THE INVERSE SCATTERING PROBLEM FOR METRIC GRAPHS AND THE TRAVELING SALESMAN PROBLEM

VADIM KOSTRYKIN AND ROBERT SCHRADER

Dedicated to Arthur Jaffe, Walter Schneider, and Roland Seneor on the occasion of their birthday celebration

ABSTRACT. We present a solution to the inverse scattering problem for differential Laplace operators on metric noncompact graphs. We prove that for almost all boundary conditions (i) the scattering matrix uniquely determines the graph and its metric structure, (ii) the boundary conditions are determined uniquely up to trivial gauge transformations. The main ingredient of our approach is a combinatorial Fourier expansion of the scattering matrix which encodes the topology of the graph into analytic properties of the scattering matrix. Using the technique developed in this work, we also propose an analytic approach to solving some combinatorial problems on graphs, in particular, the Traveling Salesman Problem.

CONTENTS

1. INTRODUCTION

The problem of reconstructing geometric objects like obstacles or manifolds from scattering data is a scattering-theoretic analogue of the famous question by M. Kac: *Can one hear the shape of a drum?* [39]. The question is whether an Euclidean domain (or more generally a compact Riemannian manifold) is determined by the spectrum of its Laplace-Beltrami operator. Although there are examples of isospectral (i.e. having the same eigenvalues with the same multiplicities) but non-isometric manifolds [27], up to now it is unknown whether Kac's question has an affirmative answer for "generic" manifolds. Another open question is how large the set of manifolds isospectral to a given manifold can be. In [67] Osgood, Phillips, and Sarnak proved that any isospectral class of two-dimensional domains is at most compact in an appropriate topology on domains. A number of further "affirmative" results are reviewed in [85].

The status of the inverse scattering problem is rather similar. We mention the following results.

Date: 21st February 2006.
2000 *Mathematics Subject Classification.* Primary 34B45, 05C35; Secondary 47A40.
Key words and phrases. Laplace operators on metric graphs; inverse problems; traveling salesman problem.

Inverse scattering problem for obstacles: Hassell and Zelditch [34] proved that the scattering phase (that is, a complex argument of the determinant of the scattering matrix) for the Dirichlet Laplace operator of an exterior domain in $\mathbb{R}^2$ with smooth boundary determines the obstacle up to a compact set of deformations.

Inverse scattering problem on noncompact Riemannian manifolds: An example of two non-isometric two-dimensional asymptotically Euclidean manifolds with the same scattering phase has been constructed by Brooks and Perry in [9].

Inverse scattering problem on compact Riemannian manifolds with infinitely thin horns: Brüning and Geyler proved in [10] that the spectrum of the Laplace operator on a low-dimensional compact Riemannian manifold is uniquely determined by the scattering matrix of the Laplace operator on this manifold with an attached semiline $\mathbb{R}_+$. Thus, the inverse scattering problem is reduced to "hearing the shape of a drum".

In the present work we address the inverse scattering problem for Laplace operators on *noncompact metric graphs* – one-dimensional noncompact piecewise linear spaces with singularities at the vertices, that is, non-smooth deformation retracts of smooth Riemannian manifolds. Alternatively, a noncompact metric graph is a metric space which can be written as a union of finitely many intervals, which are either compact or $[0, \infty)$; any two of these intervals are either disjoint or intersect only in one or both of their endpoints. The corresponding Laplace operator arises as a strong limit of Laplace-Beltrami operators on the approximating manifolds [17], [55], [56], [74], [75], [76]. A survey of results on Laplace operators on metric graphs can be found in [53] and [54].

The inverse problem consists of determining the graph, its metric structure (i.e. the lengths of its edges), and the boundary conditions at the vertices from the scattering matrix. It is known [8], [57] that in general neither the graph nor the boundary conditions can be determined uniquely from the scattering matrix. A similar situation occurs in the context of compact metric graphs (that is, unions of finitely many compact intervals): The articles [7], [28] provide examples of two different metric graphs such that the corresponding Laplace operators are isospectral.

Below we will prove, that for an arbitrary graph with *generic* metric structure and *generic* boundary conditions the inverse scattering problem has a unique solution. This is the main result of our work. Precise formulations will be presented in the next section.

The main technical ingredient of our approach to the solution of the inverse scattering problem is a combinatorial Fourier expansion of the scattering matrix (Theorems 5.2, 6.6, and 7.2 below). This expansion encodes the topology of the graph and its metric structure into analytic properties of the scattering matrix.

In [28] Gutkin and Smilansky have announced a different solution of the inverse scattering problem for graphs based on a relation between the scattering phase and lengths of all closed paths on the graph, a kind of Selberg-Gutzwiller formula [29]. A heuristic derivation of this relation has been presented by Kottos and Smilansky in [49] and [50]. The arguments in [28] seem to be applicable only to those boundary conditions which give rise to energy-independent single-vertex scattering matrices.

A solution of the inverse spectral problem for compact metric graphs has been recently given by Kurasov and Nowaczyk in [58]. This work gives a rigorous proof of the solution presented in [28]. Inverse spectral problems on finite trees have been studied in [6].

A different type of the inverse problem for Schrödinger operators on metric graphs (i.e., Laplace operators perturbed by a potential) had been solved in [24] using results obtained in [23]. In that work the graph as well as the boundary conditions were supposed to be known. We mention also the articles [32], [33], [70], and [84] devoted to determining the potentials from the spectrum of the Schrödinger operator on a given compact graph.

As an application of concepts and techniques developed in the present work, we will also propose an analytic approach to solving the symmetric Traveling Salesman Problem (TSP) as well as some other combinatorial problems. In particular, we reduce these problems to an analysis of the scattering matrix of a Laplace operator on the graph. However, it is too early to decide whether this approach may lead to an effective algorithm. Expository accounts of TSP can be found, e.g., in [3], [38], and [59]. The web pages [81] provide a large amount of information on the history of TSP as well as on-going research. Proofs of NP-completeness of TSP are given in [20], [68].

For other relations of Laplace operators on metric graphs to combinatorics we also mention the work [77] by Schanz and Smilansky, where some results of spectral analysis of Laplace operators on graphs have been applied to obtain combinatorial identities, as well as our recent work [46] on the calculation of the generating function of walks on graphs.

The article is organized as follows. In Section 2 we summarize the graph theory terminology used in the present work and describe the main results – Theorems 1 and 2. In Section 3 we will revisit the theory of (differential) Laplace operators on metric graphs for general boundary conditions at the vertices. An important case of local boundary conditions is discussed in detail in Section 4. Section 5 is devoted to the study of the scattering matrix as a function of the metric of the graph. In particular, we prove (Theorem 5.2) that the scattering matrix of the Laplace operator on a non-compact graph possesses an absolutely converging multidimensional Fourier expansion. In Section 6 we study walks on a non-compact graph, that is, sequences of edges with the property that any two successive edges have a common vertex. The main results of this section are given in Theorem 6.6, which expresses the Fourier coefficients as finite sums over walks with a given combinatorial length, and in Theorem 6.11, which relates the topology of the graph to analytic properties of the scattering matrix. Sections 7 and 8 are devoted to the proof of the main results of the present work. The two principal tools used in the proof of Theorem 1 are Theorems 7.2 and 7.6. The first result is of analytical nature and the second one is purely combinatorial. The main ingredient of the proof of Theorem 2 is Proposition 8.5. In Section 9 we treat TSP and some other combinatorial problems. The reader interested in TSP only, may skip Section 8.

Acknowledgments. The authors would like to thank M. Grötschel, M. Karowski, W. Klotz, H. Kurke, M. Schmidt, F. Sobieczky, and E. Vogt for helpful comments. One of the authors (R.S.) is indebted to the Theory Group of Microsoft Research for its kind hospitality during his stay in Redmond in the spring of 2004.

2. MAIN RESULTS

Before we turn to the description of the main results obtained in the present work, we summarize the graph theory terminology used below.

A finite noncompact graph is a 4-tuple $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$, where V is a finite set of *vertices*, $\mathcal{I}$ is a finite set of *internal edges*, $\mathcal{E}$ is a finite set of *external edges*. Elements in $\mathcal{I} \cup \mathcal{E}$ are called *edges*. The map ∂ assigns to each internal edge $i \in \mathcal{I}$ an ordered pair of (possibly equal) vertices $\partial(i) := \{v_1, v_2\}$ and to each external edge $e \in \mathcal{E}$ a single vertex v. The vertices $v_1 =: \partial^-(i)$ and $v_2 =: \partial^+(i)$ are called the *initial* and *terminal* vertex of the internal edge i, respectively. The vertex $v = \partial(e)$ is the initial vertex of the external edge e. We write $\partial(i) \doteq \{v_1, v_2\}$ if either $\partial(i) = \{v_1, v_2\}$ or $\partial(i) = \{v_2, v_1\}$. If $\partial(i) = \{v, v\}$, that is, $\partial^-(i) = \partial^+(i)$ then i is called a *tadpole*. A graph is called *compact* if $\mathcal{E} = \varnothing$, otherwise it is *noncompact*.

Two vertices v and v' are called *adjacent* if there is an internal edge $i \in \mathcal{I}$ such that $v \in \partial(i)$ and $v' \in \partial(i)$. A vertex v and the (internal or external) edge $j \in \mathcal{I} \cup \mathcal{E}$ are *incident* if $v \in \partial(j)$.

We do not require ∂ to be injective. In particular, any two vertices are allowed to be adjacent by more than one internal edge and two different external edges may be incident with the same vertex. If ∂ is injective and $\partial^-(i) \neq \partial^+(i)$ for all $i \in \mathcal{I}$, the graph $\mathcal{G}$ is called *simple*.[1]

[1] In a different terminology (see, e.g., [14]) compact graphs are called digraphs whereas simple compact graphs are designated as oriented graphs.

The *degree* $\deg(v)$ of the vertex v is defined as

$$\deg(v) = |\{e \in \mathcal{E} \mid \partial(e) = v\}| + |\{i \in \mathcal{I} \mid \partial^-(i) = v\}| + |\{i \in \mathcal{I} \mid \partial^+(i) = v\}|,$$

that is, it is the number of (internal or external) edges incident with the given vertex v by which every tadpole is counted twice. The minimum and the maximum degree of the graph $\mathcal{G}$ are defined as

$$\min_{v\in V} \deg(v) \qquad \text{and} \qquad \max_{v\in V} \deg(v),$$

respectively.

It is easy to extend the First Theorem of Graph Theory (see, e.g. [14]) to the case of noncompact graphs:

$$\sum_{v\in V} \deg(v) = |\mathcal{E}| + 2|\mathcal{I}|.$$

A vertex is called a *boundary vertex* if it is incident with some external edge. The set of all boundary vertices will be denoted by ∂V. The vertices not in ∂V, that is in $V \setminus \partial V$ are called *internal vertices*.

The compact graph $\mathcal{G}_{\mathrm{int}} = (V, \mathcal{I}, \emptyset, \partial|_{\mathcal{I}})$ will be called the *interior* of the graph $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$. It is obtained from $\mathcal{G}$ by eliminating the external edges. Similarly, the graph $\mathcal{G}_{\mathrm{ext}} = (\partial V, \emptyset, \mathcal{E}, \partial|_{\mathcal{E}})$ will be called the *exterior* of the graph $\mathcal{G}$. It is obtained from $\mathcal{G}$ by eliminating all its internal edges.

Let $\mathcal{S}(v) \subseteq \mathcal{E} \cup \mathcal{I}$ denote the *star graph* of the vertex $v \in V$, i.e., the set of the edges adjacent to v. Also, by $\mathcal{S}_-(v)$ (respectively $\mathcal{S}_+(v)$) we denote the set of the edges for which v is the initial vertex (respectively terminal vertex). Obviously, $\mathcal{S}_+(v) \cap \mathcal{S}_-(v) = \emptyset$ if $\mathcal{G}$ does not contain tadpoles.

We will endow the graph with the following metric structure. Any internal edge $i \in \mathcal{I}$ will be associated with an interval $[0, a_i]$ with $a_i > 0$ such that the initial vertex of i corresponds to $x = 0$ and the terminal one - to $x = a_i$. Any external edge $e \in \mathcal{E}$ will be associated with a semiline $[0, +\infty)$. We call the number a_i the length of the internal edge i. The set of lengths $\{a_i\}_{i\in\mathcal{I}}$, which will also be treated as an element of $\mathbb{R}^{|\mathcal{I}|}$, will be denoted by $\underline{a}$. The map $\mathcal{I} \to \underline{a}$ can be seen as a positive weight on the interior $\mathcal{G}_{\mathrm{int}}$ of the graph $\mathcal{G}$. A compact or noncompact graph $\mathcal{G}$ endowed with a metric structure is called a *metric graph* $(\mathcal{G}, \underline{a})$. In a different terminology compact metric graphs are called *positively weighted graphs* or *networks* (see, e.g., [38]).

To define a (differential) Laplace operator on the metric graph $(\mathcal{G}, \underline{a})$ consider the family $\psi = \{\psi_j\}_{j\in\mathcal{E}\cup\mathcal{I}}$ of complex valued functions ψ_j defined on $[0, \infty)$ if $j \in \mathcal{E}$ and on $[0, a_j]$ if $j \in \mathcal{I}$. The Laplace operator is defined as

$$(\Delta(A, B, \underline{a})\psi)_j(x) = \frac{d^2}{dx^2}\psi_j(x), \qquad j \in \mathcal{I} \cup \mathcal{E} \tag{2.1}$$

with the boundary conditions

$$A\underline{\psi} + B\underline{\psi}' = 0 \tag{2.2}$$

where

$$\underline{\psi} = \begin{pmatrix} \{\psi_e(0)\}_{e\in\mathcal{E}} \\ \{\psi_i(0)\}_{i\in\mathcal{I}} \\ \{\psi_i(a_i)\}_{i\in\mathcal{I}} \end{pmatrix}, \qquad \underline{\psi}' = \begin{pmatrix} \{\psi_e'(0)\}_{e\in\mathcal{E}} \\ \{\psi_i'(0)\}_{i\in\mathcal{I}} \\ \{-\psi_i'(a_i)\}_{i\in\mathcal{I}} \end{pmatrix}, \tag{2.3}$$

A and B are $(|\mathcal{E}| + 2|\mathcal{I}|) \times (|\mathcal{E}| + 2|\mathcal{I}|)$ matrices. The operator $\Delta(A, B, \underline{a})$ is self-adjoint if and only if the matrix (A, B) has maximal rank and the matrix $AB^\dagger$ is Hermitian [42]. Here and in what follows (A, B) will denote the $(|\mathcal{E}| + 2|\mathcal{I}|) \times 2(|\mathcal{E}| + 2|\mathcal{I}|)$ matrix, where A and B are put next to each other. Boundary conditions (A, B) and (A', B') define the same operator $\Delta(A, B, \underline{a}) = \Delta(A', B', \underline{a})$ if and only if the unitary matrices

$$\mathfrak{S}(A, B) = -(A + \mathrm{i}B)^{-1}(A - \mathrm{i}B) \qquad \text{and} \qquad \mathfrak{S}(A', B') = -(A' + \mathrm{i}B')^{-1}(A' - \mathrm{i}B')$$

coincide (see Proposition 3.7 below). Conversely, any unitary matrix $\mathfrak{S} \in \mathsf{U}(|\mathcal{E}| + 2|\mathcal{I}|)$ defines a self-adjoint Laplace operator corresponding to boundary conditions (2.2) with $A = \mathbb{I} + \mathfrak{S}$ and $B = -\mathrm{i}(\mathbb{I} - \mathfrak{S})$. Thus, the set of all Laplace operators on a graph $\mathcal{G}$ is uniquely parametrized by elements of the unitary group $\mathsf{U}(|\mathcal{E}| + 2|\mathcal{I}|)$.

Recall (see [42] and [45]) that the boundary conditions are called local if they couple only those boundary values of ψ and of its derivative ψ' which belong to the same vertex. The precise definition will be given in Section 4 below (Definition 4.2). The set of all local boundary conditions on a graph $\mathcal{G}$ is isomorphic to the Lie group

$$\mathsf{U}_{\mathcal{G}} = \bigtimes_{v\in V} \mathsf{U}(\deg(v)),$$

where $\mathsf{U}(n)$ is the group of all unitary transformations of $\mathbb{C}^n$. The Haar measure on $\mathsf{U}(n)$ induces a Haar measure on $\mathsf{U}_{\mathcal{G}}$. The statement that a property holds "for Haar almost all local boundary conditions" means that there is a subset $\mathcal{U} \subset \mathsf{U}_{\mathcal{G}}$ of full Haar measure such that this property holds for all boundary conditions (A, B) with $\mathfrak{S}(A, B) \in \mathcal{U}$ (see Definition 6.10 below).

We start with a discussion of the main results obtained in the present work with the formulation of the main assumptions made below. We split them into two groups.

Assumption 1 (topological properties)**.** *The graph $\mathcal{G}$ possesses the following properties:*

(i) *$\mathcal{G}$ is connected, i.e., for any $v, v' \in V$ there is an ordered sequence $\{v_1 = v, v_2, \ldots, v_n = v'\}$ such that any two successive vertices in this sequence are adjacent. In particular, this implies that any vertex of the graph $\mathcal{G}$ has nonzero degree, i.e., for any vertex there is at least one edge with which it is incident.*

(ii) *$|\mathcal{E}| \geq 1$, i.e., the graph has at least one external edge.*

(iii) *The graph has no tadpoles, i.e., for no edge its initial and terminal vertex coincide.*

Assumption 2 (metric property)**.** *The lengths a_i $(i \in \mathcal{I})$ of the internal edges of the graph $\mathcal{G}$ are rationally independent, i.e., the equation*

$$\sum_{i\in\mathcal{I}} n_i\, a_i = 0 \tag{2.4}$$

with integer *$n_i \in \mathbb{Z}$ has no non-trivial solution.*

Let $S(\mathsf{k}; A, B, \underline{a})$ denote the scattering matrix at the energy $E = \mathsf{k}^2 > 0$ associated with the Laplace operator $\Delta(A, B, \underline{a})$ on the metric graph $(\mathcal{G}, \underline{a})$ (see Subsection 3.1 below). It is an $|\mathcal{E}| \times |\mathcal{E}|$ unitary matrix indexed by the elements of $\mathcal{E}$. Its diagonal elements are reflection amplitudes while the off-diagonal elements are transmission amplitudes for the incoming plane wave $\mathrm{e}^{-\mathrm{i}\mathsf{k}x}$.

Theorem 1. *Let the metric graph $(\mathcal{G}, \underline{a})$ satisfy Assumptions 1 and 2. Then for any external edge $e \in \mathcal{E}$ the map*

$$(\mathcal{G}_{\mathrm{int}}, \partial(e), \underline{a}) \mapsto [S(\cdot; A, B, \underline{a})]_{e,e}$$

is injective for Haar almost all local boundary conditions (A, B). Furthermore, for any given $e \in \mathcal{E}$ the maps

$$(\mathcal{G}, \underline{a}) \mapsto \left\{[S(\cdot; A, B, \underline{a})]_{e,e'}\right\}_{e'\in\mathcal{E}} \qquad \textit{and} \qquad (\mathcal{G}, \underline{a}) \mapsto \left\{[S(\cdot; A, B, \underline{a})]_{e',e}\right\}_{e'\in\mathcal{E}}$$

are also injective for Haar almost all local boundary conditions (A, B).

Theorem 1 claims that it suffices to know one reflection amplitude for all $\mathsf{k} > 0$ in order to determine the sets $V, \mathcal{I}$, the map $\partial|_{\mathcal{I}}$ and, thus, the interior $\mathcal{G}_{\mathrm{int}} = (V, \mathcal{I}, \varnothing, \partial|_{\mathcal{I}})$ of the graph $\mathcal{G}$ as well as the metric $\underline{a}$ and the vertex $\partial(e)$. Furthermore, if under otherwise the same assumptions one entire row or one entire column of $S(\mathsf{k}; A, B, \underline{a})$ is known for all $\mathsf{k} > 0$, then all boundary vertices are uniquely determined.

