function using the fact that $I_{L^2(E)} - P_- = P_+$ (i. e., $\hat{H}^2_+(E)$ is the orthogonal complement of $\hat{H}^2_-(E)$ in $L^2(\mathbb{R}, E)$):

$$\begin{aligned}\widetilde{g} - P_+(\widetilde{g} + S^* g) + S^*(g - P_-(S\widetilde{g} + g)) &= (I_{L^2(E)} - P_+)(\widetilde{g} + S^* g) - S^* P_-(S\widetilde{g} + g)\\ &= P_-(\widetilde{g} + S^* g) - S^* P_-(S\widetilde{g} + g)\,.\end{aligned}$$

Note that this equality makes evident (A.18). Thus,

$$\Phi(A_\varkappa - zI)^{-1}\Phi^{-1} P_K \begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K \frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g} - P_+(\widetilde{g} + S^* g)\\ g - P_-(S\widetilde{g} + g) - \gamma(z)\end{pmatrix} \tag{A.19}$$

where

$$\gamma(z) := \chi^+_\varkappa \Theta^{-1}_\varkappa(z)\big(P_-(\widetilde{g} + S^* g)(z) - S^* P_-(S\widetilde{g} + g)(z)\big). \tag{A.20}$$

The following lemma is needed to simplify the form of $\gamma(z)$.

Lemma A.1. *For all* $\binom{\widetilde{g}}{g} \in \mathfrak{H}$ *the following identity holds:*

$$\gamma(z) = -P_-(S\widetilde{g} + g)(z) \qquad \forall z \in \mathbb{C}_-.$$

Proof.

$$\begin{aligned}&\chi^+_\varkappa \Theta^{-1}_\varkappa(z)\big(P_-(\widetilde{g} + S^* g)(z) - S^*(\overline{z}) P_-(S\widetilde{g} + g)(z)\big)\\ &= \chi^+_\varkappa\big(I + i\alpha(B_\varkappa - M(z))^{-1}\alpha\chi^+_\varkappa\big)\big(P_-(\widetilde{g} + S^* g)(z) - S^*(\overline{z}) P_-(S\widetilde{g} + g)(z)\big)\\ &= \big(I + i\chi^+_\varkappa\alpha(B_\varkappa - M(z))^{-1}\alpha\big)\chi^+_\varkappa\big(P_-(\widetilde{g} + S^* g)(z) - S^*(\overline{z}) P_-(S\widetilde{g} + g)(z)\big)\\ &= \big(I + \chi^+_\varkappa(S^*(\overline{z}) - I)\big)^{-1}\big(\chi^+_\varkappa P_-(\widetilde{g} + S^* g)(z) - \chi^+_\varkappa S^*(\overline{z}) P_-(S\widetilde{g} + g)(z)\big)\\ &= \big(I + \chi^+_\varkappa(S^*(\overline{z}) - I)\big)^{-1}\big(-\chi^-_\varkappa P_-(S\widetilde{g} + g)(z) - \chi^+_\varkappa S^*(\overline{z}) P_-(S\widetilde{g} + g)(z)\big)\\ &= \big(I + \chi^+_\varkappa(S^*(\overline{z}) - I)\big)^{-1}\big(-\chi^-_\varkappa - \chi^+_\varkappa S^*(\overline{z})\big) P_-(S\widetilde{g} + g)(z) = -P_-(S\widetilde{g} + g)(z),\end{aligned}$$

where we use the fact that

$$I + i\chi^+_\varkappa\alpha(B_\varkappa - M(z))^{-1}\alpha = \big(I + \chi^+_\varkappa(S^*(\overline{z}) - I)\big)^{-1},$$

proved in a similar way to (3.9). □

Therefore, for $\binom{\widetilde{g}}{g} \in \mathcal{N}_-^\varkappa$ the expression (A.19) can be re-written as

$$\begin{aligned}\Phi(A_\varkappa - zI)^{-1}\Phi^{-1}P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} &= P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g} - P_+(\widetilde{g} + S^*g)\\ g - P_-(S\widetilde{g} + g) + P_-(S\widetilde{g} + g)(z)\end{pmatrix}\\ &= P_K\frac{1}{\cdot - z}\left[\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} - \begin{pmatrix}P_+(\widetilde{g} + S^*g)\\ P_-(S\widetilde{g} + g) - P_-(S\widetilde{g} + g)(z)\end{pmatrix}\right]\end{aligned}$$

