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FUNCTIONAL MODEL FOR EXTENSIONS OF SYMMETRIC OPERATORS AND APPLICATIONS TO SCATTERING THEORY

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To the memory of Professor Boris Pavlov

(Communicated by Enrique Zuazua)

Abstract. On the basis of the 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, we 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.

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 [59], [60] 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 Friedrichs, Kato and Rosenblum [28, 53, 22] and subsequently by Birman and Kreĭn [7], Birman [6], Kato and Kuroda [29] and Pearson [50]. For a detailed exposition of this subject, see [51, 64]. A parallel approach, which provides a connection to the theory of dissipative operators, was developed by Lax and Phillips [39], who

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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, such as the functional model for contractions and dissipative operators by Szökefalvi-Nagy and Foiaş [56], which showed the special rôle in it of the characteristic function of Livšic [41] and allowed Pavlov [49] 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]. In a closely related development, Adamyan and Pavlov [2] established a description for the scattering matrix of a pair of self-adjoint extensions of a symmetric operator (densely or non-densely defined) with finite equal deficiency indices.

Further, Naboko [44] advanced the research initiated by Pavlov, Adamyan and Arov in two directions. Firstly, he generalised Pavlov's construction of the functional model in its spectral form to the case of non-dissipative operators, and secondly, he established its applicability to the scattering theory for pairs of non-selfadjoint operators. 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 discuss an extension of the approach of Naboko [44], which was formulated for additive perturbations of self-adjoint operators, to the case of *both self-adjoint and non-self-adjoint* extensions of symmetric operators. Our strategy is based on a version of the functional model of Pavlov and Naboko as developed by Ryzhov [54]. The work [54] stopped short of proving the crucial, from the scattering point of view, theorem on "smooth" vectors and therefore was unable 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, using the above construction, to provide an explicit solution to an open problem of inverse scattering on a finite non-compact quantum graph, namely, 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 [32]. 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 [61], [62], 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 classical problem of inverse scattering on the infinite and semi-infinite line, which was solved using the classical integral-operator techniques by Borg [9, 10], Levinson [40], Krein [35, 36, 37], Gel'fand and Levitan [23], Marchenko [42], Faddeev [21, 20], Deift and Trubowitz [13]. 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 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 Weyl-Titchmarsh M-matrix in the case of quantum graphs and, more generally, symmetric operators with finite deficiency indices. This generalisation has been exploited extensively in the study of operators, self-adjoint and 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 [25], Kochubei [30, 31], Derkach and Malamud [15]). In our view, the theory of boundary triples is convenient for the study of quantum graphs, when it can also be viewed as a version of the celebrated Birman-Kreĭn-Višik theory [5, 34, 58].

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.* [4] are known to combine 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 7 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 [54] 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 operators 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.* [16, 17, 18], 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 [15] and [54]. In Section 3 we provide several observations that motivate the strategy of our analysis. In Section 4 we recall the functional model for the above family of extensions and characterise the absolutely continuous subspace of $A_\varkappa$ as the closure of the set of "smooth" vectors in the model Hilbert space. On the basis of this characterisation, in Section 5 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 (*cf.* [3]). In Section 6 we describe the representation of the scattering operator as the scattering matrix, which is explicitly written in terms of the M-operator. All material up to this point is applicable to a general class of operators subject to the assumptions discussed in Section 2. In Section 7 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 8 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 $\mathrm{dom}(A) \subset \mathcal{H}$. For such operators, all points in the lower and upper half-planes are of regular type with deficiency indices

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

If $A = A^*$ then A is referred to as self-adjoint. A closed operator L is said to be *completely non-selfadjoint* if there is no subspace reducing L such that the restriction of L to this subspace is self-adjoint. 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 view of the importance of dissipative operators within the present work, we briefly recall that a densely defined operator L in $\mathcal{H}$ is called dissipative if

$$\mathrm{Im}\,\langle Lf, f\rangle \geq 0 \qquad \forall f \in \mathrm{dom}(L). \tag{2.1}$$

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

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

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 (see in [14] a review of the subject). This approach is particularly useful in the study of self-adjoint extensions of differential operators of second order.

Definition 2.1. For a closed symmetric operator A with equal deficiency indices, consider the linear mappings $\Gamma_1 : \mathrm{dom}(A^*) \to \mathcal{K}$, $\Gamma_0 : \mathrm{dom}(A^*) \to \mathcal{K}$, where $\mathcal{K}$ is an auxiliary separable Hilbert space, such that

$$\text{(1)} \quad \langle A^*f, g\rangle_{\mathcal{H}} - \langle f, A^*g\rangle_{\mathcal{H}} = \langle \Gamma_1 f, \Gamma_0 g\rangle_{\mathcal{K}} - \langle \Gamma_0 f, \Gamma_1 g\rangle_{\mathcal{K}}\,; \tag{2.2}$$

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

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

In this work we consider *almost solvable* extensions A_B for which there exists a triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$ and $B \in \mathcal{B}(\mathcal{K})$ such that

$$f \in \mathrm{dom}(A_B) \iff \Gamma_1 f = B\Gamma_0 f\,. \tag{2.3}$$

The following assertions, written in slightly different terms, can be found in [30, Thm. 2] and [26, Chap. 3 Sec. 1.4] (see also [54, Thm. 1.1], and [55, Sec. 14]

for alternative formulation). We compile them in the next proposition for easy reference.

Proposition 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. *$f \in \mathrm{dom}(A)$ 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 2.2. 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^*, where A is assumed to be as in Proposition 1.

The Weyl function defined above has the following properties [15].

Proposition 2. *Let M be a Weyl function of the boundary triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$ for A^*, where A is a closed symmetric operator with equal deficiency indices. 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 [27], that is,*

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

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.*

We next lay out the notation for some of the main objects in our analysis. In the auxiliary Hilbert space $\mathcal{K}$, choose a bounded positive self-adjoint operator α so that the operator

$$B_\varkappa := \frac{\alpha\varkappa\alpha}{2} \tag{2.4}$$

belongs to $\mathcal{B}(\mathcal{K})$, where $\varkappa$ is a bounded operator[1] in $\mathcal{K}$. In what follows, we deal with almost solvable extensions of a given symmetric operator A that are generated by $B_\varkappa$ via (2.3). 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

$$A_\varkappa := A_{B_\varkappa}. \tag{2.5}$$

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 1(5), $A_\varkappa$ is self-adjoint. Note also that $A_{\mathrm{i}I}$ is maximal dissipative, again by Proposition 1.

Definition 2.3. The characteristic function of the operator $A_{\mathrm{i}I}$ is the operator-valued function S on $\mathbb{C}_+$ given by

$$S(z) := I + \mathrm{i}\alpha\big(B_{\mathrm{i}I}^* - M(z)\big)^{-1}\alpha, \qquad z \in \mathbb{C}_+. \tag{2.6}$$

[1] Clearly, the assumption that $\ker(\alpha) = \{0\}$ is without loss of generality, by a suitable modification of $\varkappa$ if necessary.

Remark 1. The function S is analytic in $\mathbb{C}_+$ and, for each $z \in \mathbb{C}_+$, the mapping $S(z) : \mathcal{K} \to \mathcal{K}$ is a contraction. In particular, S has nontangential limits almost everywhere on the real line in the strong topology [56], which we henceforth denote by $S(k)$, $k \in \mathbb{R}$.