Note that "experimentally" one may only obtain the transmission and the reflection probabilities – the absolute squares of the transmission and reflection amplitudes – and not the transmission and reflection amplitudes themselves. However, as argued in [43], the missing phases may be obtained by additional "experiments".

Although we do not formulate it as a conjecture, based on our discussion below we expect that Theorem 1 remains valid under the much less stringent condition replacing Assumption 2: *There is no solution to* (2.4) *with* $|n_i| \leq N$ *for a suitable integer* N *depending on the graph* $\mathcal{G}$.

The following theorem implies that the boundary conditions can also be determined from the scattering matrix.

Theorem 2. *Let the metric graph* $(\mathcal{G}, \underline{a})$ *satisfy Assumptions 1 and 2. Then for Haar almost all local boundary conditions* (A, B) *on the graph* $\mathcal{G}$ *the map*

$$\mathfrak{S}(A, B) \mapsto S(\cdot; A, B, \underline{a})$$

is injective up to trivial gauge transformations.

The notion of *trivial gauge transformations* is introduced in Definition 8.1. Such transformations correspond to perturbations of the Laplace operator by vanishing magnetic potentials [45].

In other words, Theorem 2 states that for Haar almost all boundary conditions (A, B) on the metric graph $\mathcal{G}$ the equality $S(\mathsf{k}; A, B, \underline{a}) = S(\mathsf{k}; A', B', \underline{a})$ for all $\mathsf{k} > 0$ implies that the operators $\Delta(A, B, \underline{a})$ and $\Delta(A', B', \underline{a})$ agree up to trivial gauge transformations. A partial reconstruction of the boundary conditions from the spectrum of Laplace operator on compact metric graphs has been discussed earlier in [11] and [28].

The proof of Theorems 1 and 2 will be given in Sections 7 and 8, respectively.

By Theorem 3.12 below the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ is a meromorphic function in the complex k-plane. Therefore, we have the immediate

Corollary 3. *The function* $\mathbb{R}_+ \ni \mathsf{k} \mapsto S(\mathsf{k}; A; B; \underline{a})$ *in Theorems 1 and 2 can be replaced by* $\{S(\mathsf{k}_n; A; B; \underline{a})\}_{n \in \mathbb{N}_0}$*, where* $\mathsf{k}_n > 0$ *is an arbitrary sequence with at least one finite accumulation point different from zero.*

3. Laplace Operators and Scattering Matrices on Metric Graphs

In this section we revisit the theory of Laplace operators on a metric graph $\mathcal{G}$ and the resulting scattering theory. A large portion of the material presented in this section is borrowed from our preceding papers [42], [43], [44].

Given a finite noncompact graph $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ and a metric structure $\underline{a} = \{a_i\}_{i \in \mathcal{I}}$ consider the Hilbert space

$$\mathcal{H} \equiv \mathcal{H}(\mathcal{E}, \mathcal{I}, \underline{a}) = \mathcal{H}_{\mathcal{E}} \oplus \mathcal{H}_{\mathcal{I}}, \qquad \mathcal{H}_{\mathcal{E}} = \bigoplus_{e \in \mathcal{E}} \mathcal{H}_e, \qquad \mathcal{H}_{\mathcal{I}} = \bigoplus_{i \in \mathcal{I}} \mathcal{H}_i, \tag{3.1}$$

where $\mathcal{H}_e = L^2([0, \infty))$ for all $e \in \mathcal{E}$ and $\mathcal{H}_i = L^2([0, a_i])$ for all $i \in \mathcal{I}$.

By $\mathcal{D}_j$ with $j \in \mathcal{E} \cup \mathcal{I}$ denote the set of all $\psi_j \in \mathcal{H}_j$ such that $\psi_j(x)$ and its derivative $\psi_j'(x)$ are absolutely continuous and $\psi_j''(x)$ is square integrable. Let $\mathcal{D}_j^0$ denote the set of those elements $\psi_j \in \mathcal{D}_j$ which satisfy

$$\begin{array}{l} \psi_j(0) = 0 \\ \psi_j'(0) = 0 \end{array} \quad \text{for} \quad j \in \mathcal{E} \qquad \text{and} \qquad \begin{array}{l} \psi_j(0) = \psi_j(a_j) = 0 \\ \psi_j'(0) = \psi_j'(a_j) = 0 \end{array} \quad \text{for} \quad j \in \mathcal{I}.$$

Let Δ^0 be the differential operator

$$\left(\Delta^0 \psi\right)_j(x) = \frac{d^2}{dx^2} \psi_j(x), \qquad j \in \mathcal{I} \cup \mathcal{E} \tag{3.2}$$

with domain

$$\mathcal{D}^0 = \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} \mathcal{D}_j^0 \subset \mathcal{H}.$$

It is straightforward to verify that Δ^0 is a closed symmetric operator with deficiency indices equal to $|\mathcal{E}| + 2|\mathcal{I}|$.

We introduce an auxiliary finite-dimensional Hilbert space

$$\mathcal{K} \equiv \mathcal{K}(\mathcal{E},\mathcal{I}) = \mathcal{K}_{\mathcal{E}} \oplus \mathcal{K}_{\mathcal{I}}^{(-)} \oplus \mathcal{K}_{\mathcal{I}}^{(+)} \tag{3.3}$$

with $\mathcal{K}_{\mathcal{E}} \cong \mathbb{C}^{|\mathcal{E}|}$ and $\mathcal{K}_{\mathcal{I}}^{(\pm)} \cong \mathbb{C}^{|\mathcal{I}|}$. Let ${}^d\mathcal{K}$ denote the "double" of $\mathcal{K}$, that is, ${}^d\mathcal{K} = \mathcal{K} \oplus \mathcal{K}$.

For any $\psi \in \mathcal{D} := \bigoplus_{j\in\mathcal{E}\cup\mathcal{I}} \mathcal{D}_j$ we set

$$[\psi] := \underline{\psi} \oplus \underline{\psi}' \in {}^d\mathcal{K}, \tag{3.4}$$

with $\underline{\psi}$ and $\underline{\psi}'$ defined in (2.3).

Let J be the canonical symplectic matrix on ${}^d\mathcal{K}$,

$$J = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix} \tag{3.5}$$

with $\mathbb{I}$ the identity operator on $\mathcal{K}$. Consider the non-degenerate Hermitian symplectic form

$$\omega([\phi],[\psi]) := \langle [\phi], J[\psi]\rangle, \tag{3.6}$$

where $\langle\cdot,\cdot\rangle$ denotes the scalar product in ${}^d\mathcal{K} \cong \mathbb{C}^{2(|\mathcal{E}|+2|\mathcal{I}|)}$. Note that the Hermitian symplectic form ω differs from the standard (Euclidean) symplectic form [4], [60].

Recall that a linear subspace $\mathcal{M}$ of ${}^d\mathcal{K}$ is called *isotropic* if the form ω vanishes on $\mathcal{M}$ identically. An isotropic subspace is called *maximal* if it is not a proper subspace of a larger isotropic subspace. Every maximal isotropic subspace has complex dimension equal to $|\mathcal{E}| + 2|\mathcal{I}|$.

If $\mathcal{M}$ is a maximal isotropic subspace, then its orthogonal complement $\mathcal{M}^\perp$ (with respect to the scalar product $\langle\cdot,\cdot\rangle$) is also maximal isotropic. Moreover, as in the standard symplectic theory we have the following result (see [42, Lemma 2.1]):

Lemma 3.1. *An isotropic subspace $\mathcal{M} \subset {}^d\mathcal{K} \cong \mathbb{C}^{2(|\mathcal{E}|+2|\mathcal{I}|)}$ is maximal if and only if $\mathcal{M}^\perp = J\mathcal{M}$ such that the orthogonal decomposition*

$${}^d\mathcal{K} = \mathcal{M} \oplus J\mathcal{M} \tag{3.7}$$

holds.

By the symplectic extension theory of symmetric operators on a Hilbert space (see, e.g., [1], [12], [16], [37], [65], [69]) there is a one-to-one correspondence between all self-adjoint extensions of Δ^0 and maximal isotropic subspaces of ${}^d\mathcal{K}$. In explicit terms, any self-adjoint extension of Δ^0 is the differential operator defined by (3.2) with domain

$$\operatorname{Dom}(\Delta) = \{\psi \in \mathcal{D} |\ [\psi] \in \mathcal{M}\}, \tag{3.8}$$

where $\mathcal{M}$ is a maximal isotropic subspace of ${}^d\mathcal{K}$. Conversely, any maximal isotropic subspace $\mathcal{M}$ of ${}^d\mathcal{K}$ defines through (3.8) a self-adjoint operator $\Delta(\mathcal{M},\underline{a})$. If $\mathcal{I} = \varnothing$, we will simply write $\Delta(\mathcal{M})$. In the sequel we will call the operator $\Delta(\mathcal{M},\underline{a})$ a Laplace operator on the metric graph $(\mathcal{G},\underline{a})$.

Let A and B be linear maps of $\mathcal{K}$ onto itself. By (A,B) we denote the linear map from ${}^d\mathcal{K} = \mathcal{K}\oplus\mathcal{K}$ to $\mathcal{K}$ defined by the relation

$$(A,B)\ (\chi_1 \oplus \chi_2) := A\,\chi_1 + B\,\chi_2,$$

where $\chi_1,\chi_2 \in \mathcal{K}$. Set

$$\mathcal{M}(A,B) := \operatorname{Ker}(A,B). \tag{3.9}$$

Theorem 3.2. *A subspace $\mathcal{M} \subset {}^d\mathcal{K}$ is maximal isotropic if and only if there exist linear maps $A, B: \mathcal{K} \to \mathcal{K}$ such that $\mathcal{M} = \mathcal{M}(A,B)$ and*

$$\begin{aligned} &\text{(i) the map } (A,B): {}^d\mathcal{K} \to \mathcal{K} \text{ has maximal rank equal to } |\mathcal{E}| + 2|\mathcal{I}|,\\ &\text{(ii) } AB^\dagger \text{ is self-adjoint, } AB^\dagger = BA^\dagger. \end{aligned} \tag{3.10}$$

For the proof we refer to [42]. We note that Theorem 4 in Section 125 of [1] presents an analogous result for differential operators of even order on a compact interval.

By direct calculations one can easily verify the equality

$$J\mathcal{M}(A,B) = \mathcal{M}(B,-A),$$

which by Lemma 3.1 implies the following result.

Lemma 3.3. *A subspace $\mathcal{M}(A,B) \subset {}^d\mathcal{K}$ is maximal isotropic if and only if*

$$\mathcal{M}(A,B)^\perp = \mathcal{M}(B,-A). \tag{3.11}$$

We mention also the equalities

$$\begin{aligned} \mathcal{M}(A,B)^\perp &= \big[\mathrm{Ker}\,(A,B)\big]^\perp = \mathrm{Ran}\,(A,B)^\dagger,\\ \mathcal{M}(A,B) &= \mathrm{Ran}(-B,A)^\dagger. \end{aligned} \tag{3.12}$$

In the terminology of symplectic geometry (see, e.g., Section 2.3 in [60]) equalities (3.12) have the following interpretation: The matrix $(A,B)^\dagger$ is a (Lagrangian) *frame* for $\mathcal{M}(A,B)^\perp$ and the matrix $(-B,A)^\dagger$ is a frame for $\mathcal{M}(A,B)$.

Lemma 3.4. *If (A,B) satisfies* (3.10)*, then*

(i) $\mathrm{Ker}\, A \perp \mathrm{Ker}\, B$,
(ii) $\mathrm{Ker}\, A^\dagger \cap \mathrm{Ker}\, B^\dagger = \{0\}$.

Proof. (i). Choose arbitrary $\chi_1 \in \mathrm{Ker}\, A$ and $\chi_2 \in \mathrm{Ker}\, B$. For any complex number c we have

$$\begin{pmatrix} \chi_1 \\ c\chi_2 \end{pmatrix} \in \mathcal{M}(A,B) \qquad \text{and} \qquad \begin{pmatrix} c\chi_2 \\ \chi_1 \end{pmatrix} \in \mathcal{M}(B,-A).$$

From (3.11) it follows that

$$\left\langle \begin{pmatrix} \chi_1 \\ c\chi_2 \end{pmatrix}, \begin{pmatrix} c\chi_2 \\ \chi_1 \end{pmatrix} \right\rangle = 0.$$

Hence, $\mathrm{Re}\, c\langle \chi_1, \chi_2\rangle_{\mathcal{K}} = 0$ for all $c \in \mathbb{C}$ which implies that $\langle \chi_1, \chi_2\rangle_{\mathcal{K}} = 0$.

(ii). Since the linear map $\begin{pmatrix} A^\dagger \\ B^\dagger \end{pmatrix} = (A,B)^\dagger : \mathcal{K} \to {}^d\mathcal{K}$ has maximal rank equal to $|\mathcal{E}| + 2|\mathcal{I}|$, it follows that $\mathrm{Ker} \begin{pmatrix} A^\dagger \\ B^\dagger \end{pmatrix} = \{0\}$. Noting that $\mathrm{Ker} \begin{pmatrix} A^\dagger \\ B^\dagger \end{pmatrix} = \mathrm{Ker}\, A^\dagger \cap \mathrm{Ker}\, B^\dagger$ completes the proof. □

Definition 3.5. *The boundary conditions (A,B) and (A',B') satisfying* (3.10) *are equivalent if the corresponding maximal isotropic subspaces coincide, that is, $\mathcal{M}(A,B) = \mathcal{M}(A',B')$.*

Proposition 3.6. *The boundary conditions (A,B) and (A',B') satisfying* (3.10) *are equivalent if and only if there is an invertible map $C: \mathcal{K} \to \mathcal{K}$ such that $A' = CA$ and $B' = CB$.*

Proof. The "if" part is obvious. To prove the "only if" part assume that $\mathcal{M}(A,B) = \mathcal{M}(A',B')$. This equality is equivalent to the condition

$$\mathrm{Ker}\,\big(A,B\big) = \mathrm{Ker}\,\big(A',B'\big).$$

But this condition holds if and only if there is an invertible C such that $A' = CA$ and $B' = CB$. □

Denote by $\Delta(A, B, \underline{a})$ the Laplace operator corresponding to the maximal isotropic subspace $\mathcal{M}(A, B)$, that is, $\Delta(A, B, \underline{a}) := \Delta(\mathcal{M}(A, B), \underline{a})$. If $\mathcal{I} = \emptyset$, we will simply write $\Delta(A, B)$. From the discussion above it follows immediately that any self-adjoint Laplace operator on $\mathcal{H}$ equals $\Delta(A, B, \underline{a})$ for some A and B satisfying (3.10). Moreover, $\Delta(A, B, \underline{a}) = \Delta(A', B', \underline{a})$ if and only if $\mathcal{M}(A, B) = \mathcal{M}(A', B')$. From Theorem 3.2 it follows that the domain of the Laplace operator $\Delta(A, B, \underline{a})$ consists of the functions $\psi \in \mathcal{D}$ satisfying the boundary conditions

$$A\underline{\psi} + B\underline{\psi}' = 0, \tag{3.13}$$

where $\underline{\psi}$ and $\underline{\psi}'$ are defined by (2.3).

By comparing $\Delta(\mathcal{M}, \underline{a})$ with the Laplace operators constructed from Δ^0 by means of the von Neumann extension theory one immediately concludes that the manifold of all maximal isotropic subspaces (Lagrangian Grassmannian) is isomorphic to the unitary group $\mathsf{U}(|\mathcal{E}| + 2|\mathcal{I}|)$ of all $(|\mathcal{E}| + 2|\mathcal{I}|) \times (|\mathcal{E}| + 2|\mathcal{I}|)$ matrices, a result contained in [43].

Proposition 3.7. *A subspace $\mathcal{M}(A, B) \subset {}^d\mathcal{K}$ is maximal isotropic if and only if for an arbitrary $\mathsf{k} \in \mathbb{R} \setminus \{0\}$ the operator $A + \mathrm{i}\mathsf{k}B$ is invertible and*

$$\mathfrak{S}(\mathsf{k}; A, B) := -(A + \mathrm{i}\mathsf{k}B)^{-1}(A - \mathrm{i}\mathsf{k}B) \tag{3.14}$$

is unitary. Moreover, given any $\mathsf{k} \in \mathbb{R} \setminus \{0\}$ the correspondence between maximal isotropic subspaces $\mathcal{M} \subset {}^d\mathcal{K}$ and unitary operators $\mathfrak{S}(\mathsf{k}; A, B) \in \mathsf{U}(|\mathcal{E}| + 2|\mathcal{I}|)$ on $\mathcal{K}$ is one-to-one.

A symplectic theory proof of this fact has been recently given by Arnold [5] and Harmer [30]. For reader's convenience we present here an alternative rather elementary proof of this proposition.

Proof. The "if" part. Assume that the operator $A + \mathrm{i}\mathsf{k}B$ is invertible and (3.14) is unitary. Using $\mathfrak{S}^\dagger = \mathfrak{S}^{-1}$ we obtain that $\mathrm{Im}\,(AB^\dagger) = 0$, that is, $AB^\dagger$ is self-adjoint. By (i) of Lemma 3.4

$$\mathrm{Rank}\,(A, B) = \dim \mathcal{K} - \dim(\mathrm{Ker}\ A \cap \mathrm{Ker}\ B) = \dim \mathcal{K}$$

is maximal. By Theorem 3.2 this proves that $\mathcal{M}(A, B)$ is maximal isotropic.

The "only if" part is proven in [42]. We recall the arguments. Assume that $\mathcal{M}(A, B) \subset {}^d\mathcal{K}$ is maximal isotropic. Then, by Theorem 3.2, (A, B) satisfies (3.10). Assume that $\mathrm{Ker}(A + \mathrm{i}\mathsf{k}B) \neq \{0\}$. Then there is a $\chi \in \mathcal{K}$ such that $(A^\dagger - \mathrm{i}\mathsf{k}B^\dagger)\chi = 0$. In particular, we have

$$\langle (A^\dagger - \mathrm{i}\mathsf{k}B^\dagger)\chi, (A^\dagger - \mathrm{i}\mathsf{k}B^\dagger)\chi \rangle = 0.$$

By Theorem 3.2 this implies that

$$\langle \chi, AA^\dagger \chi \rangle + \mathsf{k}^2 \langle \chi, BB^\dagger \chi \rangle = 0.$$

Hence, $\chi \in \mathrm{Ker}\, A^\dagger \cap \mathrm{Ker}\, B^\dagger$. Applying (ii) of Lemma 3.4 we obtain $\chi = 0$. Thus, $A + \mathrm{i}\mathsf{k}B$ is invertible. To prove the unitarity of $\mathfrak{S}(\mathsf{k}; A, B)$ we observe that

$$(A \pm \mathrm{i}\mathsf{k}B)^{-1} = (A^\dagger \mp \mathrm{i}\mathsf{k}B^\dagger)(AA^\dagger + \mathsf{k}^2 BB^\dagger)^{-1}.$$

Combining this with (3.14) we obtain

$$\mathfrak{S}(\mathsf{k}; A, B)\mathfrak{S}(\mathsf{k}; A, B)^\dagger = \mathfrak{S}(\mathsf{k}; A, B)^\dagger \mathfrak{S}(\mathsf{k}; A, B) = \mathbb{I}.$$

To prove that for given $\mathsf{k} > 0$ the correspondence between maximal isotropic subspaces $\mathcal{M} \subset {}^d\mathcal{K}$ and unitary matrices $\mathfrak{S} \in \mathsf{U}(|\mathcal{E}| + 2|\mathcal{I}|)$ given by (3.14) is one-to-one, first we show that the map $\mathcal{M} \mapsto \mathfrak{S}$ is surjective. Given an arbitrary $\mathfrak{S} \in \mathsf{U}(|\mathcal{E}| + 2|\mathcal{I}|)$ we set

$$A_{\mathfrak{S}} = -\frac{1}{2}(\mathfrak{S} - \mathbb{I}), \qquad B_{\mathfrak{S}} = \frac{1}{2\mathrm{i}\mathsf{k}}(\mathfrak{S} + \mathbb{I}) \tag{3.15}$$

such that $-(A_{\mathfrak{S}} + \mathrm{i}\mathsf{k}B_{\mathfrak{S}})^{-1}(A_{\mathfrak{S}} - \mathrm{i}\mathsf{k}B_{\mathfrak{S}}) = \mathfrak{S}$. Obviously,

$$A_{\mathfrak{S}} B_{\mathfrak{S}}^\dagger = \frac{1}{2\mathsf{k}}\mathrm{Im}\ \mathfrak{S} \equiv \frac{1}{4\mathrm{i}\mathsf{k}}(\mathfrak{S} - \mathfrak{S}^\dagger) \tag{3.16}$$

is self-adjoint. Since $\mathrm{Ker}\, A_{\mathfrak{S}} \cap \mathrm{Ker}\, B_{\mathfrak{S}} = \{0\}$, the map $(A_{\mathfrak{S}}, B_{\mathfrak{S}})$ has maximal rank. By Theorem 3.2 this proves that $\mathcal{M}(A_{\mathfrak{S}}, B_{\mathfrak{S}})$ is maximal isotropic.