One completes the proof by observing that

$$\frac{P_+(\widetilde{g} + S^*g)}{\cdot - z} \in H_+^2(E), \qquad \frac{P_-(S\widetilde{g} + g) - P_-(S\widetilde{g} + g)(z)}{\cdot - z} \in H_-^2(E).$$

We have thus shown that

$$\mathcal{N}_-^\varkappa \subset \left\{\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_-\right\}.$$

The inclusion

$$\mathcal{N}_+^\varkappa \subset \left\{\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_+\right\}$$

is proved analogously.

To prove the converse inclusion, i.e.

$$\left\{\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_\pm\right\} \subset \mathcal{N}_\pm^\varkappa$$

one again follows the arguments of [48, Thm. 4]. According to (A.19), for all $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$, one has

$$\Phi(A_\varkappa - zI)^{-1}\Phi^{-1}P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g} - P_+(\widetilde{g} + S^*g)\\ g - P_-(S\widetilde{g} + g) - \gamma(z)\end{pmatrix},$$

where $\gamma(z)$ is defined in (A.20). Thus

$$\begin{aligned}\Phi(A_\varkappa - zI)^{-1}\Phi^{-1}P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} &- P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}\\ &= P_K\begin{pmatrix}0\\ -\gamma(z)(\cdot - z)^{-1}\end{pmatrix}\\ &= P_K\begin{pmatrix}P_+(S^*\gamma(z)(\cdot - z)^{-1})\\ -\gamma(z)(\cdot - z)^{-1} + P_-(\gamma(z)(\cdot - z)^{-1})\end{pmatrix}\end{aligned}$$

But in view of (A.17), one has

$$P_+\left[\frac{S^*\gamma(z)}{\cdot - z}\right] = \frac{S^*(\overline{z})\gamma(z)}{\cdot - z}$$

and, clearly,

$$P_- \left[\frac{\gamma(z)}{\cdot - z}\right] = 0\,.$$

Therefore

$$\Phi(A_\varkappa - zI)^{-1}\Phi^{-1}P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} - P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \begin{pmatrix}S^*(\overline{z})\gamma(z)(\cdot - z)^{-1}\\ -\gamma(z)(\cdot - z)^{-1}\end{pmatrix}.$$

If

$$\Phi(A_\varkappa - zI)^{-1}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_-\,,$$

then

$$\begin{pmatrix}S^*(\overline{z})\gamma(z)(\cdot - z)^{-1}\\ -\gamma(z)(\cdot - z)^{-1}\end{pmatrix} = 0$$

which in its turn implies

$$\big(S^* - S^*(\overline{z})\big)\gamma(z)(\cdot - z)^{-1} = 0\,.$$

From this equality, by virtue of the fact that the operator A_{iI} is completely non-self-adjoint, one obtains that $\gamma(z) = 0$ for any $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$ (see details in the proof of [47, Lem. 4]). Taking into account (A.20) one arrives at

$$\chi_\varkappa^- P_\pm(S\,\widetilde{g} + g) + \chi_\varkappa^+ P_\pm(\widetilde{g} + S^* g) = 0\,.$$

The inclusion

$$\left\{\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_+\right\} \subset \mathcal{N}_+^\varkappa$$

is proved in a similar way.

Proof of Theorem 4.3.

To prove the inclusion

$$\widetilde{N}_-^\varkappa \subset \left\{u \in \mathcal{H} : \chi_\varkappa^+ \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_-^2(E)\right\},$$

one has to show that $u \in \Phi^* P_K \mathcal{N}_-^\varkappa$ implies $\chi_\varkappa^+ \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_-^2(E)$. By (4.6), if $u = \Phi^* P_K\binom{\widetilde{g}}{g}$, then

$$\Phi u = \begin{pmatrix}\widetilde{g} - P_+(\widetilde{g} + S^* g)\\ g - P_-(S\,\widetilde{g} + g)\end{pmatrix}.$$