Remark 2. When $\alpha = \sqrt{2}I$, which is the case of our application to finite quantum graphs, a straightforward calculation yields that $S(z)$ is the Cayley transform of $M(z)$, *i.e.*

$$S(z) = \big(M(z) - \mathrm{i}I\big)\big(M(z) + \mathrm{i}I\big)^{-1}. \tag{2.7}$$

3. **General remarks on our approach.** Our approach to mathematical scattering theory for extensions of closed symmetric operators (direct and inverse) will be based on the functional model for a family of almost solvable extensions of the given minimal symmetric operator. Our choice of this method is based on the following considerations:

1) We would like to consider scattering problems where at least one of the two operators of the pair is non-selfadjoint. In contrast, the classical scattering results only pertain to pairs of self-adjoint operators: even the definition of $\exp(\mathrm{i}Lt)$ in the case of non-selfadjoint L needs to be clarified. While there are various ways to construct functional calculus for non-uniformly bounded groups, say the Riesz-Dunford calculus, the most attractive of them for us is via developing a functional model where the exponent is represented by an operator of multiplication on a linear set dense in the absolutely continuous subspace of its generator. The "symmetric Pavlov model" [49], which we describe in Section 4, provides such an approach.

2) Naboko [44] has shown how to construct mathematical scattering for a class of non-selfadjoint operators in the "additive" case $L = A + \mathrm{i}V$, where A, V are self-adjoint operators. This kind of method offers some advantages in comparison with other techniques: a) the difference between stationary and non-stationary theories disappears, in the sense that the same construction yields explicit expressions for both; b) the scattering operator is represented in a concise form, which, in particular, immediately yields a formula for the spectral representation in the eigenfunction basis of the unperturbed self-adjoint operator ("scattering matrix").

3) It has to be pointed out that the seemingly non-selfadjoint approach due to Naboko contains the self-adjoint setting as its particular case, and when applied this way it yields all the classical results (*e.g.* Pearson Theorem, Birman-Krein-Kuroda Theorem, as well as their generalisations). In this self-adjoint setting this approach proves to be consistent with the "smooth" scattering theory (see [64]). As in the case of the latter, the principal rôle in Naboko's construction is played by a linear dense subset of the absolutely continuous subspace ("smooth" vectors), which in the self-adjoint case is described by the so-called Rosenblum Lemma [53]. In the non-self-adjoint case the corresponding linear dense subset is identified by the property that the resolvent acts on it as the resolvent of the operator of multiplication in the symmetric Pavlov representation, *cf.* (4.9). This, in turn, facilitates the derivation of explicit formulae for wave operators on these dense sets of smooth vectors. The construction of the wave operators is then completed by passing to a closure.

In what follows we briefly describe the approach introduced above and the results obtained on this way, essentially building up on the earlier results pertaining to the analysis of non-self-adjoint extensions, due to Ryzhov. These allow us to generalise Naboko's construction of wave operators and scattering matrices to the case studied in the present paper. In order to deal with the family of extensions $\{A_\varkappa\}$ of the

operator A (where the parameter $\varkappa$ is itself an operator, see notation immediately following Proposition 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. In view of transparency, we try to reduce the technicalities to the bare minimum, at the same time pointing out that the corresponding complete proofs of the necessary statements can be found in [12].

4. **Functional model.** Following [44], 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 [49, 47, 48] and further developed in [44]. Next we recall some related necessary information. In what follows, in various formulae, we use the subscript "$\pm$" to indicate two different versions of the same formula in which the subscripts "$+$" and "$-$" are taken individually.

A $\mathcal{K}$-valued function f, analytic on $\mathbb{C}_\pm$, is said to be in the Hardy class $H^2_\pm(\mathcal{K})$ if (*cf.* [52, Sec. 4.8])

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

Whenever $f\in H^2_\pm(\mathcal{K})$, the left-hand side of the above inequality defines $\|f\|^2_{H^2_\pm(\mathcal{K})}$. 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 $H^2_\pm(\mathcal{K})$ 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 $H^2_\pm(\mathcal{K})$ are denoted by $\widehat{H}^2_\pm(\mathcal{K})$, and they are subspaces of $L^2(\mathbb{R},\mathcal{K})$ [52, Sec. 4.8, Thm. B]). By the Paley-Wiener theorem [52, Sec. 4.8, Thm. E]), these subspaces are the orthogonal complements of each other (*i.e.*, $L^2(\mathbb{R},\mathcal{K})=\widehat{H}^2_+(\mathcal{K})\oplus\widehat{H}^2_-(\mathcal{K})$).

As mentioned above, the characteristic function S has non-tangential 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 $\mathcal{K}\oplus\mathcal{K}$, one can consider the integral

$$\int_{\mathbb{R}}\left\langle\begin{pmatrix} I & S^*(s)\\ S(s) & I\end{pmatrix}\begin{pmatrix}\widetilde{g}(s)\\ g(s)\end{pmatrix},\begin{pmatrix}\widetilde{g}(s)\\ g(s)\end{pmatrix}\right\rangle_{\mathcal{K}\oplus\mathcal{K}}ds, \tag{4.1}$$

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

$$\mathfrak{H}:=L^2\left(\mathcal{K}\oplus\mathcal{K};\begin{pmatrix} I & S^*\\ S & I\end{pmatrix}\right) \tag{4.2}$$

is the completion of the linear set of two-component vector functions $\binom{\widetilde{g}}{g}:\mathbb{R}\to\mathcal{K}\oplus\mathcal{K}$ in the norm (4.1), 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 $\widetilde{g}, g \in L^2(\mathbb{R}, \mathcal{K})$ one has

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

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

Furthermore, consider the orthogonal subspaces of $\mathfrak{H}$

$$D_- := \begin{pmatrix} 0 \\ \widehat{H}^2_-(\mathcal{K}) \end{pmatrix}, \quad D_+ := \begin{pmatrix} \widehat{H}^2_+(\mathcal{K}) \\ 0 \end{pmatrix}, \tag{4.3}$$

and define the space $K := \mathfrak{H} \ominus (D_- \oplus D_+)$, which is characterised as follows, see *e.g.* [47, 48]:

$$K = \left\{ \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} : \widetilde{g} + S^* g \in \widehat{H}^2_-(\mathcal{K}) \,, S\widetilde{g} + g \in \widehat{H}^2_+(\mathcal{K}) \right\}. \tag{4.4}$$

The orthogonal projection P_K onto the subspace K is given by (see *e.g.* [43])

$$P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \begin{pmatrix} \widetilde{g} - P_+(\widetilde{g} + S^* g) \\ g - P_-(S\,\widetilde{g} + g) \end{pmatrix}, \tag{4.5}$$

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

A completely non-selfadjoint dissipative operator admits [56] a self-adjoint dilation. The dilation $\mathcal{A} = \mathcal{A}^*$ of the operator $A_{\mathrm{i}I}$ is constructed following Pavlov's procedure [47, 49, 48]: it is defined in the Hilbert space $\mathcal{H} = L^2(\mathbb{R}_-, \mathcal{K}) \oplus \mathcal{H} \oplus L^2(\mathbb{R}_+, \mathcal{K})$, so that

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

As in the case of additive non-selfadjoint perturbations [44], Ryzhov established in [54, Thm. 2.3] that $\mathfrak{H}$ serves as the functional model space for the dilation $\mathcal{A}$ *i.e.* there exists an isometry $\Phi : \mathcal{H} \to \mathfrak{H}$ such that $\mathcal{A}$ is transformed into the operator of multiplication by the independent variable: $\Phi(\mathcal{A} - zI)^{-1} = (\cdot - z)^{-1}\Phi$. Furthermore, under this isometry

$$\Phi \restriction_{\mathcal{H}} \mathcal{H} = K$$

unitarily, where $\mathcal{H}$ is understood as being embedded in $\mathcal{H}$ in the natural way, *i.e.*

$$\mathcal{H} \ni h \mapsto 0 \oplus h \oplus 0 \in \mathcal{H}.$$

In what follows we keep the label Φ for the restriction $\Phi \restriction_{\mathcal{H}}$, in hope that it does not lead to confusion.