To prove the injectivity by Proposition 3.6 it suffices to show that given an arbitrary $\mathfrak{S} \in \mathsf{U}(|\mathcal{E}| + 2|\mathcal{I}|)$ for any map (A, B) satisfying (3.10) and such that

$$\mathfrak{S}(\mathsf{k}; A, B) = \mathfrak{S} \tag{3.17}$$

there is an invertible map $C : \mathcal{K} \to \mathcal{K}$ such that

$$A = CA_{\mathfrak{S}} \qquad \text{and} \qquad B = CB_{\mathfrak{S}},$$

or, equivalently,

$$A = -\frac{1}{2}C(\mathfrak{S} - \mathbb{I}) \quad \text{and} \quad B = \frac{1}{2\mathsf{ik}}C(\mathfrak{S} + \mathbb{I}).$$

Using (3.17) these relations can equivalently be written as

$$A = C(A + \mathsf{ik}B)^{-1}A \quad \text{and} \quad B = C(A + \mathsf{ik}B)^{-1}B.$$

Thus,

$$C = A + \mathsf{ik}B,$$

which is invertible. □

Remark 3.8. *There are several results in the literature related to Proposition 3.7 (see* [41] *and references quoted therein).*

Due to Proposition 3.7, given an arbitrary maximal isotropic subspace $\mathcal{M} \subset {}^d\mathcal{K}$, we will write $\mathfrak{S}(\mathsf{k}; \mathcal{M})$ for $\mathfrak{S}(\mathsf{k}; A_{\mathcal{M}}, B_{\mathcal{M}})$ with $(A_{\mathcal{M}}, B_{\mathcal{M}})$ an arbitrary map satisfying (3.10) such that $\mathrm{Ker}(A_{\mathcal{M}}, B_{\mathcal{M}}) = \mathcal{M}$.

From (3.11) and Proposition 3.7 it follows that

$$\mathfrak{S}(\mathsf{k}; \mathcal{M}) = -\mathfrak{S}(\mathsf{k}^{-1}; \mathcal{M}^{\perp}). \tag{3.18}$$

From (3.14) it follows that

$$\mathfrak{S}(\mathsf{k}; AU, BU) = U^{\dagger}\mathfrak{S}(\mathsf{k}; A, B)U. \tag{3.19}$$

for arbitrary $U \in \mathsf{U}(|\mathcal{E}|+2|\mathcal{I}|)$. We cast this relation into the following form. Let ${}^dU : {}^d\mathcal{K} \to {}^d\mathcal{K}$ denote the "double" of U,

$${}^dU = \begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix}. \tag{3.20}$$

Since ${}^dU^{\dagger} J\, {}^dU = J$, the transformation ${}^dU$ leaves the Hermitian symplectic structure invariant. Therefore, if $\mathcal{M}$ is maximal isotropic, then so is ${}^dU\mathcal{M}$. Furthermore, by (3.9) we have

$${}^dU\mathcal{M}(A, B) = \mathcal{M}(AU^{\dagger}, BU^{\dagger}).$$

Combining this equality with (3.19) gives that

$$\mathfrak{S}(\mathsf{k}\,;\, {}^dU\mathcal{M}) = U\mathfrak{S}(\mathsf{k}\,; \mathcal{M})U^{\dagger} \tag{3.21}$$

holds for any maximal isotropic space $\mathcal{M}$ and any unitary U.

From (3.14) we obtain that the matrix $\mathfrak{S}(\mathsf{k}; A, B)$ for an arbitrary $\mathsf{k} \in \mathbb{R} \setminus \{0\}$ can be obtained from $\mathfrak{S}(\mathsf{k}_0; A, B)$ with $\mathsf{k}_0 \in \mathbb{R} \setminus \{0\}$ via

$$\mathfrak{S}(\mathsf{k}; A, B) = \big((\mathsf{k} - \mathsf{k}_0)\mathfrak{S}(\mathsf{k}_0; A, B) + (\mathsf{k} + \mathsf{k}_0)\big)^{-1}\big((\mathsf{k} + \mathsf{k}_0)\mathfrak{S}(\mathsf{k}_0; A, B) + (\mathsf{k} - \mathsf{k}_0)\big). \tag{3.22}$$

Note that for all $\mathsf{k} \in \mathbb{R} \setminus \{0, \mathsf{k}_0\}$ the inequality $|(\mathsf{k} + \mathsf{k}_0)/(\mathsf{k} - \mathsf{k}_0)| \neq 1$ holds such that $((\mathsf{k} - \mathsf{k}_0)\mathfrak{S}(\mathsf{k}_0; A, B) + (\mathsf{k} + \mathsf{k}_0))$ is invertible.

The relation (3.22) implies the somewhat surprising fact that the operators $\mathfrak{S}(\mathsf{k}; A, B)$ for different k form a commuting family, i.e.,

$$[\mathfrak{S}(\mathsf{k}_1; A, B), \mathfrak{S}(\mathsf{k}_2; A, B)] = 0 \quad \text{for all} \quad \mathsf{k}_1, \mathsf{k}_2 \in \mathbb{R} \setminus \{0\}, \tag{3.23}$$

where $[\cdot, \cdot]$ denotes the commutator.

Remark 3.9. *The matrix $\mathfrak{S}(\mathsf{k}; A, B)$ is k-independent if and only if $\mathfrak{S}(\mathsf{k}; A, B)$ is self-adjoint for at least one $\mathsf{k} > 0$ and, thus, for all $\mathsf{k} > 0$. Indeed, assume that $\mathfrak{S}(\mathsf{k}; A, B)$ is k-independent. Then for any eigenvector $\chi \in \mathcal{K}$ with eigenvalue λ*

$$(\lambda + 1)A\chi + \mathrm{i}\mathsf{k}(\lambda - 1)B\chi = 0$$

holds for all $\mathsf{k} > 0$. By Lemma 3.4 this implies $\lambda \in \{-1, 1\}$. Thus, $\mathfrak{S}(\mathsf{k}; A, B)$ is self-adjoint.

Conversely, assume that $\mathfrak{S}(\mathsf{k}; A, B)$ is self-adjoint for some $\mathsf{k} > 0$. By (3.22) *it is self-adjoint for all $\mathsf{k} > 0$. Hence, any of its eigenvalues is either $+1$ or -1. By* (3.23) *the eigenspaces do not depend on k. The same argument as above shows that the eigenvalues of $\mathfrak{S}(\mathsf{k}; A, B)$ are k-independent. Thus, $\mathfrak{S}(\mathsf{k}; A, B)$ does not depend on $\mathsf{k} > 0$.*

To sum up, the matrix $\mathfrak{S}(\mathsf{k}; A, B)$ is k-independent if and only if it is of the form $\mathfrak{S}(\mathsf{k}; A, B) = \mathbb{I} - 2P$, where P denotes an orthogonal projection.

Alternatively, the matrix $\mathfrak{S}(\mathsf{k}; A, B)$ is k-independent if and only if $AB^\dagger = 0$. To prove this fact we note that $\mathfrak{S}(\mathsf{k}; A, B)$ is self-adjoint if and only if $A_{\mathfrak{S}} B_{\mathfrak{S}}^\dagger = 0$ with $A_{\mathfrak{S}}$ and $B_{\mathfrak{S}}$ defined in (3.15). *Since the boundary conditions (A, B) and $(A_{\mathfrak{S}}, B_{\mathfrak{S}})$ are equivalent, from* (3.16) *we obtain the claim.*

3.1. **Scattering Theory.** On the exterior $\mathcal{G}_{\mathrm{ext}} = (\partial V, \varnothing, \mathcal{E}, \partial|_{\mathcal{E}})$ of the graph $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ we consider the Laplace operator $-\Delta(A_{\mathcal{E}} = 0, B_{\mathcal{E}} = \mathbb{I})$ corresponding to Neumann boundary conditions. Let $\mathcal{P}_{\mathcal{E}} : \mathcal{H} \to \mathcal{H}_{\mathcal{E}}$ be the orthogonal projection in $\mathcal{H}$ onto $\mathcal{H}_{\mathcal{E}}$. By the Kato-Rosenblum theorem (see, e.g., [83, Theorem 6.2.3 and Corollary 6.2.4]) the two-space wave operators

$$\Omega^{\pm}(-\Delta(A, B, \underline{a}), -\Delta(A_{\mathcal{E}} = 0, B_{\mathcal{E}} = \mathbb{I}); \mathcal{P}_{\mathcal{E}}) = \operatorname*{s-lim}_{t \to \mp\infty} \mathrm{e}^{-\mathrm{i}\Delta(A,B,\underline{a})t}\, \mathcal{P}_{\mathcal{E}}\, \mathrm{e}^{\mathrm{i}\Delta(A_{\mathcal{E}}=0, B_{\mathcal{E}}=\mathbb{I})t}$$

exist and are $\mathcal{P}_{\mathcal{E}}$-complete. Thus, the scattering operator

$$S(-\Delta(A, B, \underline{a}), -\Delta(A_{\mathcal{E}} = 0, B_{\mathcal{E}} = \mathbb{I}); \mathcal{P}_{\mathcal{E}}) = (\Omega^-)^\dagger \Omega^+ : \mathcal{H}_{\mathcal{E}} \to \mathcal{H}_{\mathcal{E}} \tag{3.24}$$

is unitary and its layers $S(\mathsf{k}; A, B, \underline{a}) : \mathcal{K}_{\mathcal{E}} \to \mathcal{K}_{\mathcal{E}}$ (in the direct integral representation with respect to $-\Delta(A_{\mathcal{E}} = 0, B_{\mathcal{E}} = \mathbb{I})$) are also unitary for almost all $\mathsf{k} > 0$.

The resulting scattering matrix $S(\mathsf{k}) := S(\mathsf{k}; A, B, \underline{a})$ associated to $\Delta(A, B, \underline{a})$ has the following interpretation in terms of the solutions to the Schrödinger equation (see [42] and [44]). For given $k \in \mathcal{E}$ consider the solutions $\psi^k(\mathsf{k})$ of the stationary Schrödinger equation at energy $\mathsf{k}^2 > 0$,

$$-\Delta(A, B, \underline{a})\psi^k(\mathsf{k}) = \mathsf{k}^2 \psi^k(\mathsf{k}).$$

This solution is of the form

$$\psi_j^k(x; \mathsf{k}) = \begin{cases} [S(\mathsf{k})]_{jk} \mathrm{e}^{\mathrm{i}\mathsf{k}x} & \text{for } j \in \mathcal{E}, j \neq k, \\ \mathrm{e}^{-\mathrm{i}\mathsf{k}x} + [S(\mathsf{k})]_{kk} \mathrm{e}^{\mathrm{i}\mathsf{k}x} & \text{for } j \in \mathcal{E}, j = k, \\ [\alpha(\mathsf{k})]_{jk} \mathrm{e}^{\mathrm{i}\mathsf{k}x} + [\beta(\mathsf{k})]_{jk} \mathrm{e}^{-\mathrm{i}\mathsf{k}x} & \text{for } j \in \mathcal{I}. \end{cases} \tag{3.25}$$

Thus, the number $[S(\mathsf{k})]_{jk}$ for $j \neq k$ is the transmission amplitude from channel $k \in \mathcal{E}$ to channel $j \in \mathcal{E}$ and $[S(\mathsf{k})]_{kk}$ is the reflection amplitude in channel $k \in \mathcal{E}$. Their absolute squares may be interpreted as transmission and reflection probabilities, respectively. The "interior" amplitudes $[\alpha(\mathsf{k})]_{jk}$ and $[\beta(\mathsf{k})]_{jk}$ are also of interest, since they describe how an incoming wave moves through a graph before it is scattered into an outgoing channel.

The condition for the $\psi^k(\mathsf{k})$ $(k \in \mathcal{E})$ to satisfy the boundary conditions (3.13) immediately leads to the following solution for the scattering matrix $S(\mathsf{k}) : \mathcal{K}_{\mathcal{E}} \to \mathcal{K}_{\mathcal{E}}$ and the linear maps $\alpha(\mathsf{k})$ and $\beta(\mathsf{k})$ from $\mathcal{K}_{\mathcal{E}}$ to $\mathcal{K}_{\mathcal{I}} := \mathcal{K}_{\mathcal{I}}^{(-)} \oplus \mathcal{K}_{\mathcal{I}}^{(+)}$. Indeed, by combining these operators into a map from $\mathcal{K}_{\mathcal{E}}$ to $\mathcal{K} = \mathcal{K}_{\mathcal{E}} \oplus \mathcal{K}_{\mathcal{I}} \oplus \mathcal{K}_{\mathcal{I}}$ we obtain the linear equation

$$Z(\mathsf{k}; A, B, \underline{a}) \begin{pmatrix} S(\mathsf{k}) \\ \alpha(\mathsf{k}) \\ \beta(\mathsf{k}) \end{pmatrix} = -(A - \mathrm{i}\mathsf{k}B) \begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix} \tag{3.26}$$

with

$$Z(\mathsf{k}; A, B, \underline{a}) = AX(\mathsf{k}; \underline{a}) + \mathrm{i}\mathsf{k}BY(\mathsf{k}; \underline{a}), \tag{3.27}$$

where

$$X(\mathsf{k}; \underline{a}) = \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & \mathbb{I} \\ 0 & \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}} & \mathrm{e}^{-\mathrm{i}\mathsf{k}\underline{a}} \end{pmatrix} \qquad \text{and} \qquad Y(\mathsf{k}; \underline{a}) = \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & -\mathbb{I} \\ 0 & -\mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}} & \mathrm{e}^{-\mathrm{i}\mathsf{k}\underline{a}} \end{pmatrix}. \tag{3.28}$$

The diagonal $|\mathcal{I}| \times |\mathcal{I}|$ matrices $\mathrm{e}^{\pm\mathrm{i}\mathsf{k}\underline{a}}$ are given by

$$[\mathrm{e}^{\pm\mathrm{i}\mathsf{k}\underline{a}}]_{jk} = \delta_{jk}\mathrm{e}^{\pm\mathrm{i}\mathsf{k}a_j} \quad \text{for} \quad j, k \in \mathcal{I}. \tag{3.29}$$

From (3.26) it follows that the scattering matrix is a meromorphic function in the complex k-plane. In particular, $S(\mathsf{k})$ is real analytic in $\mathsf{k} \in \mathbb{R}$ except for a discrete set of values with no finite accumulation points. Indeed, the determinant $\det Z(\mathsf{k})$ of $Z(\mathsf{k}) := Z(\mathsf{k}; A, B, \underline{a})$ is an entire function in k and, therefore, $Z(\mathsf{k})^{-1}$ is meromorphic. As proven in [42, Theorem 3.1] the set of real zeros of $\det Z(\mathsf{k})$ is discrete. This implies, in particular, that $S(\mathsf{k})$ is known if it is known for a countable set of values $\mathsf{k} \in \mathbb{R}$ with at least one finite accumulation point. So Corollary 3 is a direct consequence of Theorem 2.

Observe that

$$\begin{aligned} AX(\mathsf{k}; \underline{a}) + \mathrm{i}\mathsf{k}BY(\mathsf{k}; \underline{a}) &= (A + \mathrm{i}\mathsf{k}B)R_+(\mathsf{k}; \underline{a}) + (A - \mathrm{i}\mathsf{k}B)R_-(\mathsf{k}; \underline{a}) \\ &= (A + \mathrm{i}\mathsf{k}B)\big[\mathbb{I} + (A + \mathrm{i}\mathsf{k}B)^{-1}(A - \mathrm{i}\mathsf{k}B)T(\mathsf{k}; \underline{a})\big]R_+(\mathsf{k}; \underline{a}) \\ &= (A + \mathrm{i}\mathsf{k}B)\big[\mathbb{I} - \mathfrak{S}(\mathsf{k}; A, B)T(\mathsf{k}; \underline{a})\big]R_+(\mathsf{k}; \underline{a}), \end{aligned} \tag{3.30}$$

where

$$R_+(\mathsf{k}; \underline{a}) := \frac{1}{2}[X(\mathsf{k}; \underline{a}) + Y(\mathsf{k}; \underline{a})] = \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & \mathbb{I} & 0 \\ 0 & 0 & \mathrm{e}^{-\mathrm{i}\mathsf{k}\underline{a}} \end{pmatrix}, \tag{3.31}$$

$$R_-(\mathsf{k}; \underline{a}) := \frac{1}{2}[X(\mathsf{k}; \underline{a}) - Y(\mathsf{k}; \underline{a})] = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \mathbb{I} \\ 0 & \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}} & 0 \end{pmatrix},$$

and

$$T(\mathsf{k}; \underline{a}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}} \\ 0 & \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}} & 0 \end{pmatrix} \tag{3.32}$$

with respect to the orthogonal decomposition (3.3). Thus, from (3.26) we get

$$K(\mathsf{k}; A, B, \underline{a}) \begin{pmatrix} S(\mathsf{k}) \\ \alpha(\mathsf{k}) \\ \mathrm{e}^{-\mathrm{i}\mathsf{k}\underline{a}}\beta(\mathsf{k}) \end{pmatrix} = \mathfrak{S}(\mathsf{k}; A, B) \begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix}, \tag{3.33}$$

where

$$K(\mathsf{k}; A, B, \underline{a}) := \mathbb{I} - \mathfrak{S}(\mathsf{k}; A, B)T(\mathsf{k}; \underline{a}) \tag{3.34}$$

and $\begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix} : \mathcal{K}_{\mathcal{E}} \to \mathcal{K}$ such that $\begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix} \chi = \chi \oplus 0 \oplus 0$ with respect to orthogonal decomposition (3.3).

Theorem 3.10 (= Theorem 3.2 in [42]). *Let the boundary conditions* (A, B) *satisfy* (3.10). *For any* $\mathsf{k} \in \mathbb{R} \setminus \{0\}$

$$\operatorname{Ran}\ \mathfrak{S}(\mathsf{k}; A, B) \begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix} \subset \operatorname{Ran} K(\mathsf{k}; A, B, \underline{a}). \tag{3.35}$$

Thus, equation (3.33) *has a solution even if* $\det K(\mathsf{k}; A, B, \underline{a}) = 0$ *for some* $\mathsf{k} \in \mathbb{R} \setminus \{0\}$. *This solution defines the scattering matrix uniquely. Moreover,*

$$S(\mathsf{k}) = -\begin{pmatrix} \mathbb{I} & 0 & 0 \end{pmatrix} \Big(K(\mathsf{k}; A, B, \underline{a})|_{\operatorname{Ran} K(\mathsf{k}; A, B, \underline{a})^\dagger} \Big)^{-1} P_{\operatorname{Ran} K(\mathsf{k}; A, B, \underline{a})} \mathfrak{S}(\mathsf{k}; A, B) \begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix} \tag{3.36}$$

is unitary for all $\mathsf{k} \in \mathbb{R} \setminus \{0\}$.