Thus, in view of the inclusion $\binom{\widetilde{g}}{g} \in K$, it follows from (A.12) that

$$\begin{aligned}\mathcal{F}_+ u &= \widetilde{g} - P_+(\widetilde{g} + S^* g) + S^* g - S^* P_-(S\widetilde{g} + g)\\ &= (I - P_+)(\widetilde{g} + S^* g) - S^* P_-(S\widetilde{g} + g)\\ &= P_-(\widetilde{g} + S^* g) - S^* P_-(S\widetilde{g} + g)\,.\end{aligned}$$

By analytic continuation of $\mathcal{F}_+ u$ into the lower half-plane, taking into account (A.10), one arrives at

$$\alpha\Gamma_0(A_{\mathrm{i}I}-zI)^{-1}u=-\sqrt{2\pi}\big(P_-(\widetilde{g}+S^*g)(z)-S^*(\overline{z})P_-(S\widetilde{g}+g)(z)\big)\qquad\forall z\in\mathbb{C}_-.$$

Combining this with Lemma 3.1(ii), we write

$$\alpha\Gamma_0(A_\varkappa-zI)^{-1}u=-\sqrt{2\pi}\Theta_\varkappa^{-1}(z)\big(P_-(\widetilde{g}+S^*g)(z)-S^*(\overline{z})P_-(S\widetilde{g}+g)(z)\big).$$

Finally, using Lemma A.1 from the proof of Theorem 4.2 above, we obtain

$$\chi_\varkappa^+\alpha\Gamma_0(A_\varkappa-zI)^{-1}u=\sqrt{2\pi}P_-(S\widetilde{g}+g)(z),$$

To demonstrate the converse inclusion

$$\big\{u\in\mathcal{H}:\chi_\varkappa^+\alpha\Gamma_0(A_\varkappa-zI)^{-1}u\in H^2_-(E)\big\}\subset\widetilde{N}_-^\varkappa,$$

we show that, whenever $\chi_\varkappa^+\alpha\Gamma_0(A_\varkappa-zI)^{-1}u\in H^2_-(E)$, the vector

$$\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}=\Phi u-\frac{1}{2\pi}\begin{pmatrix}0\\ \alpha\Gamma_0(A_\varkappa-zI)^{-1}u\end{pmatrix}$$

satisfies

$$P_-\left(\chi_\varkappa^+(\widetilde{g}+S^*g)+\chi_\varkappa^-(S\widetilde{g}+g)\right)=0,$$

and hence $u=\Phi^*P_K\binom{\widetilde{g}}{g}\in\Phi^*P_K\mathcal{N}_-^\varkappa=\widetilde{N}_{\mathrm{e}}^\varkappa$. Indeed, introducing the notation

$$\Phi u=:\begin{pmatrix}\widetilde{g}_0\\ g_0\end{pmatrix},\qquad\qquad h^-:=\frac{1}{2\pi}\alpha\Gamma_0(A_{iI}-zI)^{-1}u,$$

we have

$$\begin{aligned}&P_-\left(\chi_\varkappa^+(\widetilde{g}_0+S^*(g_0+h^-))+\chi_\varkappa^-(S\widetilde{g}_0+g_0+h^-)\right)\qquad\qquad(\mathrm{A.21})\\ &=\chi_\varkappa^+(\widetilde{g}_0+S^*g_0)-P_+\chi_\varkappa^+(\widetilde{g}_0+S^*g_0)+P_-\chi_\varkappa^-(S\widetilde{g}_0+g_0)+\big(I+\chi_\varkappa^+(S^*-I)\big)h^-\\ &=\chi_\varkappa^+\mathcal{F}_+u+\big(I+\chi_\varkappa^+(S^*-I)\big)h^-,\end{aligned}$$

By the analytic continuation into the lower half-plane and using Lemma 3.1(i), it follows that (A.21) represents the boundary value on the real line of the function

$$-\frac{1}{2\pi}\chi_\varkappa^+\alpha\Gamma_0(A_{iI}-zI)^{-1}u+\big(I+\chi_\varkappa^+(S^*(\overline{z})-I)\big)h^-(z)$$

$$=-\frac{1}{2\pi}\chi_\varkappa^+\Theta_\varkappa(z)\alpha\Gamma_0(A_\varkappa-zI)^{-1}u+\big(I+\chi_\varkappa^+(S^*(\overline{z})-I)\big)h^-(z)\qquad(\mathrm{A.22})$$