Following the ideas of Naboko, in the functional model space $\mathfrak{H}$ consider two subspaces

$$\mathfrak{N}^{\varkappa}_{\pm} := \left\{ \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} : P_\pm \left(\chi^+_{\varkappa}(\widetilde{g} + S^* g) + \chi^-_{\varkappa}(S\widetilde{g} + g) \right) = 0 \right\}, \tag{4.6}$$

where

$$\chi^\pm_{\varkappa} := \frac{I \pm \mathrm{i}\varkappa}{2}.$$

These subspaces have a characterisation in terms of the resolvent of the operator $A_{\varkappa}$, whose proof, see [12], follows the approach of [44, Thm. 4].

Theorem 4.1 ([12]). *The following characterisation holds:*

$$\mathfrak{N}_\pm^\varkappa = \left\{ \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \frac{1}{\cdot - z} \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \text{ for all } z \in \mathbb{C}_\pm \right\}. \tag{4.7}$$

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

$$\widetilde{N}_\pm^\varkappa := \Phi^* P_K \mathfrak{N}_\pm^\varkappa, \tag{4.8}$$

which are linear sets albeit not necessarily subspaces. In a way similar to [44], we define the set

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

of so-called smooth vectors and its closure $N_{\mathrm{e}}^\varkappa := \operatorname{clos}(\widetilde{N}_{\mathrm{e}}^\varkappa)$. This proves to be suitable for the description of the absolutely continuous subspace and, therefore, for the construction of the wave operators.

Definition 4.2. For a symmetric operator A, in the case of a non-selfadjoint extension $A_\varkappa$ the absolutely continuous subspace $\mathcal{H}_{\mathrm{ac}}(A_\varkappa)$ is defined by the formula $\mathcal{H}_{\mathrm{ac}}(A_\varkappa) = N_{\mathrm{e}}^\varkappa$.

The next statement, the proof of which is given in [12], motivates the above definition.

Theorem 4.3 (Self-adjoint case, see [12]). *Assume that $\varkappa = \varkappa^*$ (equivalently, $A_\varkappa = A_\varkappa^*$) 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 $N_{\mathrm{e}}^\varkappa = \mathcal{H}_{\mathrm{ac}}(A_\varkappa)$.*

Definition 4.2 follows in the footsteps of the corresponding definition by Naboko [44] in the case of additive perturbations. In particular, an argument similar to [44, Corollary 1] shows that for the functional model image of $\widetilde{N}_{\mathrm{e}}^\varkappa$ the following representation holds:

$$\Phi\widetilde{N}_{\mathrm{e}}^\varkappa = \left\{ P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} : \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} \text{ satisfies } \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \frac{1}{\cdot - z} \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \quad \forall\, z \in \mathbb{C}_- \cup \mathbb{C}_+ \right\}. \tag{4.9}$$

(Note that the inclusion of the right-hand side of (4.9) into $\Phi\widetilde{N}_{\mathrm{e}}^\varkappa$ follows immediately from Theorem 4.1.) Further, we arrive at an equivalent description (*cf.* (4.6)):

$$\Phi\widetilde{N}_{\mathrm{e}}^\varkappa = \left\{ P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} : \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} \text{ satisfies } \chi_\varkappa^+(\widetilde{g} + S^* g) + \chi_\varkappa^-(S\widetilde{g} + g) = 0 \right\}. \tag{4.10}$$

The representations (4.9), (4.10) illustrate the rôle of the subspace of smooth vectors as the subspace in whose image under the isometry Φ the operator $A_\varkappa$ acts as multiplication by the independent variable. This property is crucial in the derivation of the formulae for wave operators of pairs from the family $\{A_\varkappa\}$, which we present in the next section and which are subsequently used in the solution of the inverse problem for quantum graphs in Sections 7, 8.

5. **Wave and scattering operators.** The results discussed above 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. For simplicity, and having in mind the application of the abstract construction to the problem described in Sections 7 and 8, 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 recalling 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 $\widetilde{N}_{\mathrm{e}}^{\varkappa}$, as well as a proposition describing such vectors in $\widetilde{N}_{\mathrm{e}}^{\varkappa}$ and $\widetilde{N}_{\mathrm{e}}^{0}$ that the difference between their respective dynamics vanishes as $t \to -\infty$.

Proposition 3. *([44, 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*

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

Proposition 4. *([44, Section 4]) If $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{\varkappa}$ and $\Phi^* P_K \binom{\widetilde{g}'}{g} \in \widetilde{N}_{\mathrm{e}}^{0}$ (with the same element[2] g), then*

$$\left\| \exp(-iA_\varkappa t)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} - \exp(-iA_0 t)\Phi^* P_K \begin{pmatrix} \widetilde{g}' \\ g \end{pmatrix} \right\|_{\mathfrak{H}} \xrightarrow[t\to-\infty]{} 0.$$

It follows from Proposition 4 that whenever $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{\varkappa}$ and $\Phi^* P_K \binom{\widetilde{g}'}{g} \in \widetilde{N}_{\mathrm{e}}^{0}$ (with the same second component g), one formally has

$$\lim_{t\to-\infty} e^{iA_0 t} e^{-iA_\varkappa t} \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi^* P_K \begin{pmatrix} \widetilde{g}' \\ g \end{pmatrix} = \Phi^* P_K \begin{pmatrix} -(I+S)^{-1}(I+S^*)g \\ g \end{pmatrix},$$

where in the last equality we use the inclusion $\Phi^* P_K \binom{\widetilde{g}'}{g} \in \widetilde{N}_{\mathrm{e}}^{0}$, which by (4.10) yields $\widetilde{g}' + S^* g + S\widetilde{g}' + g = 0$.

In what follows we use the standard definition of wave operators, see *e.g.* [28], allowing the operator $A_\varkappa$ to be non-selfadjoint:

$$W_\pm(A_0, A_\varkappa) := \operatorname*{s-lim}_{t\to\pm\infty} e^{iA_0 t} e^{-iA_\varkappa t} P_{\mathrm{ac}}^{\varkappa}, \qquad W_\pm(A_\varkappa, A_0) := \operatorname*{s-lim}_{t\to\pm\infty} e^{iA_\varkappa t} e^{-iA_0 t} P_{\mathrm{ac}}^{0}. \tag{5.1}$$

In the above formulae, we denote by $P_{\mathrm{ac}}^{\varkappa}$, P_{ac}^{0} the projections onto the absolutely continuous subspace of $A_\varkappa$, see Definition 4.2, and the absolutely continuous subspace of the self-adjoint operator A_0, respectively.