Here $P_{\operatorname{Ran} K(\mathsf{k}; A, B, \underline{a})}$ denotes the orthogonal projection in $\mathcal{K}$ onto $\operatorname{Ran} K(\mathsf{k}; A, B, \underline{a})$, the range of $K(\mathsf{k}; A, B, \underline{a})$ as a map on $\mathcal{K}$.

We present an elementary proof of Theorem 3.10.

Proof. For any $\chi \in \operatorname{Ker} K(\mathsf{k}; A, B, \underline{a})$ we have

$$T(\mathsf{k}; \underline{a})\chi = \mathfrak{S}(\mathsf{k}; A, B)^\dagger \chi.$$

Multiplying this equality by $\begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ from the left we obtain $\begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \mathfrak{S}(\mathsf{k}; A, B)^\dagger \chi = 0.$
Thus,

$$\operatorname{Ker} K(\mathsf{k}; A, B, \underline{a}) \subset \operatorname{Ker} \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \mathfrak{S}(\mathsf{k}; A, B)^\dagger,$$

which implies the inclusion

$$\operatorname{Ran} K(\mathsf{k}; A, B, \underline{a})^\dagger \supset \operatorname{Ran}\ \mathfrak{S}(\mathsf{k}; A, B) \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{3.37}$$

Observe that for any $\mathsf{k} > 0$ the operator $\mathfrak{S}(\mathsf{k}; A, B) T(\mathsf{k}; \underline{a})$ is a partial isometry with initial subspace $\mathcal{K}_{\mathcal{I}} := \mathcal{K}_{\mathcal{I}}^{(-)} \oplus \mathcal{K}_{\mathcal{I}}^{(+)}$ and final subspace $\mathfrak{S}(\mathsf{k}; A, B)\mathcal{K}_{\mathcal{I}}$. In particular, it is a contraction. Thus (see, e.g. [80, Theorem I.3.2] or [36, Theorem 1.6.6]), $\operatorname{Ran} K(\mathsf{k}; A, B, \underline{a})$ and $\operatorname{Ran} K(\mathsf{k}; A, B, \underline{a})^\dagger$ are equal. Hence, noting that

$$\operatorname{Ran}\ \mathfrak{S}(\mathsf{k}; A, B) \begin{pmatrix} \mathbb{I} & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \operatorname{Ran}\ \mathfrak{S}(\mathsf{k}; A, B) \begin{pmatrix} \mathbb{I} \\ 0 \\ 0 \end{pmatrix},$$

inclusion (3.37) proves (3.35). Combined with (3.33) this also establishes (3.36).

To prove the unitarity we note that equation (3.33) implies that

$$\begin{pmatrix} S(\mathsf{k}) \\ \alpha(\mathsf{k}) \\ \mathrm{e}^{-\mathrm{i}\mathsf{k}\underline{a}}\beta(\mathsf{k}) \end{pmatrix} = \mathfrak{S}(\mathsf{k}; A, B, \underline{a}) \begin{pmatrix} \mathbb{I} \\ \beta(\mathsf{k}) \\ \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}}\alpha(\mathsf{k}) \end{pmatrix}.$$

Since $\mathfrak{S}(\mathsf{k}; A, B, \underline{a})$ is unitary we obtain $S(\mathsf{k})^\dagger S(\mathsf{k}) = \mathbb{I}$. □

We turn to the study of the analytic properties of the scattering matrix as a function of $\mathsf{k} \in \mathbb{C}$.

Proposition 3.11. *Let the boundary conditions* (A, B) *satisfy* (3.10). *If* $\det(A + \mathrm{i}\mathsf{k}B) = 0$ *for some* $\mathsf{k} \in \mathbb{C}$*, then* $\mathsf{k} = \mathrm{i}\kappa$ *with* $\kappa \in \mathbb{R}$*. For any sufficiently large* $\rho > 0$ *there is a constant* $C_\rho > 0$ *such that*

$$\|(A + \mathrm{i}\mathsf{k}B)^{-1}\| \le C_\rho \tag{3.38}$$

for all $\mathsf{k} \in \mathbb{C}$ *with* $|\mathsf{k}| > \rho$.

Proof. Assume that $\det(A + \mathrm{i}\mathsf{k}B) = 0$ for some $\mathsf{k} \in \mathbb{C}$ with $\operatorname{Re}\mathsf{k} \neq 0$. Then also

$$\det(A^\dagger - \mathrm{i}\bar{\mathsf{k}}B^\dagger) = \overline{\det(A + \mathrm{i}\mathsf{k}B)} = 0.$$

Therefore, there is a $\chi \neq 0$ such that

$$(A^\dagger - \mathrm{i}\bar{\mathsf{k}}B^\dagger)\chi = 0. \tag{3.39}$$

In particular, we have $(BA^\dagger - \mathrm{i}\bar{\mathsf{k}}BB^\dagger)\chi = 0$. Therefore, since $BA^\dagger$ is self-adjoint, we get

$$\langle\chi, BA^\dagger\chi\rangle = \langle\chi, BB^\dagger\chi\rangle \operatorname{Im}\mathsf{k} \qquad \text{and} \qquad \langle\chi, BB^\dagger\chi\rangle \operatorname{Re}\mathsf{k} = 0.$$

The second equality implies that $\chi \in \operatorname{Ker} B^\dagger$. Then, by (3.39), $\chi \in \operatorname{Ker} A^\dagger$. By Lemma 3.4 we have $\operatorname{Ker} A^\dagger \cap \operatorname{Ker} B^\dagger = \{0\}$. Thus, $\chi = 0$ which contradicts the assumption and, hence, $\operatorname{Re}\mathsf{k} = 0$.

Since $\det(A + \mathrm{i}\mathsf{k}B)$ is a polynomial in k, it has a finite number of zeroes. Take an arbitrary $\rho > 0$ such that all its zeroes lie in the disk $|\mathsf{k}| < \rho$. Using the matrix inverse formula we represent any element of $(A + \mathrm{i}\mathsf{k}B)^{-1}$ as a quotient of two polynomials. Obviously, the degree of the nominator does not exceed the degree of the denominator. In turn, this implies the estimate (3.38). □

Theorem 3.12. *Let the boundary conditions* (A, B) *satisfy* (3.10). *The scattering matrix* $S(\mathsf{k}) = S(\mathsf{k}; A, B, \underline{a})$ *is a meromorphic function in the complex* k*-plane. In the upper half-plane* $\operatorname{Im}\mathsf{k} > 0$ *it has at most a finite number of poles which are located on the imaginary semiaxis* $\operatorname{Re}\mathsf{k} = 0$.

Proof. Assume that $\det K(\mathsf{k}; A, B, \underline{a}) = 0$ for some $\mathsf{k} \in \mathbb{C}$ with $\operatorname{Im}\mathsf{k} > 0$ and $\operatorname{Re}\mathsf{k} \neq 0$. This implies that the homogeneous equation

$$K(\mathsf{k}; A, B, \underline{a}) \begin{pmatrix} s \\ \alpha \\ \beta \end{pmatrix} = 0$$

has a nontrivial solution with $s \in \mathcal{K}_\mathcal{E}$, $\alpha \in \mathcal{K}_\mathcal{I}^{(-)}$, and $\beta \in \mathcal{K}_\mathcal{I}^{(+)}$. Consider the function $\psi(x) = \{\psi_j(x)\}_{j \in \mathcal{I} \cup \mathcal{E}}$ defined by

$$\psi_j(x) = \begin{cases} s_j \mathrm{e}^{\mathrm{i}\mathsf{k}x} & \text{for } j \in \mathcal{E}, \\ \alpha_j \mathrm{e}^{\mathrm{i}\mathsf{k}x} + \beta_j \mathrm{e}^{\mathrm{i}\mathsf{k}a_j} \mathrm{e}^{-\mathrm{i}\mathsf{k}x} & \text{for } j \in \mathcal{I}. \end{cases}$$

Obviously, $\psi(x)$ satisfies the boundary conditions (2.2). Moreover, $\psi \in L^2(\mathcal{G})$ since $\operatorname{Im}\mathsf{k} > 0$. Hence, $\mathsf{k}^2 \in \mathbb{C}$ with $\operatorname{Im}\mathsf{k}^2 \neq 0$ is an eigenvalue of the operator $\Delta(A, B, \underline{a})$ which contradicts the self-adjointness of $\Delta(A, B, \underline{a})$.

Since $\det K(\mathsf{k}; A, B, \underline{a})$ is an entire function in k which does not vanish identically, from (3.26) it follows that the scattering matrix $S(\mathsf{k})$ is a meromorphic function in the complex k-plane. To prove that the scattering matrix $S(\mathsf{k})$ has at most a finite number of poles on the imaginary semiaxis $\{\mathsf{k} \in \mathbb{C} | \operatorname{Re}\mathsf{k} = 0, \operatorname{Im}\mathsf{k} > 0\}$ it suffices to show that the determinant $\det K(\mathsf{k}; A, B, \underline{a})$ does not vanish for all sufficiently large $\operatorname{Im}\mathsf{k} > 0$. From Proposition 3.11 it follows that there is $\rho > 0$ and a constant $C > 0$ such that $\|\mathfrak{S}(\mathrm{i}\kappa; A, B)\| \le C$ for all $\kappa > \rho$. Observing that $\|T(\mathrm{i}\kappa; \underline{a})\| \le \mathrm{e}^{-a\kappa}$ with $a := \min_{j \in \mathcal{I}} a_j$ for all $\kappa > 0$, we obtain that $\|\mathfrak{S}(\mathrm{i}\kappa; A, B) T(\mathrm{i}\kappa; \underline{a})\| < 1$ for all $\kappa > \max\{\rho, a^{-1}\log C\}$. □

Remark 3.13. *The positive eigenvalues of the operator* $-\Delta(A,B,\underline{a})$ *on a compact metric graph* $(\mathcal{G},\underline{a})$ *are determined by the equation*

$$\det[\mathbb{I}-\mathfrak{S}(\mathsf{k};A,B)T(\mathsf{k};\underline{a})]=0 \tag{3.40}$$

with $T(\mathsf{k};\underline{a})$ *defined in* (3.32). *This fact has first been observed by Carlson in* [11, Section 3.2].

Observing that $\mathfrak{S}(\mathsf{k};A,B)T(\mathsf{k};\underline{a})$ *is strictly contractive for all* $\mathsf{k}\in\mathbb{C}$ *with* $\operatorname{Im}\mathsf{k}>0$ *and sufficiently large* $\operatorname{Re}\mathsf{k}>0$ *one obtains an absolutely convergent expansion*

$$\log\det[\mathbb{I}-\mathfrak{S}(\mathsf{k};A,B)T(\mathsf{k};\underline{a})]=1+\sum_{n=1}^{\infty}\frac{1}{n}\operatorname{tr}[\mathfrak{S}(\mathsf{k};A,B)T(\mathsf{k};\underline{a})]^n.$$

Starting from this observation Kottos and Smilansky presented in [48] *a derivation of a representation for the eigenvalues counting function in terms of closed paths on the graph. This representation strongly resembles the celebrated Selberg trace formula for compact Riemann manifolds* [78], [61] *(a generalization of the Poisson summation formula). The Selberg trace formula establishes a relation between the length spectrum of prime geodesics and the spectrum of the Laplace operator on the manifold.*

A mathematically rigorous version of the Kottos-Smilansky representation for the Laplace transform of the eigenvalues counting function has been proven earlier by Roth [72], [73] *for the case of standard boundary conditions (see Example 4.5 below). Some related results can also be found in* [21], [22], [62], [63], [64], [79]. *The Weyl asymptotics for fourth-order differential operators on compact graphs has been proven in* [13].

The representation from [48] *was used by Gutkin and Smilansky in* [28] *to determine the lengths of internal edges of a compact metric graph from the spectrum of the associated Laplace operator. A rigorous proof of this result has been recently given by Kurasov and Nowaczyk in* [58] *for standard boundary conditions.*

3.2. **Symmetry Properties of the Scattering Matrices.** We say that the boundary conditions (A,B) satisfying (3.10) are *real* if the self-adjoint operator $\Delta(A,B)$ is real, that is, its domain $\operatorname{Dom}(\Delta(A,B,\underline{a}))$ is invariant with respect to the complex conjugation. This implies that $\overline{\Delta(A,B,\underline{a})\psi}=\Delta(A,B,\underline{a})\overline{\psi}$ for all $\psi\in\operatorname{Dom}(\Delta(A,B,\underline{a}))$.

By (3.8) the operator $\Delta(A,B,\underline{a})$ is real if and only if the maximal isotropic subspace $\mathcal{M}(A,B)$ defined by (3.9) is invariant with respect to complex conjugation. This immediately implies that $\Delta(A,B,\underline{a})$ is real if and only if the boundary conditions (A,B) and $(\overline{A},\overline{B})$ are equivalent.

Lemma 3.14. *Boundary conditions* (A,B) *satisfying* (3.10) *are real if and only if there are real matrices* (A',B') *and an invertible matrix* C *such that* $A'=CA$ *and* $B'=CB$.

Proof. The "if" part is obvious. To prove the "only if" part we assume that boundary conditions (A,B) satisfying (3.10) are real such that $\overline{A}=CA$ and $\overline{B}=CB$ for some invertible C. Therefore,

$$\overline{A}+\kappa\overline{B}=C(A+\kappa B) \tag{3.41}$$

for all $\kappa\in\mathbb{C}$. Choose $\kappa>0$ sufficiently large such that $A+\kappa B$ is invertible, which is possible by Proposition 3.11. Equation (3.41) implies that

$$C=(\overline{A}+\kappa\overline{B})(A+\kappa B)^{-1}.$$

Now set $A'=(A+\kappa B)^{-1}A$ and $B'=(A+\kappa B)^{-1}B$. The matrices A' and B' are real since $\overline{A'}=(\overline{A}+\kappa\overline{B})^{-1}\overline{A}=(A+\kappa B)^{-1}C^{-1}\overline{A}=(A+\kappa B)^{-1}A=A'$ and similarly for B'. □

Lemma 3.15. *Boundary conditions* (A,B) *satisfying* (3.10) *are real if and only if the unitary matrix* $\mathfrak{S}(\mathsf{k};A,B)$ *defined by* (3.14) *is symmetric for at least one* $\mathsf{k}>0$ *and, thus, for all* $\mathsf{k}>0$, *that is*

$$\mathfrak{S}(\mathsf{k};A,B)^T=\mathfrak{S}(\mathsf{k};A,B) \tag{3.42}$$

with "T" denoting the transpose.

Proof. By Corollary 2.1 in [42] one has the relation

$$\mathfrak{S}(\mathsf{k};A,B)^T=\mathfrak{S}(\mathsf{k};\overline{A},\overline{B}). \tag{3.43}$$

If $\mathfrak{S}(\mathsf{k};A,B)$ is symmetric, then $\mathfrak{S}(\mathsf{k};A,B)=\mathfrak{S}(\mathsf{k};\overline{A},\overline{B})$. By Proposition 3.7 the boundary conditions (A,B) and $(\overline{A},\overline{B})$ are equivalent, which implies that they are real.

Conversely, if the boundary conditions (A,B) are real, then by Lemma 3.14 both matrices A and B may be chosen real. Hence, $\mathfrak{S}(\mathsf{k};A,B)=\mathfrak{S}(\mathsf{k};\overline{A},\overline{B})$, which by (3.43) implies (3.42). □

Recall that the scattering matrix $S(\mathsf{k};A,B,\underline{a})$ possesses a property similar to (3.43) (see Corollary 3.2 in [42] and Theorem 2.2 in [43]):

$$S(\mathsf{k};A,B,\underline{a})^T=S(\mathsf{k};\overline{A},\overline{B},\underline{a}).$$

Observe that for all $\mathsf{k}>0$

$$\mathfrak{S}(\mathsf{k};A,B)^\dagger=\mathfrak{S}(\mathsf{k};A,B)^{-1}=\mathfrak{S}(-\mathsf{k};A,B). \tag{3.44}$$

Corollary 3.16. *Let the boundary conditions (A,B) satisfy* (3.10). *For all complex k the relation*

$$S(-\mathsf{k};A,B,\underline{a})=S(\mathsf{k};A,B,\underline{a})^{-1} \tag{3.45}$$

is valid.

Proof. By Theorem 3.12 it suffices to prove (3.45) for almost all $\mathsf{k}>0$. Assume that $\det[\mathbb{I}-\mathfrak{S}(\mathsf{k};A,B)T(\mathsf{k};\underline{a})]\neq 0$. Taking the adjoint of (3.36) and using relations (3.44) and $T(\mathsf{k};\underline{a})^\dagger=T(-\mathsf{k};\underline{a})$, we obtain

$$S(\mathsf{k};A,B,\underline{a})^\dagger=\begin{pmatrix}\mathbb{I}&0&0\end{pmatrix}\mathfrak{S}(-\mathsf{k};A,B)(\mathbb{I}-T(-\mathsf{k};\underline{a})\mathfrak{S}(-\mathsf{k};A,B))^{-1}\begin{pmatrix}\mathbb{I}\\0\\0\end{pmatrix}.$$

Note that $K_1(\mathbb{I}+K_2K_1)^{-1}=(\mathbb{I}+K_1K_2)^{-1}K_1$ if at least one of the inverses $(\mathbb{I}+K_2K_1)^{-1}$ and $(\mathbb{I}+K_1K_2)^{-1}$ exists. Thus, we obtain

$$\begin{aligned}S(\mathsf{k};A,B,\underline{a})^\dagger&=\begin{pmatrix}\mathbb{I}&0&0\end{pmatrix}(\mathbb{I}-\mathfrak{S}(-\mathsf{k};A,B)T(-\mathsf{k};\underline{a}))^{-1}\mathfrak{S}(-\mathsf{k};A,B)\begin{pmatrix}\mathbb{I}\\0\\0\end{pmatrix}\\&=S(-\mathsf{k};A,B,\underline{a}).\end{aligned}$$

□

In the context of analytic S-matrix theory (see, e.g., [15], [66]) relation (3.45) is called Hermitian analyticity.

3.3. **Graphs With No Internal Edges.** The case with no internal edges ($\mathcal{I}=\emptyset$) deserves special attention. The relation (3.26) for the scattering matrix simplifies to

$$S(\mathsf{k};A,B)=\mathfrak{S}(\mathsf{k};A,B), \tag{3.46}$$

where $\mathfrak{S}(\mathsf{k};A,B)$ is defined in (3.14). As special cases we obtain k-independent scattering matrices for Dirichlet and Neumann boundary conditions

$$\begin{aligned}S(\mathsf{k};A=\mathbb{I},B=0)&=-\ \mathbb{I}\quad\text{(Dirichlet boundary conditions)},\\S(\mathsf{k};A=0,B=\mathbb{I})&=\ \ \mathbb{I}\quad\text{(Neumann boundary conditions)}.\end{aligned} \tag{3.47}$$

Since $\mathcal{M}(A=\mathbb{I},B=0)^\perp=\mathcal{M}(A=0,B=\mathbb{I})$, equations (3.47) provide an example to (3.18).

By Proposition 3.7, with condition (3.10) being satisfied, both matrices $A\pm\mathrm{i}\mathsf{k}B$ are invertible for all real $\mathsf{k}\neq 0$. Now by the representation (3.46) the scattering matrix $S(\mathsf{k};A,B)$ is a rational function in k. By Proposition 3.11, all possible poles of the scattering matrix are located on the imaginary axis.