$$=\big(I+\chi_\varkappa^+(S^*(\overline{z})-I)\big)\left(h^-(z)-\frac{1}{2\pi}\chi_\varkappa^+\alpha\Gamma_0(A_\varkappa-zI)^{-1}u\right)=0,\qquad(\mathrm{A.23})$$

where in order to pass from (A.22) to (A.23) we have used the fact that (see (3.1))

$$\chi_\varkappa^+\Theta_\varkappa(z)=\big(I-\mathrm{i}\chi_\varkappa^+\alpha(B_{\mathrm{i}I}-M(z))^{-1}\alpha\big)\chi_\varkappa^+=\big(I+\chi_\varkappa^+(S^*(\overline{z})-I)\big)\chi_\varkappa^+,\quad z\in\mathbb{C}_-.$$

Hence, the expression (A.21) vanishes, which concludes the proof.

The property

$$\widetilde{N}_+^{\varkappa} = \{u \in \mathcal{H} : \chi_{\varkappa}^{-}\alpha\Gamma_0(A_{\varkappa} - zI)^{-1}u \in H_+^2(E)\}$$

is proved in a similar way.

Proof of Proposition 5.1.

Suppose that $z \in \mathbb{C}_+$. If

$$\int_{\mathbb{R}} \frac{d\mu(s)}{s-z} \in H_+^2 \,,$$

then, by [57, Thm. 5.19], there exists a function $f \in L^2(\mathbb{R})$ such that

$$\int_{\mathbb{R}} \frac{f(s)ds - d\mu(s)}{s-z} = 0\,.$$

Fix a $z_0 \in \mathbb{C}_+$, then

$$\begin{aligned} 0 =& \int_{\mathbb{R}} \frac{f(s)ds - d\mu(s)}{s-z} - \int_{\mathbb{R}} \frac{f(s)ds - d\mu(s)}{s-z_0} \\ =&(z-z_0)\int_{\mathbb{R}} \frac{f(s)ds - d\mu(s)}{(s-z)(s-z_0)}\,. \end{aligned}$$

Thus, one has

$$\int_{\mathbb{R}} \frac{1}{s-z}\frac{f(s)ds - d\mu(s)}{s-z_0} = 0\,, \qquad \text{for all } z \in \mathbb{C}_+ \setminus \{z_0\}\,,$$

where now $(s-z_0)^{-1}(f(s)ds - d\mu(s))$ is a complex measure on $\mathbb{R}$. Further, we invoke to the upper half-plane counterpart of the theorem by F. and M. Riesz obtained by applying the conformal mapping from the unit circle onto the upper half plane [32, Chap. 2, Sec. A]. This theorem implies that $(s-z_0)^{-1}(f(s)dt - d\mu(s))$ is absolutely continuous with respect to the Lebesgue measure and, therefore, the same applies to $d\mu(s)$.

The case of H_-^2 is treated likewise.

References

[1] V. M. Adamjan, D. Z. Arov. Unitary couplings of semi-unitary operators. (Russian) *Mat. Issled.*, 1(2):3–64, 1966; English translation in Amer. Math Soc. Transl. Ser. 2, 95, 1970

[2] G. Berkolaiko and P. Kuchment. *Introduction to quantum graphs*, volume 186 of *Mathematical Surveys and Monographs*. American Mathematical Society, Providence, RI, 2013.

[3] M. Š. Birman. On the theory of self-adjoint extensions of positive definite operators. *Math. Sb. N. S.*, 38(80):431–450, 1956.

[4] M. Š. Birman Existence conditions for wave operators. (Russian) *Izv. Akad. Nauk SSSR Ser. Mat.*, 27, 883–906, 1963.

[5] M. Š. Birman, M. G. Kreĭn. On the theory of wave operators and scattering operators. (Russian) *Dokl. Akad. Nauk SSSR* 144:475–478, 1962.

[6] M. Š. Birman and M. Z. Solomjak. *Spectral theory of selfadjoint operators in Hilbert space*. Mathematics and its Applications (Soviet Series). D. Reidel Publishing Co., Dordrecht, 1987. Translated from the 1980 Russian original by S. Khrushchëv and V. Peller.

[7] G. Borg. Eine Umkehrung der Sturm-Liouvilleschen Eigenwertaufgabe. Bestimmung der Differentialgleichung durch die Eigenwerte. (German) Acta Math. 78:1–96, 1946.