It follows that for $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{\varkappa}$ one has

$$W_-(A_0, A_\varkappa)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi^* P_K \begin{pmatrix} -(I+S)^{-1}(I+S^*)g \\ g \end{pmatrix}. \tag{5.2}$$

One argues in a similar way in the case of the wave operator $W_+(A_0, A_\varkappa)$, as well as in the case of the wave operators $W_\pm(A_\varkappa, A_0)$, which we define by

$$\left\| e^{-iA_\varkappa t} W_\pm(A_\varkappa, A_0)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} - e^{-iA_0 t}\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \right\|_{\mathfrak{H}} \xrightarrow[t\to\pm\infty]{} 0, \quad \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \widetilde{N}_{\mathrm{e}}^{0}.$$

[2]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 $L^2(\mathcal{K})$ spaces with operators "weights", see details below in Section 6. 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.

Theorem 5.1 ([12]). *Let A be a closed, symmetric, completely non-selfadjoint operator with equal deficiency indices and consider its extension $A_\varkappa$, as described in Section 2, under the assumption that $A_\varkappa$ has at least one regular point in $\mathbb{C}_+$ and in $\mathbb{C}_-$. If $S-I$ is compact in $\overline{\mathbb{C}}_+$, then the wave operators $W_\pm(A_0, A_\varkappa)$ exist on dense sets in $N_{\mathrm{e}}^\varkappa$ and for all $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^\varkappa$ one has (5.2) and*

$$W_+(A_0, A_\varkappa)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ -(I+S^*)^{-1}(I+S)\widetilde{g} \end{pmatrix}. \tag{5.3}$$

Similarly, the wave operators and $W_\pm(A_\varkappa, A_0)$ exist on dense sets in $\mathcal{H}_{\mathrm{ac}}(A_0)$ and for all $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^0$ one has

$$W_-(A_\varkappa, A_0)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi^* P_K \begin{pmatrix} -\big(I+\chi_\varkappa^-(S-I)\big)^{-1}\big(I+\chi_\varkappa^+(S^*-I)\big)g \\ g \end{pmatrix}, \tag{5.4}$$

$$W_+(A_\varkappa, A_0)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ -\big(I+\chi_\varkappa^+(S^*-I)\big)^{-1}\big(I+\chi_\varkappa^-(S-I)\big)\widetilde{g} \end{pmatrix}, \tag{5.5}$$

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.[3]

Sketch of the proof. In order to rigorously justify the above formal derivation of (5.2)–(5.5), *i.e.* in order to prove the existence and completeness of the wave operators, one needs to show that the right-hand sides of the formulae (5.2)–(5.5) make sense on dense subsets of the corresponding absolutely continuous subspaces. Noting that (5.2)–(5.5) have the form identical to the expressions for wave operators derived in [44, Section 4], [46], this justification is an appropriate modification of the argument of [46].

Indeed, consider the formula (5.2). Here one needs to attribute a correct sense to the expression $(I+S(k))^{-1}$ a.e. on the real line. Let $S(z)-I$ satisfy the assumption of the theorem. Then, using the strategy of [46], one has non-tangential boundedness of $(I+S(z))^{-1}$ for almost all points of the real line. On the other hand, the latter inverse can be computed in $\mathbb{C}_+$:

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

It follows from the analytic properties of $M(z)$ that the inverse $(I+S(z))^{-1}$ exists everywhere in the upper half-plane. Thus, [46] yields that $(I+S(z))^{-1}$ is $\mathbb{R}$-a.e. non-tangentially bounded and 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 presented argument allows one to verify the correctness of the formula (5.2). Indeed, consider $\mathbb{1}_n(k)$, the indicator of the set $\{k \in \mathbb{R} : \|(I+S(k))^{-1}\| \le n\}$.

[3] 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.* [44, Section 4], [46] and references therein.

Clearly, $\mathbb{1}_n(k) \to 1$ as $n \to \infty$ for almost all $k \in \mathbb{R}$. Next, suppose that $P_K(\widetilde{g}, g) \in \widetilde{N}_{\mathrm{e}}^{\varkappa}$. Then $P_K \mathbb{1}_n(\widetilde{g}, g)$ is also a smooth vector and

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

It follows, by the Lebesgue dominated convergence theorem, that the set of vectors $P_K \mathbb{1}_n(\widetilde{g}, g)$ is dense in $N_{\mathrm{e}}^{\varkappa}$.

The remaining three wave operators are treated in a similar way, see the complete details in [12]. 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.* [64]. □

Remark 3 ([12])**.** 1. The condition of the above theorem that $S(z) - I$ is compact in $\overline{\mathbb{C}}_+$ is satisfied [24, 12], 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.

2. 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 [45] for details.

3. 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 (2.4), then one "shifts" the boundary triple: $\widehat{\Gamma}_0 = \Gamma_0$, $\widehat{\Gamma}_1 = \Gamma_1 - C_0\Gamma_0$. 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 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 2 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.

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 formulae (5.2)–(5.5) lead (see (*cf.* [44])) to the following formula for the action of Σ in the model representation:

$$\Phi\Sigma\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \begin{pmatrix} -(I + \chi_{\varkappa}^-(S-I))^{-1}(I + \chi_{\varkappa}^+(S^*-I))g \\ (I+S^*)^{-1}(I+S)(I+\chi_{\varkappa}^-(S-I))^{-1}(I+\chi_{\varkappa}^+(S^*-I))g \end{pmatrix}, \tag{5.6}$$

whenever $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^0$. This representation holds on a dense linear set in $\widetilde{N}_{\mathrm{e}}^0$ within the conditions of Theorem 5.1, which guarantees that all the objects on the right-hand side of the formula (5.6) are correctly defined.

6. **Spectral representation for the absolutely continuous part of A_0.** The identity

$$\left\| P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \right\|_{\mathfrak{H}}^2 = \big\langle (I - S^*S)\widetilde{g}, \widetilde{g} \big\rangle \qquad \forall P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \widetilde{N}_{\mathrm{e}}^0,$$

which is derived in the same way as in [44, Section 7] for all $P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^0$, which is equivalent to the condition $(\widetilde{g} + S^*g) + (S\widetilde{g} + g) = 0$, see (4.10), allows us to consider the isometry $F : \Phi\widetilde{N}_{\mathrm{e}}^0 \mapsto L^2(\mathcal{K}; I - S^*S)$ defined by

$$F P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \widetilde{g}. \tag{6.1}$$

Here $L^2(\mathcal{K}; I - S^*S)$ is the Hilbert space of $\mathcal{K}$-valued functions on $\mathbb{R}$ square summable with the matrix "weight" $I - S^*S$, *cf.* (4.2). Similarly, the formula

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

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

Proposition 5 ([12])**.** *Suppose that the assumptions of Theorem 5.1 hold. Then the ranges of the operators F and F_* are dense in the spaces $L^2(\mathcal{K}; I - S^*S)$ and $L^2(\mathcal{K}; I - SS^*)$, respectively.*

The above statement immediately implies the next result, which allows us to obtain the required spectral representation.