We collect some properties of the single-vertex scattering matrix (3.46) associated to (A, B). By Proposition 3.7 we conclude that the scattering matrix $S(\mathsf{k}; A, B)$ is uniquely determined by the maximal isotropic space $\mathcal{M}(A, B)$, i.e., the equality

$$S(\mathsf{k}; A, B) = S(\mathsf{k}; A', B')$$

holds for all $\mathsf{k} \neq 0$ if and only if $\mathcal{M}(A, B) = \mathcal{M}(A', B')$. Conversely, again by Proposition 3.7, the scattering matrix $S(\mathsf{k})$ for arbitrarily fixed $\mathsf{k} > 0$ uniquely fixes the boundary conditions,

$$A(\mathsf{k}) = -\frac{1}{2}(S(\mathsf{k}) - \mathbb{I}), \qquad B(\mathsf{k}) = \frac{1}{2i\mathsf{k}}(S(\mathsf{k}) + \mathbb{I}). \tag{3.48}$$

Relation (3.46) and Proposition 3.11 imply the following result.

Lemma 3.17. *For any boundary conditions (A, B) satisfying* (3.10) *the scattering matrix $S(\mathsf{k})$ $:= S(\mathsf{k}; A, B)$ possesses the following properties for all $\mathsf{k} \in \mathbb{R} \setminus \{0\}$:*

$$\operatorname{Ker} B = \operatorname{Ker}(S(\mathsf{k}) + \mathbb{I}), \qquad \operatorname{Ker} A = \operatorname{Ker}(S(\mathsf{k}) - \mathbb{I}). \tag{3.49}$$

Therefore, -1 is an eigenvalue of $S(\mathsf{k})$ for all $\mathsf{k} \in \mathbb{R}$ if and only if $\det B = 0$ and 1 is an eigenvalue of $S(\mathsf{k})$ for all $\mathsf{k} \in \mathbb{R}$ if and only if $\det A = 0$.

Let $\mathcal{M}_{\mathrm{D}} = \mathcal{M}(A = \mathbb{I}, B = 0)$ and $\mathcal{M}_{\mathrm{N}} = \mathcal{M}(A = 0, B = \mathbb{I})$ denote the maximal isotropic subspaces corresponding to Dirichlet and Neumann boundary conditions, respectively. As an immediate consequence of definition (3.9) of $\mathcal{M}(A, B)$ we obtain that

$$\mathcal{M} \cap \mathcal{M}_{\mathrm{D}} = \{0\} \oplus \operatorname{Ker} B \qquad \text{and} \qquad \mathcal{M} \cap \mathcal{M}_{\mathrm{N}} = \operatorname{Ker} A \oplus \{0\}$$

with respect to the orthogonal decomposition ${}^d\mathcal{K} = \mathcal{K} \oplus \mathcal{K}$. Thus, if (A, B) satisfies (3.10), then

$$\dim \operatorname{Ker} A = \dim(\mathcal{M}(A, B) \cap \mathcal{M}_{\mathrm{N}}) \quad \text{and} \quad \dim \operatorname{Ker} B = \dim(\mathcal{M}(A, B) \cap \mathcal{M}_{\mathrm{D}}).$$

Let $P_{\operatorname{Ker} A}$ and $P_{\operatorname{Ker} B}$ be the orthogonal projections in $\mathcal{K}$ onto the kernel of A and of B, respectively. Note that since $\operatorname{Ker} A = \operatorname{Ker} CA$ and $\operatorname{Ker} B = \operatorname{Ker} CB$ for any invertible $C : \mathcal{K} \to \mathcal{K}$, the projections $P_{\operatorname{Ker} A}$ and $P_{\operatorname{Ker} B}$ depend on $\mathcal{M}(A, B)$ only.

Corollary 3.18. *Any single vertex scattering matrix satisfies the limit relations*

$$\begin{aligned} \lim_{\mathsf{k} \to +\infty} S(\mathsf{k}; A, B) &= \mathbb{I} - 2P_{\operatorname{Ker} B}, \\ \lim_{\mathsf{k} \to 0} S(\mathsf{k}; A, B) &= -\mathbb{I} + 2P_{\operatorname{Ker} A}. \end{aligned} \tag{3.50}$$

Moreover, the scattering matrix admits an expansion

$$S(\mathsf{k}; A, B) = \sum_{m=0}^{\infty} S^{(m)}(A, B)\mathsf{k}^{-m}, \tag{3.51}$$

absolutely converging for all sufficiently large $\mathsf{k} \in \mathbb{C}$.

Proof. Fix an arbitrary $\mathsf{k}_0 > 0$. For arbitrary $\mathsf{k} > \mathsf{k}_0$ relations (3.22) and (3.46) imply that

$$S(\mathsf{k}; A, B) = \frac{\mathsf{k} + \mathsf{k}_0}{\mathsf{k} - \mathsf{k}_0}\mathbb{I} - \frac{4\mathsf{k}\mathsf{k}_0}{(\mathsf{k} - \mathsf{k}_0)^2}\left[S(\mathsf{k}_0; A, B) + \frac{\mathsf{k} + \mathsf{k}_0}{\mathsf{k} - \mathsf{k}_0}\mathbb{I}\right]^{-1}.$$

Observe that for large k

$$\left[S(\mathsf{k}_0; A, B) + \frac{\mathsf{k} + \mathsf{k}_0}{\mathsf{k} - \mathsf{k}_0}\mathbb{I}\right]^{-1} = \frac{\mathsf{k} - \mathsf{k}_0}{2\mathsf{k}_0} P_{\operatorname{Ker}(S(\mathsf{k}_0; A, B) + \mathbb{I})} + O(1),$$

where $P_{\operatorname{Ker}(S(\mathsf{k}_0; A, B) + \mathbb{I})}$ is the orthogonal projection in $\mathcal{K}$ onto $\operatorname{Ker}(S(\mathsf{k}_0; A, B) + \mathbb{I})$. By Lemma 3.17 this leads to the first relation in (3.50). The second relation in (3.50) follows from the first one using (3.18) and (3.11). The expansion (3.51) can be proved by applying standard perturbation theory [40]. $\square$

Proposition 3.19. *For any boundary conditions (A,B) satisfying* (3.10) *with* $\operatorname{Ker} B=\{0\}$ *the resulting scattering matrix $S(\mathsf{k},A,B)$ has a representation*

$$S(\mathsf{k};A,B)=\frac{\mathsf{k}+\mathrm{i}H/2}{\mathsf{k}-\mathrm{i}H/2}, \tag{3.52}$$

where H is an $|\mathcal{E}|\times|\mathcal{E}|$ Hermitian matrix.

Proof. Note that $B^{-1}A$ is self-adjoint since $AB^{\dagger}$ is:

$$B^{-1}A-A^{\dagger}{B^{\dagger}}^{-1}=B^{-1}(A-BA^{\dagger}{B^{\dagger}}^{-1})=B^{-1}(A-AB^{\dagger}{B^{\dagger}}^{-1})=0.$$

From (3.46) it follows that

$$\begin{aligned} S(\mathsf{k};A,B)&=-(A+\mathrm{i}\mathsf{k}B)^{-1}BB^{-1}(A-\mathrm{i}\mathsf{k}B)\\ &=-(B^{-1}A+\mathrm{i}\mathsf{k})^{-1}(B^{-1}A-\mathrm{i}\mathsf{k}), \end{aligned} \tag{3.53}$$

which implies (3.52) with $H=2B^{-1}A$. □

Lemma 3.20. *Given an arbitrary Hermitian $|\mathcal{E}|\times|\mathcal{E}|$ matrix H there are boundary conditions (A,B) satisfying* (3.10) *and* $\operatorname{Ker} B=\{0\}$ *such that*

$$\lim_{\mathsf{k}\to+\infty}\mathsf{k}(S(\mathsf{k};A,B)-\mathbb{I})=\mathrm{i}H.$$

These boundary conditions are unique up to the equivalence in the sense of Definition 3.5.

Proof. Fix $\mathsf{k}_0>0$ arbitrarily. Obviously, the matrix

$$R=\frac{\mathsf{k}_0+\mathrm{i}H/2}{\mathsf{k}_0-\mathrm{i}H/2}$$

is unitary. Now set

$$A=-\frac{1}{2}(R-\mathbb{I})\qquad\text{and}\qquad B=\frac{1}{2\mathrm{i}\mathsf{k}_0}(R+\mathbb{I}).$$

It is easy to check that (A,B) satisfies (3.10) and $\operatorname{Ker} B=\{0\}$. Furthermore, for $\mathsf{k}=\mathsf{k}_0$ the scattering matrix $S(\mathsf{k};A,B)$ coincides with R. Proposition 3.19 implies the claim.

To prove the uniqueness assume that there are boundary conditions (A',B') satisfying (3.10) such that

$$\lim_{\mathsf{k}\to+\infty}\mathsf{k}(S(\mathsf{k};A',B')-\mathbb{I})=\mathrm{i}H. \tag{3.54}$$

By Corollary 3.18, $\operatorname{Ker} B'=\{0\}$ such that, by Proposition 3.19,

$$S(\mathsf{k};A',B')=\frac{\mathsf{k}+\mathrm{i}H'/2}{\mathsf{k}-\mathrm{i}H'/2}\quad\text{with}\quad H'=2{B'}^{-1}A'.$$

Comparing this with (3.54) shows that $H=H'$ and, therefore, $S(\mathsf{k};A,B)=S(\mathsf{k};A',B')$ for all $\mathsf{k}>0$. Applying Proposition 3.7 completes the proof. □

To proceed further we introduce some new notions. Recall that the set of all maximal isotropic subspaces (the Lagrangian Grassmannian) is isomorphic to the group $\mathsf{U}(|\mathcal{E}|)$ of all $|\mathcal{E}|\times|\mathcal{E}|$ unitary matrices. Proposition 3.7 provides an explicit parametrization $\mathcal{M}(U)$ of the maximal isotropic subspaces by the elements of the group $\mathsf{U}(|\mathcal{E}|)$. Let μ be the normalized Haar measure on $\mathsf{U}(|\mathcal{E}|)$.

Definition 3.21. *A property P holds for Haar almost all boundary conditions if*

$$\begin{aligned}\mu\{U\in\mathsf{U}(|\mathcal{E}|)|\ &P \textit{ holds for the boundary conditions}\\ &\textit{defined by the maximal isotropic subspace } \mathcal{M}(U)\}=\mu(\mathsf{U}(|\mathcal{E}|))=1.\end{aligned}$$

is valid.

We recall the following well-known result:

Lemma 3.22. *For arbitrary $N \in \mathbb{N}$ the set of all unitary matrices $U \in \mathsf{U}(N)$ with simple spectrum is of full Haar measure. Moreover,*

(i) *for any given $\lambda \in \mathbb{C}$ such that $|\lambda| = 1$ the set*

$$\{U \in \mathsf{U}(N) | \ \lambda \text{ is an eigenvalue of } U\} \tag{3.55}$$

is of zero Haar measure;

(ii) *for any given $\chi \in \mathbb{C}^N$ both set*

$$\{U \in \mathsf{U}(N) | \ \chi \text{ is an eigenvector of } U\}$$

is of zero Haar measure;

(iii) *for any given $\chi_1, \chi_2 \in \mathbb{C}^N$ the sets*

$$\{U \in \mathsf{U}(N) | \ \langle \chi_1, U\chi_2 \rangle = 0\} \tag{3.56}$$

and

$$\left\{U \in \mathsf{U}(N) | \left\langle \chi_1, \frac{U - \mathbb{I}}{U + \mathbb{I}} \chi_2 \right\rangle = 0 \right\} \tag{3.57}$$

are of zero Haar measure.

The proof of Lemma 3.22 is based on the fact that any proper analytic subvariety of $\mathsf{U}(N)$ has Haar measure zero [82]. The proof of the main claim can be found in [82]. The details of the proof of claims (i) – (iii) are left to the reader.

Proposition 3.23. *For Haar almost all boundary conditions* $\operatorname{Ker} A = \{0\}$ *and* $\operatorname{Ker} B = \{0\}$.

Proof. By Lemma 3.22, for an arbitrary $\mathsf{k} > 0$ the numbers ± 1 are not eigenvalues of $S(\mathsf{k}; A, B)$ for Haar almost all boundary conditions (A, B). By Lemma 3.17 this implies the claim. □

We obtain the following consequence of Proposition 3.19 and Lemma 3.22.

Theorem 3.24. *For Haar almost all boundary conditions (A, B) the associated scattering matrix $S(\mathsf{k}; A, B)$ has a representation in the form*

$$S(\mathsf{k}; A, B) = \frac{\mathsf{k} + \mathrm{i}H/2}{\mathsf{k} - \mathrm{i}H/2}, \tag{3.58}$$

where H is a Hermitian matrix with non-vanishing entries and simple eigenvalues. Furthermore, for Haar almost all boundary conditions (A, B)

(i) *given an arbitrary $\chi \in \mathcal{K}$ neither of the eigenvectors of $S(\mathsf{k}; A, B)$ is orthogonal to χ;*
(ii) *there are no $\chi_1, \chi_2 \in \mathcal{K}$, $\langle \chi_1, \chi_2 \rangle = 0$ and $\chi_{1,2} \neq 0$ such that the inner product $\langle \chi_1, S(\mathsf{k}; A, B)\chi_2 \rangle$ vanishes identically for all $\mathsf{k} > 0$.*

Proof. Representation (3.58) follows from Propositions 3.19 and 3.23. Observe that $\lambda \in \mathbb{R}$ is a degenerated eigenvalue of H if and only if $(\mathsf{k} + \mathrm{i}\lambda/2)(\mathsf{k} - \mathrm{i}\lambda/2)^{-1}$ is a degenerated eigenvalue of $S(\mathsf{k}; A, B)$ for all $\mathsf{k} > 0$. Thus, by Lemma 3.22 all eigenvalues of H are simple.

To prove that all entries of the matrix H are non-vanishing we note that by Lemma 3.17 and Proposition 3.23 $\mathbb{I} + S(\mathsf{k}; A, B)$ is invertible for Haar almost all boundary conditions. Thus, (3.58) implies that

$$H = -2\mathrm{i}\mathsf{k} \frac{S(\mathsf{k}; A, B) - \mathbb{I}}{S(\mathsf{k}; A, B) + \mathbb{I}} \tag{3.59}$$

for all $\mathsf{k} > 0$. By (iii) of Proposition 3.22 the claim follows.

To prove the claim (i) we note that the eigenvectors of $S(\mathsf{k}; A, B)$ are those of the Hermitian matrix H and, thus, are independent of $\mathsf{k} > 0$. Therefore, (i) follows from Lemma 3.22. The claim (ii) also follows from Lemma 3.22. □

Let $\mathfrak{M}_N$ be the set of all Hermitian $N\times N$ matrices endowed with the metric topology induced by the operator norm. Consider the probability measure $\varkappa$ on $\mathfrak{M}_N$ defined for any Borel set $M\subset\mathfrak{M}_N$ via

$$\varkappa(M)=\mu\Big(\Big\{\frac{\mathbb{I}+\mathrm{i}H/2}{\mathbb{I}-\mathrm{i}H/2}\Big|\, H\in M\Big\}\Big), \tag{3.60}$$

where μ is the normalized Haar measure on $\mathsf{U}(N)$. For example, if $N=1$, then

$$\varkappa(M)=\frac{1}{\pi}\int_M\frac{dh}{1+h^2},\qquad M\subset\mathbb{R}.$$

On $\mathfrak{M}_N$ we also consider the measure

$$\begin{aligned} d\nu &= \prod_{k=1}^N dH_{kk}\prod_{1\le m<k\le N} d\,\mathrm{Re}\,H_{mk}\; d\,\mathrm{Im}\,H_{mk}\\ &= \prod_{k=1}^N dH_{kk}\prod_{1\le m<k\le N} d|H_{mk}|\,d(\arg H_{mk}) \end{aligned}\tag{3.61}$$

Recall (see, e.g., [82]) that on any chart of the manifold $\mathsf{U}(N)$ the Haar measure is absolutely continuous with respect the measure induced by the $N(N+1)/2$-dimensional Lebesgue measure via a coordinate map. In particular, this implies the following

Lemma 3.25. *The measure $\varkappa$ is absolutely continuous with respect to the measure ν.*

4. Local Boundary Conditions

The notion of local boundary conditions has been introduced in our paper [42] and discussed in more detail in [45]. Local boundary conditions couple only those boundary values of ψ and of its derivative ψ' which belong to the same vertex.

In this section we show that given boundary conditions (A,B) satisfying (3.10) and the sets $\mathcal{E}$ and $\mathcal{I}$ there exists a graph $\mathcal{G}$ for which these boundary conditions are *local*. Moreover, among all such graphs there exists a unique maximal graph.

The precise definition of local boundary conditions is as follows. With respect to the orthogonal decomposition $\mathcal{K}=\mathcal{K}_{\mathcal{E}}=\oplus\mathcal{K}_{\mathcal{I}}^{(-)}\oplus\mathcal{K}_{\mathcal{I}}^{(+)}$ any element χ of $\mathcal{K}$ can be represented as a vector

$$\chi=\begin{pmatrix}\{\chi_e\}_{e\in\mathcal{E}}\\ \{\chi_i^{(-)}\}_{i\in\mathcal{I}}\\ \{\chi_i^{(+)}\}_{i\in\mathcal{I}}\end{pmatrix}. \tag{4.1}$$

Consider the orthogonal decomposition

$$\mathcal{K}=\bigoplus_{v\in V}\mathcal{L}_v \tag{4.2}$$

with $\mathcal{L}_v$ the linear subspace of dimension $\deg(v)$ spanned by those elements (4.1) of $\mathcal{K}$ which satisfy

$$\begin{aligned} \chi_e&=0 \quad\text{if}\quad e\in\mathcal{E}\quad\text{is not incident with the vertex}\quad v,\\ \chi_i^{(-)}&=0\quad\text{if}\quad v\quad\text{is not an initial vertex of}\quad i\in\mathcal{I},\\ \chi_i^{(+)}&=0\quad\text{if}\quad v\quad\text{is not a terminal vertex of}\quad i\in\mathcal{I}. \end{aligned}\tag{4.3}$$

Obviously, the subspaces $\mathcal{L}_{v_1}$ and $\mathcal{L}_{v_2}$ are orthogonal if $v_1\neq v_2$.

Set ${}^{d}\mathcal{L}_v := \mathcal{L}_v \oplus \mathcal{L}_v \cong \mathbb{C}^{2\deg(v)}$. Obviously, each ${}^{d}\mathcal{L}_v$ inherits a symplectic structure from ${}^{d}\mathcal{K}$ in a canonical way, such that the orthogonal decomposition

$$\bigoplus_{v\in V} {}^{d}\mathcal{L}_v = {}^{d}\mathcal{K}$$

holds.

Definition 4.1. *Given the graph $\mathcal{G} = \mathcal{G}(V, \mathcal{I}, \mathcal{E}, \partial)$, boundary conditions (A, B) satisfying* (3.10) *are called* local on $\mathcal{G}$ *if the maximal isotropic subspace $\mathcal{M}(A, B)$ of $\mathcal{K}$ has an orthogonal decomposition*

$$\mathcal{M}(A, B) = \bigoplus_{v\in V} \mathcal{M}(v),$$

with $\mathcal{M}(v)$ maximal isotropic subspaces of ${}^{d}\mathcal{L}_v$.

Otherwise the boundary conditions are called non-local.

For instance, for a single-vertex graph any boundary conditions are local. The boundary conditions considered in Example 3.4 of [45] are non-local.

Recall (see Section 3) that $\mathcal{M}(A, B)$ denotes the maximal isotropic subspace of $\mathcal{K}$ corresponding to the boundary conditions (A, B). It is defined through (3.9).

The following proposition gives another characterization of local boundary conditions (cf. [45]).

Proposition 4.2. *Given the graph $\mathcal{G} = \mathcal{G}(V, \mathcal{I}, \mathcal{E}, \partial)$, the boundary conditions (A, B) satisfying* (3.10) *are local on $\mathcal{G}$ if and only if there is an invertible map $C : \mathcal{K} \to \mathcal{K}$ and linear transformations $A(v)$ and $B(v)$ in $\mathcal{L}_v$ such that the simultaneous orthogonal decompositions*

$$CA = \bigoplus_{v\in V} A(v) \quad \textit{and} \quad CB = \bigoplus_{v\in V} B(v) \tag{4.4}$$

are valid.