[8] G. Borg. Uniqueness theorems in the spectral theory of $y'' + (\lambda - q(x))y = 0$. In *Den 11te Skandinaviske Matematikerkongress, Trondheim, 1949*, pages 276–287. Johan Grundt Tanums Forlag, Oslo, 1952.

[9] M. S. Brodskij *Triangular and jordan representations of linear operators*, Translations of Mathematical Monographs. Vol. 32. Providence, R.I.: American Mathematical Society, 1971.

[10] M. Brown, M. Marletta, S. Naboko, and I. Wood. Boundary triples and M-functions for non-selfadjoint operators, with applications to elliptic PDEs and block operator matrices. *J. Lond. Math. Soc. (2)*, 77(3):700–718, 2008.

[11] P. Deift, E. Trubowitz. Inverse scattering on the line. *Comm. Pure Appl. Math.* 32 (2): 121–251, 1979.

[12] V. Derkach. Boundary triples, Weyl functions, and the Kreĭn formula. *Operator Theory: Living Reference Work*, DOI 10.1007/978-3-0348-0692-3_32-1 Springer Basel, 2015

[13] V. A. Derkach and M. M. Malamud. Generalized resolvents and the boundary value problems for Hermitian operators with gaps. *J. Funct. Anal.*, 95(1):1–95, 1991.

[14] Y. Ershova, I. I. Karpenko, and A. V. Kiselev. Isospectrality for graph Laplacians under the change of coupling at graph vertices. *J. Spectr. Theory*, 6(1):43–66, 2016.

[15] Y. Ershova, I. I. Karpenko, and A. V. Kiselev. Isospectrality for graph Laplacians under the change of coupling at graph vertices: necessary and sufficient conditions. *Mathematika*, 62(1):210–242, 2016.

[16] Y. Y. Ershova, I. I. Karpenko, and A. V. Kiselev. On inverse topology problem for Laplace operators on graphs. *Carpathian Math. Publ.*, 6(2):230–236, 2014.

[17] P. Exner. A duality between Schrödinger operators on graphs and certain Jacobi matrices. *Ann. Inst. H. Poincaré Phys. Théor.*, 66(4):359–371, 1997.

[18] L. D. Faddeyev. The inverse problem in the quantum theory of scattering. *J. Mathematical Phys.*, 4:72–104, 1963.

[19] L. D. Faddeev The inverse problem in the quantum theory of scattering. II. (Russian) Current problems in mathematics, Vol. 3 (Russian), Akad. Nauk SSSR Vsesojuz. Inst. Naučn. i Tehn. Informacii, Moscow, 93–180, 1974. English translation in: *J. Sov. Math.*, 5: 334–396, 1976.

[20] K. O. Friedrichs. On the perturbation of continuous spectra. *Communications on Appl. Math.* 1: 361–406, 1948.

[21] I. M. Gel'fand, B. M. Levitan. On the determination of a differential equation from its spectral function. (Russian) Izvestiya Akad. Nauk SSSR. Ser. Mat. 15:309–360, 1951.

[22] Gohberg, I. C., Krein, M. G., *Introduction to the theory of linear nonself-adjoint operators*, Translations of Mathematical Monographs, Vol. 18. AMS, Providence, R.I., 1969.

[23] M. L. Gorbachuk and V. I. Gorbachuk. The theory of selfadjoint extensions of symmetric operators; entire operators and boundary value problems. *Ukraïn. Mat. Zh.*, 46(1-2):55–62, 1994.

[24] M. L. Gorbachuk and V. I. Gorbachuk. *M. G. Krein's lectures on entire operators*, volume 97 of *Operator Theory: Advances and Applications*. Birkhäuser Verlag, Basel, 1997.

[25] V. I. Gorbachuk and M. L. Gorbachuk. *Boundary value problems for operator differential equations*, volume 48 of *Mathematics and its Applications (Soviet Series)*. Kluwer Academic Publishers Group, Dordrecht, 1991. Translated and revised from the 1984 Russian original.

[26] I. Kac and M. G. Kreĭn. R-functions–analytic functions mapping upper half-plane into itself. *Amer. Math. Soc. Transl. Series 2*, 103:1–18, 1974.

[27] T. Kato. *Perturbation theory for linear operators.* Springer-Verlag, Berlin, Second edition, 1976. Grundlehren der Mathematischen Wissenschaften, Band 132.