Theorem 6.1. *The operator F, respectively F_*, admits an extension to the unitary mapping between ΦN_{e}^0 and $L^2(\mathcal{K}; I - S^*S)$, respectively $L^2(\mathcal{K}; I - SS^*)$.*

It follows that the operator $(A_0 - z)^{-1}$ considered on $\widetilde{N}_{\mathrm{e}}^0$ acts as the multiplication by $(k - z)^{-1}$, $k \in \mathbb{R}$, both in $L^2(\mathcal{K}; I - S^*S)$ and $L^2(\mathcal{K}; I - SS^*)$. 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 $L^2(\mathcal{K}; I - S^*S)$ and $L^2(\mathcal{K}; I - SS^*)$, respectively.

In order to obtain a spectral representation from the above result, we need 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 5.1 *e.g.* when the boundary space $\mathcal{K}$ is finite-dimensional, which is the case we deal with in the application discussed in Sections 7, 8. The corresponding diagonalisation in the general setting will be treated elsewhere.) In this particular case one has (*cf.* (2.7))

$$S = (M - iI)(M + iI)^{-1}, \tag{6.2}$$

and consequently

$$I - S^*S = -2i(M^* - iI)^{-1}(M - M^*)(M + iI)^{-1}, \tag{6.3}$$

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

Introducing the unitary transformations

$$G : L^2(\mathcal{K}; I - S^*S) \mapsto L^2\big(\mathcal{K}; -2i(M - M^*)\big), \tag{6.4}$$

$$G_* : L^2(\mathcal{K}; I - SS^*) \mapsto L^2\big(\mathcal{K}; -2i(M - M^*)\big) \tag{6.5}$$

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 $L^2(\mathcal{K}; -2i(M - M^*))$. We show next that this amounts to the spectral representation in particular in the case of (non-compact) quantum graphs.

7. **Quantum graphs and their scattering matrices.** 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.* [8, Chapter 7]). Nevertheless, it proves 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. Namely, we prove the following statement.

Theorem 7.1. *The following formula holds:*

$$\widehat{\Sigma} = GF\Sigma(GF)^* = (M - \varkappa)^{-1}(M^* - \varkappa)(M^*)^{-1}M, \tag{7.1}$$

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

Proof. Using the definition (6.1) of the isometry F along with the relationship (4.10) between $\widetilde{g}$ and g whenever $P_K\binom{\widetilde{g}}{g} \in \Phi\widetilde{N}_{\mathrm{e}}^{\varkappa}$ with $\varkappa = 0$, we obtain from (5.6):

$$F\Sigma F^* = \big(I + \chi_\varkappa^-(S - I)\big)^{-1}\big(I + \chi_\varkappa^+(S^* - I)\big)(I + S^*)^{-1}(I + S), \tag{7.2}$$

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

Furthermore, substituting the expression (2.6) 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 $L^2(\mathcal{K}; I - S^*S)$. Using (6.3), we now obtain the following identity for all $f, g \in L^2(\mathcal{K}; I - S^*S)$:

$$\begin{aligned}
\langle F\Sigma F^* f, g\rangle_{L^2(\mathcal{K}; I - S^*S)} = \\
&\langle (I - S^*S)(M + iI)(M - \varkappa)^{-1}(M^* - \varkappa)(M^*)^{-1}M(M + iI)f, g\rangle \\
&= \langle -2i(M^* - iI)^{-1}(M - M^*)(M + iI)^{-1}(M + iI)(M - \varkappa)^{-1} \\
&\qquad \times (M^* - \varkappa)(M^*)^{-1}M(M + iI)f, g\rangle \\
&= \big\langle -2i(M - M^*)(M - \varkappa)^{-1}(M^* - \varkappa)(M^*)^{-1}M(M + iI)f, (M + iI)g\big\rangle,
\end{aligned}$$

which is equivalent to (7.1), 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 (6.4), (6.5)) is degenerate: more precisely, $M(s) - M(s)^* = 2i\sqrt{s}P_{\mathrm{e}}$, $s \in \mathbb{R}$, where P_{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.

Remark 4. From this point on, for simplicity of presentation we consider the case of a finite non-compact quantum graph, when the deficiency indices are finite. However, our approach allows us to consider the general setting of infinite deficiency indices, which in the quantum graph setting leads to an infinite graph. In particular, on could consider the case of an infinite compact part of the graph.

In what follows, we denote by $\mathbb{G} = \mathbb{G}(\mathcal{E}, \sigma)$ a finite metric graph, *i.e.* a pair consisting 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 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, $m = 1, 2, \dots, N$, 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:

$$\partial_n f(x_j) := \begin{cases} f'(x_j), & \text{if } x_j \text{ is the left endpoint of the edge,} \\ -f'(x_j), & \text{if } x_j \text{ is the right endpoint of the edge.} \end{cases} \tag{7.3}$$

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

Definition 7.2. 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 5. Note that the δ-type matching condition in a particular case when $a_m = 0$ gives the standard Kirchhoff matching condition at the vertex V_m, see *e.g.* [4].

Definition 7.3. The quantum 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, $m = 1, 2, \dots, N$. The Schrödinger operator on the same graph is defined likewise on the same domain in the case of summable edge potentials (*cf.* [16]).

If all coupling constants a_m, $m = 1, \dots, N$, are real, it is shown that the operator A_a is a proper self-adjoint extension (see (2.3)) of a closed symmetric operator A in $L^2(\mathbb{G})$ [19, 33]. 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 $l_j := x_{2j} - x_{2j-1}$, $j = 1, \dots, n$ is the

length of the corresponding edge. Throughout the present paper we will therefore only consider this situation.

In [16] the following result is obtained for the case of finite *compact* metric graphs.

Proposition 6 ([16]). *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 $\varkappa$ (see (2.3)) is given by $\varkappa = \mathrm{diag}\{a_1, \dots, a_N\}$, whereas the Weyl function is an $N \times N$ matrix with elements*

$$m_{jk}(z) = \begin{cases} -\sqrt{z}\Big(\sum\limits_{e_p \in E_k} \cot \sqrt{z} l_p - 2 \sum\limits_{e_p \in L_k} \tan \frac{\sqrt{z} l_p}{2}\Big), & j = k, \\ \sqrt{z} \sum\limits_{e_p \in C_{jk}} \dfrac{1}{\sin \sqrt{z} l_p}, & j \neq k;\ V_j, V_k \text{ adjacent}, \\ 0, & j \neq k;\ V_j, V_k \text{ non-adjacent}. \end{cases} \tag{7.4}$$

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 [16] 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 6 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 7.4. *The matrix functions M, $M^{(\mathrm{i})}$ described above are related by the formula*

$$M(z) = M^{(\mathrm{i})}(z) + i\sqrt{z} P_{\mathrm{e}}, \qquad z \in \mathbb{C}_+, \tag{7.5}$$

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 6 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 6.