Proof. By Theorem 3.2 the boundary conditions (A, B) are local if and only if there exist linear maps $(A(v), B(v)) : {}^{d}\mathcal{L}_v \to \mathcal{L}_v$ such that $\mathcal{M}(v) = \mathrm{Ker}\,(A(v), B(v))$ for all $v \in V$ and

$$\mathrm{Ker}\,(A, B) = \bigoplus_{v\in V} \mathrm{Ker}\,(A(v), B(v)).$$

In turn, the last condition holds if and only if there is an invertible map $C : \mathcal{K} \to \mathcal{K}$ such that (4.4) holds. $\square$

Remark 4.3. *Let $P_{\mathcal{L}_v}$ be the orthogonal projection in $\mathcal{K}$ onto $\mathcal{L}_v$. For an arbitrary graph $\mathcal{G}$ the number*

$$A_{v,v'} := \mathrm{tr}\, P_{\mathcal{L}_v} T(0; \underline{a}) P_{\mathcal{L}_{v'}}$$

is the (v, v')-entry of the adjacency matrix of $\mathcal{G}$. In particular, for simple graphs $A_{v,v'} = 1$ if and only if the vertices $v \neq v'$ are adjacent and $A_{v,v'} = 0$ otherwise.

Definition 4.4. *Given a $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ to any vertex $v \in V = V$ we associate the graph $\mathcal{G}_v = (\{v\}, \mathcal{I}_v, \mathcal{E}_v, \partial_v)$ with the following properties*

(i) $\mathcal{I}_v = \varnothing$,
(ii) $\partial_v(e) = v$ *for all* $e \in \mathcal{E}_v$,
(iii) $|\mathcal{E}_v| = \deg_{\mathcal{G}}(v)$, *the degree of the vertex v in the graph $\mathcal{G}$,*
(iv) *there is an injective map $\Psi_v : \mathcal{E}_v \to \mathcal{E} \cup \mathcal{I}$ such that $v \in \partial \circ \Psi_v(e)$ for all $e \in \mathcal{E}_v$.*

Boundary conditions $(A(v), B(v))$ on each of the graphs $\mathcal{G}_v$ induce local boundary conditions (A, B) on the graph $\mathcal{G}$ with

$$A = \bigoplus_{v\in V} A(v) \quad \text{and} \quad B = \bigoplus_{v\in V} B(v).$$

Example 4.5 (Standard boundary conditions)**.** *Given a graph $\mathcal{G}$ with $|V| \geq 2$ and minimum degree not less than two, define the boundary conditions $(A(v), B(v))$ on $\mathcal{G}_v$ for every $v \in V$ by the* $\deg(v) \times \deg(v)$ *matrices*

$$A(v) = \begin{pmatrix} 1 & -1 & 0 & \ldots & 0 & 0 \\ 0 & 1 & -1 & \ldots & 0 & 0 \\ 0 & 0 & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 1 & -1 \\ 0 & 0 & 0 & \ldots & 0 & 0 \end{pmatrix}, \qquad B(v) = \begin{pmatrix} 0 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & 0 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & 0 & 0 \\ 1 & 1 & 1 & \ldots & 1 & 1 \end{pmatrix}. \tag{4.5}$$

Obviously, $A(v)B(v)^\dagger = 0$ and $(A(v), B(v))$ has maximal rank. Thus, for every $v \in V$ the boundary conditions (4.5) *define self-adjoint Laplace operators $\Delta(A(v), B(v))$ on $L^2(\mathcal{G}_v)$. By Lemma 3.14 they are real. The corresponding scattering matrices are given by*

$$[S_v(\mathsf{k})]_{e,e'} = -\frac{\deg(v) - 2}{\deg(v)}\delta_{e,e'} + \frac{2}{\deg(v)}(1 - \delta_{e,e'})$$

with $\delta_{e,e'}$ Kronecker symbol. They do not depend on k and are permutation invariant and symmetric. Except for the case $\deg(v) = 2$ *all their entries are non-vanishing.*

The boundary conditions (4.5) *induce local boundary conditions (A, B) on the graph $\mathcal{G}$. The resulting boundary conditions (under various names) are widely used in different models (see, e.g., the review* [52] *and references quoted there).*

Now we are in position to discuss the question how to reconstruct the graph from the boundary conditions. First we present the main result of this section.

Theorem 4.6. *Given the sets $\mathcal{E}$ and $\mathcal{I}$ let the boundary conditions (A, B) satisfy* (3.10)*. Then, there is a graph $\mathcal{G} = \mathcal{G}(V, \mathcal{I}, \mathcal{E}, \partial)$ with $|\mathcal{I}|$ internal and $|\mathcal{E}|$ external edges for which these boundary conditions are local. This graph is unique under the requirement that the number of vertices $|V|$ is maximal.*

Theorem 4.6 as well as a sketch of its proof was presented by the authors in [42]. Below we will give a complete proof. We emphasize that the graph referred to in this theorem need not satisfy Assumption 1, that is, it may be disconnected and may have tadpoles.

Consider the completely disjoint graph $\widehat{\mathcal{G}}$ with $|\mathcal{E}|$ external and $|\mathcal{I}|$ internal edges having $|\mathcal{I}| + |\mathcal{E}|$ disjoint components, i.e., any vertex of this graph is of degree 1. Let $\widehat{V}$ be the vertex set of this graph,

$$\widehat{V} = \{\partial(e)\}_{e\in\mathcal{E}} \cup \{\partial^-(i)\}_{i\in\mathcal{I}} \cup \{\partial^+(i)\}_{i\in\mathcal{I}}. \tag{4.6}$$

Now consider an arbitrary partition $\underline{\mathcal{O}}$ of the set $\widehat{V}$,

$$\underline{\mathcal{O}} = \{\mathcal{O}(v)\}_{v\in V},$$

where $\mathcal{O}(v)$ are subsets of $\widehat{V}$ satisfying

$$\bigcup_{v\in V} \mathcal{O}(v) = \widehat{V} \qquad \text{and} \qquad \mathcal{O}(v) \cap \mathcal{O}(v') = \varnothing \quad \text{for} \quad v \neq v'.$$

Here $V(\underline{\mathcal{O}})$ is a set labeling the blocks $\mathcal{O}(v)$ of the partition $\underline{\mathcal{O}}$. Let $\mathcal{G}(\underline{\mathcal{O}})$ be the graph obtained from $\widehat{\mathcal{G}}$ by identifying points in $\widehat{V}$ whenever they lie in the same $\mathcal{O}(v)$ for some $v \in V(\underline{\mathcal{O}})$. The vertex set $V(\mathcal{G}(\underline{\mathcal{O}}))$ of the graph $\mathcal{G}(\underline{\mathcal{O}})$ is then, obviously, equipotent to $V(\underline{\mathcal{O}})$ and, thus, can be identified with $V(\underline{\mathcal{O}})$. Since the property for two points to belong to the same $\mathcal{O}(v)$ is an equivalence relation, we can write

$$\mathcal{G}(\underline{\mathcal{O}}) = \widehat{\mathcal{G}}/\underline{\mathcal{O}}. \tag{4.7}$$

We will call the graph $\mathcal{G}(\underline{\mathcal{O}})$ the *contraction* of the graph $\widehat{\mathcal{G}}$ associated with the partition $\underline{\mathcal{O}}$. In the case of the trivial partition $\underline{\mathcal{O}}_{\mathrm{trivial}} = \{\widehat{V}\}$, the resulting graph has exactly one vertex.

We will say that a partition $\underline{\mathcal{O}}'$ of $\widehat{V}$ is *finer* than $\underline{\mathcal{O}}$ and write $\underline{\mathcal{O}}' \succeq \underline{\mathcal{O}}$ if to any $\mathcal{O}'(v') \in \underline{\mathcal{O}}'$ there is $\mathcal{O}(v) \in \underline{\mathcal{O}}$ with $\mathcal{O}'(v') \subseteq \mathcal{O}(v)$. We will also write $\underline{\mathcal{O}}' \succ \underline{\mathcal{O}}$ if $\underline{\mathcal{O}}' \succeq \underline{\mathcal{O}}$ and $\underline{\mathcal{O}}' \neq \underline{\mathcal{O}}$.

The finest partition $\underline{\mathcal{O}}_{\mathrm{finest}}$ is the partition which is formed by all one-element subsets of $\widehat{V}$. Note that $\widehat{\mathcal{G}} = \mathcal{G}(\underline{\mathcal{O}}_{\mathrm{finest}})$.

For a given partition $\underline{\mathcal{O}}$ the condition that the graph $\mathcal{G}(\underline{\mathcal{O}})$ has no tadpoles, i.e. for no edge its initial and terminal vertices coincide, is equivalent to the condition that all $\partial^-(i)$ and $\partial^+(i)$ lie in different $\mathcal{O}(v)$. The condition that the graph $\mathcal{G}(\underline{\mathcal{O}})$ is connected is equivalent to the statement that to each pair of vertices $v, v' \in V(\mathcal{G}(\underline{\mathcal{O}}))$ there is a sequence $i_1, i_2, \cdots, i_K$ of elements in $\mathcal{I}$ and vertices $v = v_1, \cdots, v_{K+1} = v'$ such that $i_k \in \mathcal{S}(v_k) \cap \mathcal{S}(v_{k+1})$ for all $1 \leq k \leq K$.

Definition 4.7. *A partition $\underline{\mathcal{O}}$ of the set $\widehat{V}$ (defined in* (4.6)*) is* admissible *for the boundary conditions (A, B) if the maximal isotropic subspace $\mathcal{M}(A, B)$ of ${}^d\mathcal{K}$ has an orthogonal decomposition*

$$\mathcal{M}(A, B) = \bigoplus_{v \in V(\underline{\mathcal{O}})} \mathcal{M}(v),$$

with $\mathcal{M}(v)$ maximal isotropic subspaces of ${}^d\mathcal{L}_v$.

By definition, if a partition $\underline{\mathcal{O}}$ is admissible for boundary conditions (A, B), then it is also admissible for all boundary conditions (A', B') such that $\mathcal{M}(A', B') = \mathcal{M}(A, B)$ and it also makes sense to speak of admissibility for a maximal isotropic subspace $\mathcal{M}$. Furthermore, a partition $\underline{\mathcal{O}}$ is admissible for the boundary conditions (A, B) if and only if ${}^d\mathcal{L}_v \cap \mathcal{M}(A, B)$ is a maximal isotropic subspace of ${}^d\mathcal{L}_v$ for each $v \in V(\underline{\mathcal{O}})$. For each $\mathcal{M}$ there is at least one admissible partition for each $\mathcal{M}$, namely the trivial one, where $\underline{\mathcal{O}} = \{\widehat{V}\}$. In this case the resulting graph $\mathcal{G}(\underline{\mathcal{O}})$ has exactly one vertex.

Definitions 4.1 and 4.7 immediately imply the following proposition.

Proposition 4.8. *Let $\underline{\mathcal{O}}$ be an arbitrary partition of the set $\widehat{V}$. The boundary conditions (A, B) are local on the graph $\mathcal{G}(\underline{\mathcal{O}})$ if and only if the partition $\underline{\mathcal{O}}$ is admissible for these boundary conditions.*

Definition 4.9. *An admissible partition $\underline{\mathcal{O}}$ for boundary conditions (A, B) is* maximal *if there is no admissible partition $\underline{\mathcal{O}}'$ such that $\underline{\mathcal{O}}' \succ \underline{\mathcal{O}}$.*

Proposition 4.10. *For any boundary conditions (A, B) satisfying* (3.10) *there is a unique maximal admissible partition $\underline{\mathcal{O}}(A, B)$ of the set $\widehat{V}$.*

We start the proof of the proposition with the following observation.

Let $\underline{\mathcal{O}}_1 = \{\mathcal{O}_1(v_1)\}_{v_1 \in V_1}$ and $\underline{\mathcal{O}}_2 = \{\mathcal{O}_2(v_2)\}_{v_2 \in V_2}$ be two partitions of $\widehat{V}$. By $\underline{\mathcal{O}}_1 \cap \underline{\mathcal{O}}_2$ we denote the set of all nonempty intersections $\mathcal{O}_1(v_1) \cap \mathcal{O}_2(v_2) \neq \emptyset$. Obviously, any two distinct elements of $\underline{\mathcal{O}}_1 \cap \underline{\mathcal{O}}_2$ have empty intersection. Furthermore, the union of all elements of $\mathcal{O}_1(v_1) \cap \mathcal{O}_2(v_2)$ gives the whole $\widehat{V}$. Thus, $\underline{\mathcal{O}}_1 \cap \underline{\mathcal{O}}_2$ is also a partition of $\widehat{V}$. Obviously, $\underline{\mathcal{O}}_1 \cap \underline{\mathcal{O}}_2 \succeq \underline{\mathcal{O}}_1$ and $\underline{\mathcal{O}}_1 \cap \underline{\mathcal{O}}_2 \succeq \underline{\mathcal{O}}_2$.

For any $\mathcal{O} \subset \underline{\mathcal{O}}$ we set

$$(4.8)\qquad {}^d\mathcal{L}_{\mathcal{O}} := \bigoplus_{v \in \mathcal{O}} {}^d\mathcal{L}_v.$$

Lemma 4.11. *Let $\underline{\mathcal{O}}_1$ and $\underline{\mathcal{O}}_2$ be two admissible partitions for the maximal isotropic subspace $\mathcal{M}$. Then the partition $\underline{\mathcal{O}}_1 \cap \underline{\mathcal{O}}_2$ is also admissible for $\mathcal{M}$.*

Proof. Let $\mathcal{O}_1$ and $\mathcal{O}_2$ be any two subsets of $\widehat{V}$ with empty intersection and such that

$$\mathcal{M}_{\mathcal{O}_q} := \mathcal{M} \cap {}^d\mathcal{L}_{\mathcal{O}_q}$$

is maximal isotropic in $\mathcal{L}_{\mathcal{O}_q}$ for $q=1,2$. Then, obviously, $\mathcal{M}_{\mathcal{O}_1}\oplus\mathcal{M}_{\mathcal{O}_2}$ is maximal isotropic in ${}^d\mathcal{L}_{\mathcal{O}_1\cup\mathcal{O}_2} = {}^d\mathcal{L}_{\mathcal{O}_1}\oplus{}^d\mathcal{L}_{\mathcal{O}_2}$ such that the relation $\mathcal{M}_{\mathcal{O}_1\cup\mathcal{O}_2}=\mathcal{M}_{\mathcal{O}_1}\oplus\mathcal{M}_{\mathcal{O}_2}$ holds.

With this observation it suffices to prove the following: Given a maximal isotropic subspace $\mathcal{M}$, let $\mathcal{O}$ and $\mathcal{O}'$ be two subsets of $\widehat{V}$ having nonempty intersection. Assume that both subspaces $\mathcal{M}_{\mathcal{O}} := \mathcal{M}\cap {}^d\mathcal{L}_{\mathcal{O}}$ and $\mathcal{M}_{\mathcal{O}'} := \mathcal{M}\cap {}^d\mathcal{L}_{\mathcal{O}'}$ are maximal isotropic in ${}^d\mathcal{L}_{\mathcal{O}}$ and ${}^d\mathcal{L}_{\mathcal{O}'}$, respectively. Then $\mathcal{M}_{\mathcal{O}\cap\mathcal{O}'} := \mathcal{M}\cap {}^d\mathcal{L}_{\mathcal{O}\cap\mathcal{O}'}$ is maximal isotropic in ${}^d\mathcal{L}_{\mathcal{O}\cap\mathcal{O}'}$.

The isotropy is obvious. By Lemma 3.1 to prove the maximality it suffices to show the relation

$$\mathcal{M}^{\perp}_{\mathcal{O}\cap\mathcal{O}'} = J\mathcal{M}_{\mathcal{O}\cap\mathcal{O}'} \tag{4.9}$$

with J the canonical symplectic matrix on ${}^d\mathcal{L}_{\mathcal{O}\cap\mathcal{O}'}$. From the definition (4.8) of ${}^d\mathcal{L}_{\mathcal{O}}$ it follows that ${}^d\mathcal{L}_{\mathcal{O}\cap\mathcal{O}'} = {}^d\mathcal{L}_{\mathcal{O}}\cap{}^d\mathcal{L}_{\mathcal{O}'}$. Thus,

$$\mathcal{M}_{\mathcal{O}\cap\mathcal{O}'} = \mathcal{M}\cap{}^d\mathcal{L}_{\mathcal{O}}\cap{}^d\mathcal{L}_{\mathcal{O}'} = \mathcal{M}_{\mathcal{O}}\cap\mathcal{M}_{\mathcal{O}'}.$$

Since $\mathcal{M}_{\mathcal{O}}$ and $\mathcal{M}_{\mathcal{O}'}$ are maximal isotropic, by Lemma 3.1 we have $\mathcal{M}^{\perp}_{\mathcal{O}} = J\mathcal{M}_{\mathcal{O}}$ and $\mathcal{M}^{\perp}_{\mathcal{O}'} = J\mathcal{M}_{\mathcal{O}'}$. Therefore, for any $\chi\in{}^d\mathcal{L}_{\mathcal{O}\cap\mathcal{O}'}$ there are $\chi_1,\chi_2\in\mathcal{M}_{\mathcal{O}}$ and $\chi_1',\chi_2'\in\mathcal{M}_{\mathcal{O}'}$ such that

$$\chi = \chi_1 + J\chi_2 = \chi_1' + J\chi_2'.$$

This implies that $\chi_1-\chi_1' = -J(\chi_2-\chi_2')$. Since both $\chi_1-\chi_1'$ and $\chi_2-\chi_2'$ are elements of $\mathcal{M}$ from Lemma 3.1 again it follows that they both are null vectors. Therefore, $\chi_1=\chi_1'\in\mathcal{M}_{\mathcal{O}\cap\mathcal{O}'}$ and $\chi_2=\chi_2'\in\mathcal{M}_{\mathcal{O}\cap\mathcal{O}'}$. Thus, we obtain ${}^d\mathcal{L}_{\mathcal{O}\cap\mathcal{O}'} = \mathcal{M}_{\mathcal{O}\cap\mathcal{O}'}\oplus J\mathcal{M}_{\mathcal{O}\cap\mathcal{O}'}$ which implies (4.9). □

Proof of Proposition 4.10. The relation $\succeq$ is a partial order on the set of all admissible partitions of $\widehat{V}$. Thus, by the Zorn lemma there exists an admissible partition $\underline{\mathcal{O}}_{\max}$ such that

$$\text{there is no admissible partition}\quad \underline{\mathcal{O}}\quad\text{such that}\quad \underline{\mathcal{O}}\succ\underline{\mathcal{O}}_{\max}. \tag{4.10}$$

Assume there is an admissible partition $\underline{\mathcal{O}}$ incomparable with $\underline{\mathcal{O}}_{\max}$, that is, neither $\underline{\mathcal{O}}\succeq\underline{\mathcal{O}}_{\max}$ nor $\underline{\mathcal{O}}_{\max}\succeq\underline{\mathcal{O}}$ is valid. By Lemma 4.11 the partition $\underline{\mathcal{O}}\cap\underline{\mathcal{O}}_{\max}$ is admissible. Moreover, $\underline{\mathcal{O}}\cap\underline{\mathcal{O}}_{\max}\succeq\underline{\mathcal{O}}$ and $\underline{\mathcal{O}}\cap\underline{\mathcal{O}}_{\max}\succeq\underline{\mathcal{O}}_{\max}$, which contradicts (4.10). Thus, $\underline{\mathcal{O}}_{\max}$ is a maximal admissible partition in the sense of Definition 4.9. Its uniqueness is now obvious. □

Proof of Theorem 4.6. The claim follows immediately from Propositions 4.8 and 4.10. □

We conclude this section with two comments. First, an admissible partition $\underline{\mathcal{O}}$ for the maximal isotropic subspace $\mathcal{M}$ is also admissible for $\mathcal{M}^{\perp}$. If $\underline{\mathcal{O}}$ is maximal for $\mathcal{M}$, then it is also maximal for $\mathcal{M}^{\perp}$. Indeed, let $\underline{\mathcal{O}}$ be an admissible partition for the maximal isotropic subspace $\mathcal{M}$. Observe that the canonical symplectic matrix J (3.5) leaves the subspace ${}^d\mathcal{L}_{\mathcal{O}}$ invariant for any $\mathcal{O}\in\underline{\mathcal{O}}$. Hence,

$$(\mathcal{M}^{\perp})_{\mathcal{O}} = \mathcal{M}^{\perp}\cap{}^d\mathcal{L}_{\mathcal{O}} = J\mathcal{M}\cap{}^d\mathcal{L}_{\mathcal{O}} = J(\mathcal{M}\cap{}^d\mathcal{L}_{\mathcal{O}}) = J\mathcal{M}_{\mathcal{O}}.$$

But then we obtain

$$\bigoplus_{\mathcal{O}\in\underline{\mathcal{O}}}(\mathcal{M}^{\perp})_{\mathcal{O}} = \bigoplus_{\mathcal{O}\in\underline{\mathcal{O}}} J\mathcal{M}_{\mathcal{O}} = J\mathcal{M} = \mathcal{M}^{\perp},$$

which implies that the partition $\underline{\mathcal{O}}$ is admissible for $\mathcal{M}^{\perp}$.