[28] T. Kato and S. T. Kuroda. The abstract theory of scattering. *Rocky Mountain J. Math.*, 1(1):127–171, 1971.

[29] A. V. Kiselev. Similarity problem for non-self-adjoint extensions of symmetric operators. In *Methods of spectral analysis in mathematical physics*, volume 186 of *Oper. Theory Adv. Appl.*, pages 267–283. Birkhäuser Verlag, Basel, 2009.

[30] A. N. Kočubeĭ. Extensions of symmetric operators and of symmetric binary relations. *Mat. Zametki*, 17:41–48, 1975.

[31] A. N. Kočubeĭ. Characteristic functions of symmetric operators and their extensions (in Russian). *Izv. Akad. Nauk Arm. SSR Ser. Mat.*, 15(3):219–232, 1980

[32] P. Koosis. *Introduction to H_p spaces*, volume 115 of *Cambridge Tracts in Mathematics.* Cambridge University Press, Cambridge, second edition, 1998. With two appendices by V. P. Havin [Viktor Petrovich Khavin].

[33] V. Kostrykin and R. Schrader. The inverse scattering problem for metric graphs and the traveling salesman problem. *Preprint arXiv:math-ph/0603010*, 2006.

[34] V. Kostrykin and R. Schrader. Kirchhoff's rule for quantum wires. *J. Phys. A*, 32(4):595–630, 1999.

[35] M. G. Kreĭn. Theory of self-adjoint extensions of semi-bounded Hermitian operators and applications II. (Russian) *Mat. Sb. N. S.*, 21(63):365–404, 1947.

[36] M. G. Kreĭn. Solution of the inverse Sturm-Liouville problem. (Russian) *Doklady Akad. Nauk SSSR (N.S.)* 76:21–24, 1951.

[37] M. G. Kreĭn. On the transfer function of a one-dimensional boundary problem of the second order. (Russian) *Doklady Akad. Nauk SSSR (N.S.)* 88:405–408, 1953.

[38] M. G. Kreĭn. On determination of the potential of a particle from its S-function. (Russian) Dokl. Akad. Nauk SSSR (N.S.) 105:433–436, 1955.

[39] M. G. Kreĭn. The fundamental propositions of the theory of representations of Hermitian operators with deficiency index (m, m). *Ukrain. Mat. Žurnal*, 1(2):3–66, 1949.

[40] P. Kurasov. Inverse problems for Aharonov-Bohm rings. *Math. Proc. Cambridge Philos. Soc.*, 148(2):331–362, 2010.

[41] P. D. Lax and R. S. Phillips. *Scattering theory.* Pure and Applied Mathematics, Vol. 26. Academic Press, New York-London, 1967.

[42] N. Levinson. The inverse Sturm-Liouville problem. *Mat. Tidsskr. B.* 1949:25–30, 1949.

[43] N. Levinson. A certain explicit relation between the phase shift and scattering potential *Phys. Rev.* 89:755-757, 1953

[44] M. S. Livshitz. On a certain class of linear operators in Hilbert space. *Rec. Math. [Mat. Sbornik] N.S.*, 19(61):239–262, 1946.

[45] V. A. Marčenko. On reconstruction of the potential energy from phases of the scattered waves. (Russian) *Dokl. Akad. Nauk SSSR (N.S.)* 104:695–698, 1955.

[46] V. A. Marčenko. *Sturm-Liouville Operators and Applications (2nd ed.)* Providence: American Mathematical Society, 2011.

[47] S. N. Naboko. Absolutely continuous spectrum of a nondissipative operator, and a functional model. I. *Zap. Naučn. Sem. Leningrad. Otdel Mat. Inst. Steklov. (LOMI)*, 65:90–102, 204–205, 1976. Investigations on linear operators and the theory of functions, VII.

[48] S. N. Naboko. Functional model of perturbation theory and its applications to scattering theory. *Trudy Mat. Inst. Steklov.*, 147:86–114, 203, 1980. Boundary Value Problems of Mathematical Physics, 10.

[49] S. N. Naboko. Nontangential boundary values of operator R-functions in a half-plane. *Algebra i Analiz*, 1(5):197–222, 1989.

[50] S. N. Naboko. On the conditions for existence of wave operators in the nonselfadjoint case. *Wave propagation. Scattering theory, Amer. Math. Soc. Transl. Ser. 2*, 157:127–149, Amer. Math. Soc., Providence, RI, 1993.