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

$$-f''(x) = zf(x), \quad x \in [0, +\infty), \qquad f \in W^{2,2}(0, +\infty), \tag{7.6}$$

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 (7.6) 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 (7.3) 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 2.2, 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. □

The formula (7.5) leads to $M(s)-M^*(s) = 2i\sqrt{s}P_\mathrm{e}$ a.e. $s\in\mathbb{R}$, and the expression (7.1) for $\widehat{\Sigma}$ results in the classical scattering matrix $\widehat{\Sigma}_\mathrm{e}(k)$ 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 $\varkappa = \varkappa = \mathrm{diag}\{a_1,\dots,a_N\}$:

$$\widehat{\Sigma}_\mathrm{e}(s) = P_\mathrm{e}(M(s)-\varkappa)^{-1}(M(s)^*-\varkappa)(M(s)^*)^{-1}M(s)P_\mathrm{e}, \qquad s\in\mathbb{R}, \tag{7.7}$$

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

Remark 6. In the more common approach to the construction of scattering matrices, based on comparing the asymptotic expansions of solutions to spectral equations, see *e.g.* [20], one obtains $\widehat{\Sigma}_\mathrm{e}$ as the scattering matrix. Our approach yields an explicit factorisation of $\widehat{\Sigma}_\mathrm{e}$ into expressions involving the matrices M and $\varkappa$ only, sandwiched between two projections. (Recall that M and $\varkappa$ contain the information about the geometry of the graph and the coupling constants, respectively.) From the same formula (7.7), it is obvious that without the factorisation the pieces of information pertaining to the geometry of the graph and the coupling constants at the vertices are present in the final answer in an entangled form.

Remark 7. The concrete choice of boundary triple in accordance with Proposition 6 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, *cf.* Part 3 of Remark 3. In particular, we point out that the formula (7.2) is written in a triple-independent way.

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 5.1.

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

$$(M-\varkappa)^{-1}(M^*-\varkappa) = I + (M-\varkappa)^{-1}(M^*-M) = I - 2i\sqrt{s}(M-\varkappa)^{-1}P_\mathrm{e} \tag{7.8}$$

and

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

a factorisation of $\widehat{\Sigma}_\mathrm{e}$ into a product of $\varkappa$–dependent and $\varkappa$–independent factors (*cf.* (7.1)) still holds in this case in $P_\mathrm{e}\mathcal{K}$, namely

$$\widehat{\Sigma}_\mathrm{e} = \big[P_\mathrm{e}(M-\varkappa)^{-1}(M^*-\varkappa)P_\mathrm{e}\big]\big[P_\mathrm{e}(M^*)^{-1}MP_\mathrm{e}\big]. \tag{7.9}$$

8. **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 $\widehat{\Sigma}_\mathrm{e}(s)$, defined by (7.9), 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

$\{a_j\}_{j=1}^N$, see Definitions 7.2, 7.3. 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 $\widehat{\Sigma}_{\mathrm{e}}(s)$ for almost all $s>0$, we reconstruct the meromorphic matrix-function $P_{\mathrm{e}}(M^{(\mathrm{i})}(z)-\varkappa)^{-1}P_{\mathrm{e}}$ for all complex z, excluding the poles. This is an explicit calculation based on the second resolvent identity (see *e.g.* [63, Thm. 5.13]). Namely, almost everywhere on the positive half-line one has

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

and hence

$$P_{\mathrm{e}}(M-\varkappa)^{-1}P_{\mathrm{e}} = \big[P_{\mathrm{e}} - i\sqrt{s}P_{\mathrm{e}}(M-\varkappa)^{-1}P_{\mathrm{e}}\big]P_{\mathrm{e}}(M^{(\mathrm{i})}-\varkappa)^{-1}P_{\mathrm{e}}. \tag{8.1}$$

Further, the first factor on the right-hand side of (8.1) is invertible for almost all $s>0$. Indeed, we note first that $\widehat{\Sigma}_{\mathrm{e}}^{\varkappa} := P_{\mathrm{e}}(M(s)-\varkappa)^{-1}(M(s)^*-\varkappa)$ is unitary in $P_{\mathrm{e}}\mathcal{K}$ for almost all $s>0$, since

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

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

$$P_{\mathrm{e}} - i\sqrt{s}P_{\mathrm{e}}(M-\varkappa)^{-1}P_{\mathrm{e}} = \big(P_{\mathrm{e}}+\widehat{\Sigma}_{\mathrm{e}}^{\varkappa}\big)/2$$

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

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

A straightforward calculation then yields

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

from where

$$(M(s)-\varkappa)^{-1}u_s \in \ker\big(M^{(\mathrm{i})}(s)-\varkappa\big).$$

The latter kernel is non-trivial only at the points s which belong to the (discrete) spectrum of the Laplacian on the compact part $\mathbb{G}^{(\mathrm{i})}$ 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 $P_{\mathrm{e}}(M-\varkappa)^{-1}P_{\mathrm{e}}$ is found by combining (7.8) and (7.9):

$$P_{\mathrm{e}}(M-\varkappa)^{-1}P_{\mathrm{e}} = \frac{1}{2i\sqrt{s}}\big(P_{\mathrm{e}} - \widehat{\Sigma}_{\mathrm{e}}[P_{\mathrm{e}}(M^*)^{-1}MP_{\mathrm{e}}]^{-1}\big), \tag{8.2}$$

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

It follows from (8.1) and (8.2) that for given M, $\widehat{\Sigma}_{\mathrm{e}}$ the expression $P_{\mathrm{e}}(M^{(\mathrm{i})}-\varkappa)^{-1}P_{\mathrm{e}}$ is determined uniquely for almost all $s>0$:

$$\begin{aligned} P_{\mathrm{e}}(M^{(\mathrm{i})}-\varkappa)^{-1}P_{\mathrm{e}} &= \big[P_{\mathrm{e}}-i\sqrt{s}P_{\mathrm{e}}(M-\varkappa)^{-1}P_{\mathrm{e}}\big]^{-1}P_{\mathrm{e}}(M-\varkappa)^{-1}P_{\mathrm{e}} \\ &= \frac{1}{i\sqrt{s}}\big(P_{\mathrm{e}}+\widehat{\Sigma}_{\mathrm{e}}[P_{\mathrm{e}}(M^*)^{-1}MP_{\mathrm{e}}]^{-1}\big)^{-1}\big(P_{\mathrm{e}}-\widehat{\Sigma}_{\mathrm{e}}[P_{\mathrm{e}}(M^*)^{-1}MP_{\mathrm{e}}]^{-1}\big) \\ &= \frac{1}{i\sqrt{s}}\Big(2\big(P_{\mathrm{e}}+\widehat{\Sigma}_{\mathrm{e}}[P_{\mathrm{e}}(M^*)^{-1}MP_{\mathrm{e}}]^{-1}\big)^{-1}-I\Big)P_{\mathrm{e}}. \end{aligned} \tag{8.3}$$

In particular, due to the property of analytic continuation, the expression $P_{\mathrm{e}}(M^{(\mathrm{i})}-\varkappa)^{-1}P_{\mathrm{e}}$ 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 $A^{(\mathrm{i})}_{\varkappa}$ on the compact part $\mathbb{G}^{(\mathrm{i})}$ of the graph $\mathbb{G}$ with matching conditions at the graph vertices given by the matrix $\varkappa$, *cf.* Proposition 6.

Definition 8.1. 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 u_z 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

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

The *Robin-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 $\varkappa^{\mathcal{V}_1}:=\mathrm{diag}\{a_m:\ V_m\in\mathcal{V}_1\}$. (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 8. 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.* [4], [38].