Second, there is an alternative way of proving Theorem 4.6 based on the concept of reducible matrices (see [25] and the literature quoted therein) which goes back to Frobenius. An $n\times n$ matrix M is called *reducible* (by Frobenius *zerlegbar* or *zerfallend*) if there is a permutation matrix Π such that $\Pi M\Pi^{-1}$ has triangular block form

$$\Pi M\Pi^{-1} = \begin{pmatrix} M_{00} & M_{01}\\ 0 & M_{11}\end{pmatrix}.$$

Otherwise Z is called *irreducible*. Recall that any permutation matrix is unitary. Hence, if M is unitary, then necessary $M_{01} = 0$ and both M_{00} and M_{11} are also unitary. If for a unitary matrix $U \in \mathsf{U}(n)$ there is a permutation matrix Π such that

$$\Pi U \Pi^{-1} = \begin{pmatrix} U_1 & 0 & \cdots & 0 \\ 0 & U_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & U_m \end{pmatrix}, \qquad m \leq n,$$

where every U_k is irreducible, then Π is called *maximal*. One can prove that a maximal permutation matrix does exist and it is unique up to a permutation of the blocks and permutations within each of the blocks.

Now fix $\mathsf{k}_0 > 0$ arbitrarily and determine a maximal permutation matrix Π for $\mathfrak{S}(\mathsf{k}_0; A, B)$. Then by relation (3.22) this gives

$$\Pi \mathfrak{S}(\mathsf{k}) \Pi^{-1} = \begin{pmatrix} \mathfrak{S}_1(\mathsf{k}) & 0 & \cdots & 0 \\ 0 & \mathfrak{S}_2(\mathsf{k}) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathfrak{S}_m(\mathsf{k}) \end{pmatrix} \tag{4.11}$$

for all $\mathsf{k} \in \mathbb{R}$. Obviously, Π and m determine uniquely the graph for which the boundary conditions (A, B) are local. The number m in (4.11) is the number of vertices of this graph, the blocks $\mathfrak{S}_1(\mathsf{k}), \ldots, \mathfrak{S}_m(\mathsf{k})$ represent the matrices (3.14) associated with maximal isotropic subspaces $\mathcal{M}(v)$ from Definition 4.1.

5. Harmonic Analysis of Scattering Matrices

In this section we perform harmonic analysis of the scattering matrix with respect to the lengths $\underline{a} = \{a_i\}_{i \in \mathcal{I}} \in (\mathbb{R}_+)^{|\mathcal{I}|}$ of the internal edges of the graph $\mathcal{G}$. Throughout the whole section we will assume that the (topological) graph $\mathcal{G}$ as well as the boundary conditions (A, B) are fixed. To carry out the analysis we will now treat $\underline{a}$ as a parameter which may belong to $\mathbb{R}^{|\mathcal{I}|}$ or even $\mathbb{C}^{|\mathcal{I}|}$.

We start with the following simple but important observation.

Lemma 5.1. *For arbitrary $\mathsf{k} > 0$ the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ is uniquely defined as a solution of (3.26) for all $\underline{a} \in \mathbb{R}^{|\mathcal{I}|}$. Moreover, the scattering matrix is periodic with respect to $\underline{a}$,*

$$S\left(\mathsf{k}; A, B, \underline{a} + \frac{2\pi}{\mathsf{k}}\underline{\ell}\right) = S(\mathsf{k}; A, B, \underline{a}), \qquad \underline{a} \in \mathbb{R}^{|\mathcal{I}|}$$

for arbitrary $\underline{\ell} \in \mathbb{Z}^{|\mathcal{I}|}$.

Proof. It suffices to consider those $\underline{a} \in \mathbb{R}^{|\mathcal{I}|}$ for which $\det K(\mathsf{k}; A, B, \underline{a}) = 0$, since the claim is obvious when the determinant is non-vanishing. For $\underline{a} \in (\mathbb{R}_+)^{|\mathcal{I}|}$ the fact that $S(\mathsf{k}; A, B, \underline{a})$ is uniquely defined as a solution of (3.26) is guaranteed by Theorem 3.10. The case of arbitrary $\underline{a} \in \mathbb{R}^{|\mathcal{I}|}$ can be treated in exactly the same way (see the proof of Theorem 3.2 in [42]).

The periodicity follows immediately from (3.33) and the fact that the matrix $T(\mathsf{k}; \underline{a})$ defined in (3.32) is $\frac{2\pi}{\mathsf{k}}\mathbb{Z}^{|\mathcal{I}|}$-periodic. □

Lemma 5.1 suggests to consider a Fourier expansion of the scattering matrix. The following theorem ensures the absolute convergence of the corresponding Fourier series.

Theorem 5.2. *Let $\mathsf{k} > 0$ be arbitrary. For all $\underline{a} \in \mathbb{R}^{|\mathcal{I}|}$ the Fourier expansion of the scattering matrix*

$$S(\mathsf{k}; A, B, \underline{a}) = \sum_{\underline{n} \in \mathbb{Z}^{|\mathcal{I}|}} \widehat{S}_{\underline{n}}(\mathsf{k}; A, B)\, \mathrm{e}^{\mathrm{i}\mathsf{k}\langle \underline{n}, \underline{a} \rangle} \tag{5.1}$$

with

$$\widehat{S}_{\underline{n}}(\mathsf{k}; A, B) = \left(\frac{\mathsf{k}}{2\pi}\right)^{|\mathcal{I}|} \int\limits_{[0,2\pi/\mathsf{k}]^{|\mathcal{I}|}} d\underline{a}\, S(\mathsf{k}; A, B, \underline{a})\, \mathrm{e}^{-\mathrm{i}\mathsf{k}\langle \underline{n}, \underline{a}\rangle} \tag{5.2}$$

converges absolutely and uniformly on compact subsets of $\mathbb{R}^{|\mathcal{I}|}$. *The Fourier coefficients* (5.2) *vanish for all* $\underline{n} = \{n_i\}_{i\in\mathcal{I}} \in \mathbb{Z}^{|\mathcal{I}|}$ *for which* $n_i < 0$ *for at least one* $i \in \mathcal{I}$.

For the proof we need a couple of auxiliary results. Set

$$\mathcal{A} = \left\{\underline{a} = \{a_i\}_{i\in\mathcal{I}} \middle|\, \operatorname{Re} a_i \in \mathbb{R},\ \operatorname{Im} a_i > 0\right\} \subset \mathbb{C}^{|\mathcal{I}|}.$$

Lemma 5.3. *For any* $\mathsf{k} > 0$ *the determinant* $\det K(\mathsf{k}; A, B, \underline{a})$ *does not vanish for all* $\underline{a} \in \mathcal{A}$.

Proof. If $\underline{a} \in \mathcal{A}$, then $\|\mathfrak{S}(\mathsf{k}; A, B)T(\mathsf{k}; \underline{a})\| < 1$. Thus, all eigenvalues of $\mathfrak{S}(\mathsf{k}; A, B)T(\mathsf{k}; \underline{a})$ are strictly less than 1. Therefore, $\det K(\mathsf{k}; A, B, \underline{a}) \neq 0$ for all $\underline{a} \in \mathcal{A}$. □

Set

$$\Sigma(\mathsf{k}; A, B) := \{\underline{a} \in \operatorname{clos}(\mathcal{A}) |\ \det K(\mathsf{k}; A, B, \underline{a}) = 0\}.$$

By Lemma 5.3 we have the inclusion $\Sigma(\mathsf{k}; A, B) \subset \partial\mathcal{A}$. If $\Sigma(\mathsf{k}; A, B) \neq \emptyset$, then it is a real analytic subvariety of $\mathcal{A}$ of codimension at least 1. The following example shows that the set $\Sigma(\mathsf{k}; A, B)$ in general need not to belong to $\mathbb{R}^{|\mathcal{I}|} \subset \partial\mathcal{A}$.

Example 5.4. *Consider the graph* $\mathcal{G}$ *with* $\mathcal{I} = \{i_1, i_2, i_3\}$ *and* $\mathcal{E} = \{e_1, e_2\}$ *depicted in Fig. 1. The local boundary conditions* (A, B) *are defined by the standard boundary conditions (see Example 4.5) at the vertices of the graph.*

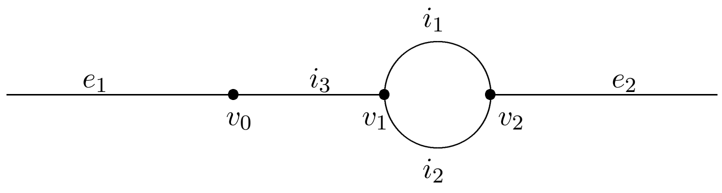

FIG. 1. The graph from Example 5.4.

A simple calculation shows that

$$\Sigma(\mathsf{k}; A, B) = \left\{a_{i_1} = \frac{\pi n_1}{\mathsf{k}},\ a_{i_2} = \frac{\pi n_2}{\mathsf{k}},\ a_{i_3} \in \mathbb{C}_+ \middle|\, n_1, n_2 \in \mathbb{Z},\ n_1 + n_2 \in 2\mathbb{Z}\right\},$$

which is a subset of the boundary $\partial\mathcal{A}$ *but not of* $\mathbb{R}^{|\mathcal{I}|}$. *Here* $\mathbb{C}_+$ *denotes the closed upper complex half-plane.*

Proposition 5.5. *Let* $\mathsf{k} > 0$ *be arbitrary. For all*

$$\underline{a} \in \operatorname{clos}(\mathcal{A}) := \left\{\underline{a} = \{a_i\}_{i\in\mathcal{I}} \middle|\, \operatorname{Re} a_i \in \mathbb{R},\ \operatorname{Im} a_i \geq 0\right\}$$

the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ *is uniquely defined as a solution of* (3.26) *and satisfies the bound*

$$\|S(\mathsf{k}; A, B, \underline{a})\| \leq 1. \tag{5.3}$$

Moreover, it is a rational function of $\underline{t} = \{t_i\}_{i\in\mathcal{I}} \in \mathbb{D}^{|\mathcal{I}|} = \{\zeta \in \mathbb{C} | \, |\zeta| < 1\}^{|\mathcal{I}|}$ *with* $t_i := \mathrm{e}^{\mathrm{i}\mathsf{k}a_i}$, *i.e. a quotient of a* $\mathcal{B}(\mathcal{K}_{\mathcal{E}})$*-valued polynomial and a* $\mathbb{C}$*-valued polynomial in the variables* t_i. *Thus, for all* $\underline{a} \in \mathrm{clos}(\mathcal{A})$ *the scattering matrix is* $\frac{2\pi}{\mathsf{k}}\mathbb{Z}^{|\mathcal{I}|}$*-periodic,*

$$S\left(\mathsf{k}; A, B, \underline{a} + \frac{2\pi}{\mathsf{k}}\underline{\ell}\right) = S(\mathsf{k}, A, B, \underline{a}), \qquad \underline{\ell} \in \mathbb{Z}^{|\mathcal{I}|}.$$

Proof. By Lemma 5.3 equation (3.33) has a unique solution for all $\underline{a} \in \mathcal{A}$. Equations (3.34) and (3.28) imply that $K(\mathsf{k}; A, B, \underline{a})$ is a polynomial function of the components of $\underline{t}$. Obviously, $K(\mathsf{k}; A, B, \underline{a})^{-1}$ is a rational function of $\underline{t}$. Thus, by (3.33) the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ is a rational function of $\underline{t}$. Thus, it is $\frac{2\pi}{\mathsf{k}}\mathbb{Z}^{|\mathcal{I}|}$-periodic.

Using (3.33) it is easy to check that this solution satisfies the relation

$$\begin{pmatrix} S(\mathsf{k}; A, B, \underline{a}) \\ \alpha(\mathsf{k}; A, B, \underline{a}) \\ \mathrm{e}^{-\mathrm{i}\mathsf{k}\underline{a}}\beta(\mathsf{k}; A, B, \underline{a}) \end{pmatrix} = \mathfrak{S}(\mathsf{k}; A, B) \begin{pmatrix} \mathbb{I} \\ \beta(\mathsf{k}; A, B, \underline{a}) \\ \mathrm{e}^{\mathrm{i}\mathsf{k}\underline{a}}\alpha(\mathsf{k}; A, B, \underline{a}) \end{pmatrix},$$

where $\mathfrak{S}(\mathsf{k}; A, B)$ is defined in (3.14). Since $\mathfrak{S}(\mathsf{k}; A, B)$ is unitary we obtain

$$\begin{aligned} S(\mathsf{k}; A, B, \underline{a})^\dagger S(\mathsf{k}; A, B, \underline{a}) + \alpha(\mathsf{k}; A, B, \underline{a})^\dagger(\mathbb{I} - \mathrm{e}^{-2\mathsf{k}\operatorname{Im}\underline{a}})\alpha(\mathsf{k}; A, B, \underline{a}) \\ + \beta(\mathsf{k}; A, B, \underline{a})^\dagger(\mathrm{e}^{2\mathsf{k}\operatorname{Im}\underline{a}} - \mathbb{I})\beta(\mathsf{k}; A, B, \underline{a}) = \mathbb{I}, \end{aligned} \tag{5.4}$$

where $\mathrm{e}^{\pm 2\mathsf{k}\operatorname{Im}\underline{a}} := \mathrm{diag}\{\mathrm{e}^{\pm 2\mathsf{k}\operatorname{Im} a_i}\}_{i\in\mathcal{I}}$. From (5.4) it follows immediately that

$$0 \leq S(\mathsf{k}; A, B, \underline{a})^\dagger S(\mathsf{k}; A, B, \underline{a}) \leq \mathbb{I}$$

in the sense of quadratic forms. This proves the bound (5.3) for all $\underline{a} \in \mathcal{A}$. Recalling Lemma 5.1 completes the proof. □

By Proposition 5.5 the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ is continuous at all points $\underline{a} \in \mathcal{A}$. A priori it is not clear whether its boundary values coincide with those given by equation (3.36) for all $\underline{a}$ in the subset $\Sigma(\mathsf{k}; A, B)$ of $\partial\mathcal{A}$ where $\det K(\mathsf{k}; A, B, \underline{a}) = 0$.

The following result shows the continuity of the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ at points $\underline{a} \in \Sigma(\mathsf{k}; A, B)$ along some non-tangential directions. Actually this result and an analyticity argument presented below will imply that the scattering matrix is continuous at all points $\underline{a} \in \mathrm{clos}(\mathcal{A})$.

Proposition 5.6. *Let* $\underline{a} \in \partial\mathcal{A}$ *and* $\mathsf{k} > 0$ *be arbitrary. For any sequence* $\{\underline{a}^{(n)}\}_{n\in\mathbb{N}}$, $\underline{a}^{(n)} \in \mathcal{A}$ *converging to* $\underline{a} \in \partial\mathcal{A}$ *and for all* $i \in \mathcal{I}$ *satisfying*

$$\lim_{n\to\infty} \frac{a_i^{(n)} - a_i}{|\underline{a}^{(n)} - \underline{a}|} = \gamma \in \mathbb{C} \setminus \{0\}, \tag{5.5}$$

where γ *is independent of* i, *the relation*

$$\lim_{n\to\infty} S(\mathsf{k}; A, B, \underline{a}^{(n)}) = S(\mathsf{k}; A, B, \underline{a}) \tag{5.6}$$

holds.

For the proof we need the following lemma, for which we introduce the shorthand notation

$$K(\underline{a}) \equiv K(\mathsf{k}; A, B, \underline{a}), \quad S(\underline{a}) \equiv S(\mathsf{k}; A, B, \underline{a}), \quad \Sigma \equiv \Sigma(\mathsf{k}; A, B), \quad \mathfrak{S} \equiv \mathfrak{S}(\mathsf{k}; A, B).$$

Lemma 5.7. *For arbitrary* $\mathsf{k} > 0$ *and arbitrary* $\underline{a} \in \partial\mathcal{A}\backslash\Sigma$ *let* $\underline{a}^{(n)} \in \mathcal{A}$ *be a sequence converging to* $\underline{a} \in \mathbb{R}$ *and satisfying* (5.5). *Then*

$$\lim_{n\to\infty} P_{\operatorname{Ran} K(\underline{a})^\dagger} K(\underline{a}^{(n)})^{-1} P_{\operatorname{Ran} K(\underline{a})} = \left(K(\underline{a})|_{\operatorname{Ran} K(\underline{a})^\dagger}\right)^{-1} P_{\operatorname{Ran} K(\underline{a})}.$$

Proof. It suffices to show that

$$\lim_{n\to\infty} P_{\operatorname{Ran} K(\underline{a})^\dagger} K(\underline{a}^{(n)})^{-1} K(\underline{a}) = P_{\operatorname{Ran} K(\underline{a})^\dagger}. \tag{5.7}$$

Indeed, for arbitrary $\widetilde{\chi} \in \operatorname{Ran} K(\underline{a})$ there is a unique $\chi \in \operatorname{Ran} K(\underline{a})^\dagger$ such that $K(\underline{a})\chi = \widetilde{\chi}$. Applying (5.7) to the vector $\chi \in \operatorname{Ran} K(\underline{a})$ we obtain

$$\lim_{n\to\infty} P_{\operatorname{Ran} K(\underline{a})^\dagger} K(\underline{a}^{(n)})^{-1} \widetilde{\chi} = \chi \equiv \Big(K(\underline{a})|_{\operatorname{Ran} K(\underline{a})^\dagger} \Big)^{-1} \widetilde{\chi},$$

from which the claim follows.

Since $T(\mathsf{k};\underline{a})$ is a contraction for all $\underline{a} \in \partial\mathcal{A}$ and $\mathfrak{S}$ is unitary, similarly to the observation made in the proof of Theorem 3.10 we conclude that $\operatorname{Ran} K(\underline{a})^\dagger = \operatorname{Ran} K(\underline{a})$. Thus, (5.7) is equivalent to the condition

$$\lim_{n\to\infty} P_{\operatorname{Ran} K(\underline{a})} K(\underline{a}^{(n)})^{-1} K(\underline{a}) = P_{\operatorname{Ran} K(\underline{a})}. \tag{5.8}$$

We represent $K(\underline{a})$ and $K(\underline{a}^{(n)})$ as block matrices

$$K(\underline{a}) = \begin{pmatrix} K_{00}(\underline{a}) & 0 \\ 0 & 0 \end{pmatrix}, \qquad K(\underline{a}^{(n)}) = \begin{pmatrix} K_{00}(\underline{a}^{(n)}) & K_{01}(\underline{a}^{(n)}) \\ K_{10}(\underline{a}^{(n)}) & K_{11}(\underline{a}^{(n)}) \end{pmatrix}$$

with respect to the orthogonal decomposition $\mathcal{K} = \operatorname{Ran} K(\underline{a}) \oplus \operatorname{Ker} K(\underline{a})$.