[51] B. S. Pavlov. Conditions for separation of the spectral components of a dissipative operator. *Izv. Akad. Nauk SSSR Ser. Mat.*, 39:123–148, 240, 1975. English translation in: *Math. USSR Izvestija*, 9:113–137, 1975.

[52] B. S. Pavlov. Diation theory and the spectral analysis of non-selfadjoint differential operators. *Proc. 7th Winter School, Drogobych, 1974*, TsEMI, Moscow, 2–69, 1976. English translation: *Transl., II Ser., Am. Math. Soc* 115: 103–142, 1981.

[53] B. S. Pavlov. Selfadjoint dilation of a dissipative Schrödinger operator, and expansion in its eigenfunction. (Russian) *Mat. Sb. (N.S.)* 102(144): 511–536, 631, 1977.

[54] D. B. Pearson. Conditions for the existence of the generalized wave operators. *J. Mathematical Phys.* 13:1490–1499, 1972.

[55] M. Reed and B. Simon. *Methods of modern mathematical physics. III.* Academic Press [Harcourt Brace Jovanovich Publishers], New York, 1979. Scattering theory.

[56] M. Rosenblum and J. Rovnyak. *Hardy classes and operator theory.* Oxford Mathematical Monographs. The Clarendon Press Oxford University Press, New York, 1985. Oxford Science Publications.

[57] M. Rosenblum and J. Rovnyak. *Topics in Hardy classes and univalent functions.* Birkhäuser Advanced Texts: Basler Lehrbücher. [Birkhäuser Advanced Texts: Basel Textbooks]. Birkhäuser Verlag, Basel, 1994.

[58] V. Ryzhov. Functional model of a class of non-selfadjoint extensions of symmetric operators. In *Operator theory, analysis and mathematical physics*, Volume 174 of *Oper. Theory Adv. Appl.*, pp. 117–158. Birkhäuser, Basel, 2007.

[59] K. Schmüdgen. *Unbounded self-adjoint operators on Hilbert space*, Volume 265 of *Graduate Texts in Mathematics.* Springer, Dordrecht, 2012.

[60] I. M. Stein *Singular integrals and differentiability properties of functions.* Princeton Math Ser. vol. 30, Princeton Univ. Press, Princeton, NJ, 1970.

[61] B. Sz.-Nagy, C. Foias, H. Bercovici, and L. Kérchy. *Harmonic Analysis of Operators on Hilbert Space.* Universitext. Springer, New York, Second enlarged edition, 2010.

[62] J. von Neumann. Über adjungierte Funktionaloperatoren. *Ann. Math.* 33(2), 294–310, 1932

[63] J. von Neumann. *Mathematical foundations of quantum mechanics.* Princeton University Press, Princeton, 1955. Translated by Robert T. Beyer.

[64] M. Rosenblum. On the operator equation $BX - XA = Q$. *Duke Math. J.*, 23:263–269, 1956.

[65] M. Rosenblum. Perturbation of the continuous spectrum and unitary equivalence. *Pacific J. Math.*, 7:997–1010, 1957.

[66] W. T. Tutte. *Graph theory. With a foreword by C. St. J. A. Nash-Williams.* Encyclopedia of Mathematics and its Applications, 21. Addison-Wesley Publishing Company, Advanced Book Program, Reading, MA, 1984.

[67] M. I. Višik. On general boundary problems for elliptic differential equations (Russian). *Trudy Moskov. Mat. Obšč.*, 1: 187–246, 1952.

[68] R. Weder. Scattering theory for the matrix Schrödinger operator on the half line with general boundary conditions. J. Math. Phys. 56(9): 092103, 24 pp, 2015.

[69] R. Weder. Trace formulas for the matrix Schrödinger operator on the half-line with general boundary conditions. J. Math. Phys. 57(11): 112101, 11 pp, 2016.

[70] J. Weidmann. *Linear operators in Hilbert spaces*, volume 68 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, 1980. Translated from the German by Joseph Szücs.

[71] D. R. Yafaev. *Mathematical scattering theory*, volume 105 of *Translations of Mathematical Monographs*. American Mathematical Society, Providence, RI, 1992. General theory, Translated from the Russian by J. R. Schulenberger.