We argue that the matrix $P_{\mathrm{e}}(M^{(\mathrm{i})}-\varkappa)^{-1}P_{\mathrm{e}}$ is the Robin-to-Dirichlet map for the set $\mathcal{V}^{(\mathrm{e})}$. Indeed, assuming $\phi:=\Gamma_1u_z-\varkappa\Gamma_0u_z$ and $\phi=P_{\mathrm{e}}\phi$, where the latter condition ensures the correct δ-type matching on the set $\mathcal{V}^{(\mathrm{i})}$, one has $P_{\mathrm{e}}\phi=(M^{(\mathrm{i})}-\varkappa)\Gamma_0u_z$ and hence $\Gamma_0u_z=(M^{(\mathrm{i})}-\varkappa)^{-1}P_{\mathrm{e}}\phi$. Applying P_{e} to the last identity yields the claim, in accordance with Definition 8.1.

We have thus proved the following theorem.

Theorem 8.2. *The Robin-to-Dirichlet map for the vertices $\mathcal{V}^{(\mathrm{e})}$ is determined uniquely by the scattering matrix $\widehat{\Sigma}_{\mathrm{e}}(s)$, $s\in\mathbb{R}$, via the formula (8.3).*

The following definition, required for the formulation of the next theorem, is a generalisation of the procedure of graph contraction, which is well studied in the algebraic graph theory, see *e.g.* [57].

Definition 8.3 (Contraction procedure[4] for graphs and associated quantum graph Laplacians)**.** For a given graph $\mathbb{G}$, vertices V and W connected by an edge e are

[4]One of the referees pointed out that this procedure is sometimes referred to a "layer peeling". We have opted to keep the term "contraction" for it, in line with the terminology of the algebraic literature.

"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 quantum graph Laplacian A_a defined on $\mathbb{G}$ is contracted to the quantum graph Laplacian $\widetilde{A}_{\widetilde{a}}$ 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 quantum graph Laplacians are described by Definition 7.3.

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

Theorem 8.4. *Suppose that the edge lengths of the graph $\mathbb{G}^{(\mathrm{i})}$ are rationally independent. The element*[5] $(1,1)$ *of the Robin-to-Dirichlet map described above yields the element* $(1,1)$ *for the "contracted" graph $\widetilde{\mathbb{G}}^{(\mathrm{i})}$ obtained from $\mathbb{G}^{(\mathrm{i})}$ 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 8.3.*

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 expressed 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 $M^{(\mathrm{i})}$, see (7.4). 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 explicit expression for f_1 mentioned above. 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:

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

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

$$\lim_{l_1\to 0} f_1(\sqrt{z}; l_1, \dots, l_n; a) = \frac{\lim\limits_{l_1\to 0}(-l_1)\mathcal{D}^{(1)}(\sqrt{z}; l_1, \dots, l_n; a)}{\lim\limits_{l_1\to 0}(-l_1)\det\big(M^{(\mathrm{i})}(z) - \varkappa\big)} \tag{8.4}$$

The numerator of (8.4) 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 (8.4), 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.

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

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.* 8.4) 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 (8.4) to the determinant of a matrix of the size reduced by one. As in [17], 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.*

$$\lim_{l_1\to 0} f_1(\sqrt{z};l_1,\dots,l_n;a)=f_1^{(1)}(\sqrt{z};l_2,\dots,l_n;\widetilde{a}),\tag{8.5}$$

where $f_1^{(1)}$ is the element (1,1) of the Robin-to-Dirichlet map of the contracted graph $\widetilde{\mathbb{G}}^{(\mathrm{i})}$, and $\widetilde{a}$ is given by Definition 8.3. □

The main result of this section is the theorem below, which is a corollary of Theorems 8.2 and 8.4. 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 Robin-to-Dirichlet map for the set $\mathcal{V}^{(\mathrm{e})}$. We set the following notation. Fix a spanning tree $\mathbb{T}$ (see *e.g.* [57]) 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 ($m=1,\dots,N$). 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 8.5. *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 Robin-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, $m=1,\dots,N$:*

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

where

$$f_1^{(l)}(\sqrt{z}):=\lim_{l^{(l)}_{N^{(l)}-1}\to 0}\ \dots\ \lim_{l_2^{(l)}\to 0}\lim_{l_1^{(l)}\to 0} f_1(\sqrt{z}),\tag{8.6}$$

where in the case $l=1$ no limits are taken in (8.6).

Proof. We first apply Theorem 8.2 to determine the Robin-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 Robin-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 6. Indeed, setting $\sqrt{z} = i\tau$, $\tau \to +\infty$, one has (*cf.* (7.4))

$$\frac{1}{f_1} = i\tau\Big(-\sum_{e_p \in E_1} \cot(i\tau l_p) + 2\sum_{e_p \in L_1} \tan\frac{i\tau l_p}{2}\Big) - a_1 + o\big(\tau^{-K}\big) \tag{8.7}$$

$$= -\tau\deg(V_1) - a_1 + o\big(\tau^{-K}\big), \quad \tau \to +\infty \tag{8.8}$$

for all $K > 0$, where the first sum in (8.7) 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 (8.8).

In order to determine the coupling constant a_2, we apply Theorem 8.4. 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 (8.5), together with asymptotics (8.8) 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 8.4, is equal to $a_1 + a_2$:

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

$$= \lim_{\tau\to+\infty}\left\{-\tau\big(\deg(V_1) + \deg(V_2) - 2\big) - \frac{1}{f_1^{(1)}}\right\}, \tag{8.9}$$

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 (8.5), is the element (1,1) of the Robin-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 (8.5)) and "$\infty - \infty$" (see (8.9)).

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 9. 1. Notice that each step of the above iterative process generates a set of loops, which is treated according to the formula (8.7). Alternatively, these loops can be discarded by an elementary recalculation of the corresponding element of the Robin-to-Dirichlet map in the application of Theorem 8.4.

2. From the proof of Theorem 8.5 it actually follows that the inverse problem of determining matching conditions based on the Robin-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 Robin-to-Dirichlet map.

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REFERENCES

[1] V. M. Adamjan and D. Z. Arov, Unitary couplings of semi-unitary operators, (Russian) *Mat. Issled.*, **1** (1966), 3–64; English translation in *Amer. Math Soc. Transl. Ser.,* **2** (1970), p95.

[2] V. M. Adamyan and B. S. Pavlov, Zero-radius potentials and M. G. Kreĭn's formula for generalized resolvents, (Russian)translated from *Zap. Nauchn. Sem. Leningrad. Otdel. Mat. Inst. Steklov. (LOMI)*, **149** (1986), Issled. Lineĭn. Teor. Funktsiĭ. XV, 7–23, 186; *J. Soviet Math.* **42** (1988), 1537–1550.

[3] J. Behrndt,M. M. Malamud and H. Neidhardt, Scattering theory for open quantum systems with finite rank coupling, *Math. Phys. Anal. Geom.*, **10** (2007), 313–358.

[4] G. Berkolaiko and P. Kuchment, *Introduction to Quantum Graphs*, volume **186** of Mathematical Surveys and Monographs, American Mathematical Society, Providence, RI, 2013.

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

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

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

[8] 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.

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

[10] 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.

[11] 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** (2008), 700–718.

[12] K. Cherednichenko, A. Kiselev and L. Silva, Scattering theory for non-selfadjoint extensions of symmetric operators, Preprint, arXiv:1712.09293, 2017.

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

[14] V. Derkach, Boundary triples, Weyl functions, and the Kreĭn formula, *Operator Theory: Living Reference Work*, Springer Basel, 2014, 1–33.

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

[16] 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** (2016), 43–66.

[17] 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** (2016), 210–242.

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

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

[20] 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, (1974), 93–180. English translation in:*J. Sov. Math.*, **5** (1976), 334–396.

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

[22] K. O. Friedrichs, On the perturbation of continuous spectra, *Communications on Appl. Math.*, **1** (1948), 361–406.
[23] I. M. Gel'fand and B. M. Levitan, On the determination of a differential equation from its spectral function, (Russian) *Izvestiya Akad. Nauk SSSR. Ser. Mat.,* **15** (1951), 309–360.
[24] I. C. Gohberg and M. G. Krein, *Introduction to the Theory of Linear Nonself-Adjoint Operators*, Translations of Mathematical Monographs, vol. 18 AMS, Providence, R.I., 1969.
[25] 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** (1994), 55–62.
[26] 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.
[27] I. Kac and M. G. Kreĭn, *R*-functions–analytic functions mapping upper half-plane into itself, *Amer. Math. Soc. Transl. Series 2*, **103** (1974), 1–18.
[28] T. Kato, *Perturbation Theory for Linear Operators*, Springer-Verlag, Berlin, Second edition, 1976. Grundlehren der Mathematischen Wissenschaften, Band 132.
[29] T. Kato and S. T. Kuroda, The abstract theory of scattering, *Rocky Mountain J. Math.*, **1** (1971), 127–171.
[30] A. N. Kočubeĭ, Extensions of symmetric operators and of symmetric binary relations, *Mat. Zametki*, **17** (1975), 41–48.
[31] A. N. Kočubeĭ, Characteristic functions of symmetric operators and their extensions (in Russian), *Izv. Akad. Nauk Arm. SSR Ser. Mat.*, **15** (1980), 219–232.
[32] V. Kostrykin and R. Schrader, The inverse scattering problem for metric graphs and the traveling salesman problem, Preprint, `arXiv:math-ph/0603010`, 2006.
[33] V. Kostrykin and R. Schrader, Kirchhoff's rule for quantum wires, *J. Phys. A*, **32** (1999), 595–630.
[34] M. G. Kreĭn, Theory of self-adjoint extensions of semi-bounded Hermitian operators and applications II, (Russian) *Mat. Sb. N. S.*, **21** (1947), 365–404.
[35] M. G. Kreĭn, Solution of the inverse Sturm-Liouville problem, (Russian) *Doklady Akad. Nauk SSSR (N.S.)*, **76** (1951), 21–24.
[36] 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** (1953), 405–408.
[37] M. G. Kreĭn, On determination of the potential of a particle from its S-function, (Russian) *Dokl. Akad. Nauk SSSR (N.S.),* **105** (1955), 433–436.
[38] P. Kurasov, Inverse problems for Aharonov-Bohm rings, *Math. Proc. Cambridge Philos. Soc.*, **148** (2010), 331–362.
[39] P. D. Lax and R. S. Phillips, *Scattering Theory*, Pure and Applied Mathematics, **26**. Academic Press, New York-London, 1967.
[40] N. Levinson, The inverse Sturm-Liouville problem, *Mat. Tidsskr. B.*, **1949** (1949), 25–30.
[41] M. S. Livshitz, On a certain class of linear operators in Hilbert space, *Rec. Math. [Mat. Sbornik] N.S.*, **19** (1946), 239–262.
[42] V. A. Marčenko, On reconstruction of the potential energy from phases of the scattered waves, (Russian) *Dokl. Akad. Nauk SSSR (N.S.)*, **104** (1955), 695–698.
[43] 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** (1976), 90–102, 204–205. Investigations on linear operators and the theory of functions, VII.
[44] S. N. Naboko, Functional model of perturbation theory and its applications to scattering theory, *Trudy Mat. Inst. Steklov.*, **147** (1980), 86–114, 203. Boundary Value Problems of Mathematical Physics, 10.
[45] S. N. Naboko, Nontangential boundary values of operator *R*-functions in a half-plane, *Algebra i Analiz*, **1** (1989), 197–222.
[46] 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*, Amer. Math. Soc., Providence, RI, **157** (1993), 127–149.
[47] B. S. Pavlov, Conditions for separation of the spectral components of a dissipative operator, *Izv. Akad. Nauk SSSR Ser. Mat.*, **39** (1975), 123–148, 240. English translation in: *Math. USSR Izvestija*, **9** (1975), 113–137.

[48] B. S. Pavlov, Dilation theory and the spectral analysis of non-selfadjoint differential operators, *Proc. 7th Winter School, Drogobych, 1974*, TsEMI, Moscow, 1976, 3–69. English translation: *Transl., II Ser., Am. Math. Soc.*, **115** (1981), 103–142.
[49] B. S. Pavlov, Selfadjoint dilation of a dissipative Schrödinger operator, and expansion in its eigenfunction, (Russian) *Mat. Sb. (N.S.)*, **102** (1977), 511–536, 631.
[50] D. B. Pearson, Conditions for the existence of the generalized wave operators, *J. Mathematical Phys.* **13** (1972), 1490–1499.
[51] M. Reed and B. Simon, *Methods of Modern Mathematical Physics. III*, Academic Press [Harcourt Brace Jovanovich Publishers], New York, 1979.
[52] 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.
[53] M. Rosenblum, Perturbation of the continuous spectrum and unitary equivalence, *Pacific J. Math.*, **7** (1957), 997–1010.
[54] V. Ryzhov. Functional model of a class of non-selfadjoint extensions of symmetric operators, In *Operator Theory, Analysis and Mathematical Physics*, **174** of *Oper. Theory Adv. Appl.*, Birkhäuser, Basel, (2007), 117–158.
[55] K. Schmüdgen, *Unbounded Self-Adjoint Operators on Hilbert Space*, Volume 265 of Graduate Texts in Mathematics. Springer, Dordrecht, 2012.
[56] 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.
[57] W. T. Tutte, *Graph theory. With a foreword by C. St. J. A. Nash-Williams,* Reprint of the 1984 original. Encyclopedia of Mathematics and its Applications, 21. Cambridge University Press, Cambridge, 2001.
[58] M. I. Višik, On general boundary problems for elliptic differential equations (Russian), *Trudy Moskov. Mat. Obšč.*, **86** (1952), 645–648.
[59] J. von Neumann, Über adjungierte Funktionaloperatoren, *Ann. Math.*, **33** (1932), 294–310.
[60] J. von Neumann, *Mathematical Foundations of Quantum Mechanics*, Princeton University Press, Princeton, 1955. Translated by Robert T. Beyer.
[61] R. Weder, Scattering theory for the matrix Schrödinger operator on the half line with general boundary conditions, *J. Math. Phys.*, **56** (2015), 092103, 24 pp.
[62] R. Weder, Trace formulas for the matrix Schrödinger operator on the half-line with general boundary conditions, *J. Math. Phys.*, **57** (2016), 112101, 11 pp.
[63] 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.
[64] 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.

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