For arbitrary $\widetilde{\chi}_0 \in \operatorname{Ran} K(\underline{a})$ we consider the linear equation

$$\begin{aligned} K_{00}(\underline{a}^{(n)})\chi_0^{(n)} + K_{01}(\underline{a}^{(n)})\chi_1^{(n)} &= \widetilde{\chi}_0, \\ K_{10}(\underline{a}^{(n)})\chi_0^{(n)} + K_{11}(\underline{a}^{(n)})\chi_1^{(n)} &= 0. \end{aligned}$$

By the assumption that $K(\underline{a}^{(n)})$ is invertible, this equation is uniquely solvable for all $n \in \mathbb{N}$. Since $K_{00}(\underline{a})$ is invertible and $K_{00}(\underline{a}^{(n)}) \to K_{00}(\underline{a})$ as $n \to \infty$, we have that $K_{00}(\underline{a}^{(n)})$ is invertible for all sufficiently large $n \in \mathbb{N}$ and $\|[K_{00}(\underline{a}^{(n)})]^{-1}\|$ is uniformly bounded. In particular, we have

$$\Big[K_{11}(\underline{a}^{(n)}) - K_{10}(\underline{a}^{(n)})[K_{00}(\underline{a}^{(n)})]^{-1}K_{01}(\underline{a}^{(n)})\Big]\,\chi_1^{(n)} = -K_{10}(\underline{a}^{(n)})[K_{00}(\underline{a}^{(n)})]^{-1}\widetilde{\chi}_0 \tag{5.9}$$

and

$$\chi_0^{(n)} = [K_{00}(\underline{a}^{(n)})]^{-1}\widetilde{\chi}_0 - [K_{00}(\underline{a}^{(n)})]^{-1}K_{01}(\underline{a}^{(n)})\chi_1^{(n)}. \tag{5.10}$$

Observe now that

$$\begin{aligned} K_{01}(\underline{a}^{(n)}) &= -P_0\mathfrak{S}[T(\mathsf{k};\underline{a}^{(n)}) - T(\mathsf{k};\underline{a})]P_1, \\ K_{10}(\underline{a}^{(n)}) &= -P_1\mathfrak{S}[T(\mathsf{k};\underline{a}^{(n)}) - T(\mathsf{k};\underline{a})]P_0, \\ K_{11}(\underline{a}^{(n)}) &= -P_1\mathfrak{S}[T(\mathsf{k};\underline{a}^{(n)}) - T(\mathsf{k};\underline{a})]P_1, \end{aligned}$$

where P_0 and P_1 abbreviate the orthogonal projections onto $\operatorname{Ran} K(\underline{a})$ and $\operatorname{Ker} K(\underline{a})$, respectively. Therefore, by (5.5) the limits

$$\begin{aligned} \widetilde{K}_{01} &:= \lim_{n\to\infty} |\underline{a} - \underline{a}^{(n)}|^{-1} K_{01}(\underline{a}^{(n)}), \\ \widetilde{K}_{10} &:= \lim_{n\to\infty} |\underline{a} - \underline{a}^{(n)}|^{-1} K_{10}(\underline{a}^{(n)}), \\ \widetilde{K}_{11} &:= \lim_{n\to\infty} |\underline{a} - \underline{a}^{(n)}|^{-1} K_{11}(\underline{a}^{(n)}) \end{aligned}$$

exist. The matrix $\widetilde{K}_{11}$ is invertible. Indeed, observe that

$$\operatorname{Ker} K(\underline{a}) \subset \mathcal{K}_{\mathcal{I}}. \tag{5.11}$$

By condition (5.5)

$$\lim_{n\to\infty} |\underline{a} - \underline{a}^{(n)}|^{-1} \Big[T(\mathsf{k};\underline{a}^{(n)}) - T(\mathsf{k};\underline{a})\Big]$$

is equal to $\mathrm{i}\mathsf{k}\gamma T(\mathsf{k};\underline{a})$. Therefore,

$$\lim_{n\to\infty}|\underline{a}-\underline{a}^{(n)}|^{-1}\mathfrak{S}[T(\mathsf{k};\underline{a}^{(n)})-T(\mathsf{k};\underline{a})]\chi_1=\mathrm{i}\mathsf{k}\gamma\mathfrak{S}T(\mathsf{k};\underline{a})\chi_1=\mathrm{i}\mathsf{k}\gamma\chi_1$$

for all $\chi_1\in\operatorname{Ker}K(\underline{a})$, which implies that $\widetilde{K}_{11}$ is invertible.

Divide equation (5.10) by $|\underline{a}-\underline{a}^{(n)}|$. Since $\widetilde{K}_{11}$ is invertible, we have that $|\underline{a}-\underline{a}^{(n)}|^{-1}K_{11}(\underline{a}^{(n)})$ is invertible for all sufficiently large $n\in\mathbb{N}$ and its inverse is uniformly bounded. Since

$$\lim_{n\to\infty}K_{01}(\underline{a}^{(n)})=0\qquad\text{and}\qquad\lim_{n\to\infty}K_{10}(\underline{a}^{(n)})=0,$$

the matrix

$$|\underline{a}-\underline{a}^{(n)}|^{-1}K_{10}(\underline{a}^{(n)})[K_{00}(\underline{a}^{(n)})]^{-1}K_{01}(\underline{a}^{(n)})$$

vanishes in the limit $n\to\infty$. Thus, taking the limit $n\to\infty$ we obtain that the solutions $\chi_1^{(n)}$ of equation (5.9) are uniformly bounded in n and, thus, by (5.10)

$$\lim_{n\to\infty}\chi_0^{(n)}=[K_{00}(\underline{a})]^{-1}\widetilde{\chi}_0.$$

This equality implies (5.8). □

Proof of Proposition 5.6. From Theorem 3.10 and Lemma 5.3 it follows that

$$S(\underline{a})=-\begin{pmatrix}\mathbb{I}&0&0\end{pmatrix}\Big(K(\underline{a})|_{\operatorname{Ran}K(\underline{a})^\dagger}\Big)^{-1}P_{\operatorname{Ran}K(\underline{a})}\mathfrak{S}\begin{pmatrix}\mathbb{I}\\0\\0\end{pmatrix}$$

and

$$\begin{aligned}S(\underline{a}^{(n)})&=-\begin{pmatrix}\mathbb{I}&0&0\end{pmatrix}K(\underline{a}^{(n)})^{-1}\mathfrak{S}\begin{pmatrix}\mathbb{I}\\0\\0\end{pmatrix}\\&=-\begin{pmatrix}\mathbb{I}&0&0\end{pmatrix}K(\underline{a}^{(n)})^{-1}P_{\operatorname{Ran}K(\underline{a})}\mathfrak{S}\begin{pmatrix}\mathbb{I}\\0\\0\end{pmatrix}.\end{aligned}$$

Thus, to prove the claim it suffices to show that

$$\lim_{n\to\infty}\begin{pmatrix}\mathbb{I}&0&0\end{pmatrix}K(\underline{a}^{(n)})^{-1}P_{\operatorname{Ran}K(\underline{a})}=\begin{pmatrix}\mathbb{I}&0&0\end{pmatrix}\Big(K(\underline{a})|_{\operatorname{Ran}K(\underline{a})^\dagger}\Big)^{-1}P_{\operatorname{Ran}K(\underline{a})}.\tag{5.12}$$

From (5.11) it follows that $\operatorname{Ker}K(\underline{a})$ is orthogonal to $\mathcal{K}_{\mathcal{E}}$. Thus,

$$\begin{pmatrix}\mathbb{I}&0&0\end{pmatrix}K(\underline{a}^{(n)})^{-1}P_{\operatorname{Ran}K(\underline{a})}=\begin{pmatrix}\mathbb{I}&0&0\end{pmatrix}P_{\operatorname{Ran}K(\underline{a})}K(\underline{a}^{(n)})^{-1}P_{\operatorname{Ran}K(\underline{a})}$$

for any $n\in\mathbb{N}$. Applying Lemma 5.7 we obtain (5.12). □

For fixed $\mathsf{k}>0$, consider

$$F(\underline{t}):=S(\mathsf{k};A,B,\underline{a})\quad\text{with}\quad\underline{t}=\{t_i\}_{i\in\mathcal{I}},\quad t_i=\mathrm{e}^{\mathrm{i}a_i\mathsf{k}}.\tag{5.13}$$

The map $\underline{a}\mapsto\underline{t}$ maps the set

$$\Big\{\underline{a}\in\mathbb{C}^{|\mathcal{I}|}\,\big|\,\underline{a}=\{a_i\}_{i\in\mathcal{I}}\text{ with }0<\operatorname{Re}a_i\leq 2\pi/\mathsf{k}\text{ and }\operatorname{Im}a_i>0\text{ for all }i\in\mathcal{I}\Big\}.$$

bijectively onto the polydisc $\mathbb{D}^{|\mathcal{I}|}=\{\zeta\in\mathbb{C}|\,|\zeta|<1\}^{|\mathcal{I}|}$. The interval $(0,2\pi/\mathsf{k}]$ is mapped onto the torus $\mathbb{T}^{|\mathcal{I}|}=\{\zeta\in\mathbb{C}|\,|\zeta|=1\}^{|\mathcal{I}|}$.

Lemma 5.8. *The function F is inner.*

Remark 5.9. *We recall that an operator-valued function on a polydisc $\mathbb{D}^d$ is said to be inner if it is holomorphic in $\mathbb{D}^d$ and takes unitary values for almost all points of $\mathbb{T}^d \subset \partial(\mathbb{D}^d)$ (the so called distinguished boundary of $\mathbb{D}^d$* [35]*). For $d = 1$ matrix-valued inner functions are studied, e.g., in* [71]. *In particular, an analog of the canonical factorization theorem for matrix-valued inner functions has been proven there. For the case $|\mathcal{E}| \geq 1$ arbitrary but $|\mathcal{I}| = 1$ by this result one can obtain a representation of the scattering matrix as a finite Blaschke product.*

Proof of Lemma 5.8. From Proposition 5.5 it follows that F is holomorphic in the punctured open polydisc $\mathbb{D}^{|\mathcal{I}|} \setminus \{0\}$. By (5.3) we have $\|F(\underline{t})\| \leq 1$ for all $\underline{t} \in \mathbb{D}^{|\mathcal{I}|} \setminus \{0\}$. Therefore, the Laurent expansion of F contains no terms with negative powers. Thus, F is holomorphic in $\mathbb{D}^{|\mathcal{I}|}$. For every $\underline{t} \in \mathbb{T}^{|\mathcal{I}|}$ the operator $F(\underline{t})$ is unitary, which means that F is an inner function. □

Proof of Theorem 5.2. Since by Proposition 5.5 $F(\underline{t})$ is a rational function, it can be analytically continued on all of $\underline{t} \in \mathbb{C}^{|\mathcal{I}|}$. Moreover, it is holomorphic in the polydisc $\mathbb{D}^{|\mathcal{I}|}_{1+\epsilon} = \{\zeta \in \mathbb{C} |\, |\zeta| < 1+\epsilon\}^{|\mathcal{I}|}$ for some $\epsilon > 0$. To show this, by Hartogs' theorem it suffices to consider the analytic continuation with respect to a single variable $t_i \in \mathbb{C}$ keeping all other variables fixed. By the bound (5.3) all possible poles of this continuation lie outside a disc $\{t_i \in \mathbb{C} |\, |t_i| < r\}$ with $r > 1$.

In turn, this implies (see, e.g., Theorem 2.4.5 in [35]) that the Taylor series of the function $F(\underline{t})$ converges absolutely and uniformly for all $\underline{t} \in \mathbb{T}^{|\mathcal{I}|}$. Combining this with Lemma 5.6 proves the absolute and uniform convergence of the Fourier expansion (5.1).

By Lemma 5.8 the Fourier coefficients (5.2) satisfy $\widehat{S}_{\underline{n}}(\mathsf{k}; A, B) = 0$ for any $\underline{n} \in \mathbb{Z}^{|\mathcal{I}|}$ with $n_i < 0$ for at least one $i \in \mathcal{I}$. □

Remark 5.10. *Lemma 5.8 reduces the calculation of the Fourier coefficients* (5.2) *to the determination of the coefficients of the Taylor series for the function* (5.13).

6. Walks on Graphs

This section provides concepts and results which will be needed for the discussion of the inverse problem as well as of the combinatorial problems in Section 9. Throughout the entire section we will assume that the graph $\mathcal{G}$ is connected.

A nontrivial *walk* $\mathbf{w}$ on the graph $\mathcal{G}$ from $e' \in \mathcal{E}$ to $e \in \mathcal{E}$ is a sequence

$$\{e', i_1, \ldots, i_N, e\}$$

of edges such that

(i) $i_1, \ldots, i_N \in \mathcal{I}$,
(ii) $v_0 := \partial(e') \in \partial(i_1)$ and $v_N := \partial(e) \in \partial(i_N)$;
(iii) for any $k \in \{1, \ldots, N-1\}$ there is a vertex $v_k \in V$ such that $v_k \in \partial(i_k)$ and $v_k \in \partial(i_{k+1})$;
(iv) $v_k = v_{k+1}$ for some $k \in \{0, \ldots, N-1\}$ if and only if i_k is a tadpole.

Remark 6.1. *We emphasize that the definition of walks on the graph $\mathcal{G}$ is independent of the particular choice of the orientation of the edges. In particular, the vertex $v_k \in \partial(i_k)$, $v_k \in \partial(i_{k+1})$ need not to be the terminal vertex of the edge i_k and the initial vertex of the edge i_{k+1}.*

More general walks than those considered here are used in [47] *to study positivity preserving semigroups generated by Laplace operators on metric graphs.*

The number N is the *combinatorial length* $|\mathbf{w}|_{\mathrm{comb}} \in \mathbb{N}$ and the number

$$|\mathbf{w}| = \sum_{k=1}^{N} a_{i_k} > 0$$

is the *metric length* of the walk $\mathbf{w}$.

Example 6.2. *Let $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ with $V = \{v_0, v_1\}$, $\mathcal{I} = \{i\}$, $\mathcal{E} = \{e\}$, $\partial(e) = v_0$, and $\partial(i) = \{v_0, v_1\}$. Then the sequence $\{e,i,e\}$ is not a walk, whereas $\{e,i,i,e\}$ is a walk from e to e.*

Proposition 6.3. *Given an arbitrary nontrivial walk $\mathbf{w} = \{e', i_1, \ldots, i_N, e\}$ there is a unique sequence $\{v_k\}_{k=0}^N$ of vertices such that $v_0 = \partial(e') \in \partial(i_1)$, $v_N = \partial(e) \in \partial(i_N)$, $v_k \in \partial(i_k)$, and $v_k \in \partial(i_{k+1})$.*

Proof. Assume on the contrary that there are two different sequences $\{v_k\}_{k=0}^N$ and $\{v_k'\}_{k=0}^N$ satisfying the assumption of the proposition. This implies that there is a number $\ell \in \{0, \ldots, N-2\}$ such that $v_k = v_k'$ for all $k \in \{0, \ldots, \ell\}$ but $v_{\ell+1} \neq v_{\ell+1}'$. Obviously, the vertices v_ℓ, $v_{\ell+1}$, and $v_{\ell+1}'$ are incident with the same edge. Thus, either $v_\ell = v_{\ell+1}$ or $v_\ell = v_{\ell+1}'$, which is a contradiction. □

A *trivial* walk $\mathbf{w}$ on the graph $\mathcal{G}$ from $e' \in \mathcal{E}$ to $e \in \mathcal{E}$ is a tuple $\{e', e\}$ with $\partial(e) = \partial(e')$. Both the combinatorial and the metric length of a trivial walk are zero.

A *chain* $\mathbf{c}$ on the graph $\mathcal{G}$ is an ordered sequence $\{v_0, \ldots, v_N\}$ of vertices of the graph $\mathcal{G}$ such that any two consecutive vertices are adjacent. Any vertex of $\mathcal{G}$ may appear more than once in this sequence. By Proposition 6.3 to any nontrivial walk $\mathbf{w} = \{e', i_1, \ldots, i_N, e\}$ we can uniquely associate the chain

$$\mathbf{c}(\mathbf{w}) = \big\{v_0 = \partial(e'), v_1, \cdots, v_N = \partial(e)\big\}, \qquad N = |\mathbf{w}|_{\mathrm{comb}}$$

such that $v_k \in \partial(i_k) \cap \partial(i_{k+1})$ for all $k \in \{1, \ldots, N-1\}$. The chain of a trivial walk is a one element set. Conversely, a chain $\mathbf{c}$ specifies a walk on $\mathcal{G}$. This walk is unique if any two vertices are adjacent by no more than one internal edge.

A walk $\mathbf{w} = \{e', i_1, \ldots, i_N, e\}$ *traverses* an internal edge $i \in \mathcal{I}$ if $i_k = i$ for some $1 \leq k \leq N$. It *visits* the vertex v if $v \in \mathbf{c}(\mathbf{w})$.

A *tour* $\mathfrak{T}$ is an unordered set $\{i_1, \ldots, i_M\}$ of pairwise different internal edges such that there is a walk $\mathbf{w}$ which traverses every internal edge i_k of the tour at least once and no other internal edge. The tour associated with a trivial walk is the empty tour $\mathfrak{T}^{(0)}$.

The *score* $\underline{n}(\mathbf{w})$ of a walk $\mathbf{w}$ is the set $\{n_i(\mathbf{w})\}_{i\in\mathcal{I}}$ with $n_i(\mathbf{w}) \geq 0$ the number of times the walk $\mathbf{w}$ traverses the internal edge $i \in \mathcal{I}$. In particular, the tour associated with a walk $\mathbf{w}$ is the set

$$\mathfrak{T}(\mathbf{w}) := \big\{i \in \mathcal{I} |\; n_i(\mathbf{w}) > 0\big\}.$$

Any trivial walk has the score $\underline{n} = \underline{0} := \{0, \ldots, 0\}$.

Let $\mathcal{W}_{e,e'}$, $e, e' \in \mathcal{E}$ be the (infinite if $\mathcal{I} \neq \emptyset$) set of all walks $\mathbf{w}$ on $\mathcal{G}$ from e' to e. By reversing a walk $\mathbf{w}$ from e' to e into a walk $\mathbf{w}_{\mathrm{rev}}$ from e to e' we obtain a natural one-to-one correspondence between $\mathcal{W}_{e,e'}$ and $\mathcal{W}_{e',e}$. Obviously, $|\mathbf{w}| = |\mathbf{w}_{\mathrm{rev}}|$ and $\underline{n}(\mathbf{w}) = \underline{n}(\mathbf{w}_{\mathrm{rev}})$.

Obviously, the combinatorial length of a walk $\mathbf{w}$ is given by

$$|\mathbf{w}|_{\mathrm{comb}} = \sum_{i\in\mathcal{I}} n_i(\mathbf{w})$$

and the metric length of a walk $\mathbf{w}$ can be represented as a sum

$$|\mathbf{w}| = \sum_{i\in\mathcal{I}} n_i(\mathbf{w}) a_i = \langle \underline{n}(\mathbf{w}), \underline{a} \rangle, \tag{6.1}$$

where $\langle\cdot,\cdot\rangle$ is the scalar product in $\mathbb{R}^{|\mathcal{I}|}$ and the sets $\underline{a}$ and $\underline{n}$ are understood as elements of $\mathbb{R}^{|\mathcal{I}|}$.

We have the following obvious result.

Lemma 6.4. *If the Assumption 2 holds, i.e., the lengths $\{a_i\}_{i\in\mathcal{I}}$ are rationally independent, then the metric length $|\mathbf{w}|$ of a walk $\mathbf{w}$ uniquely determines its score $\underline{n}(\mathbf{w})$.*

In other words once we know the length of a walk, we know how often any internal edge has been traversed during that walk.

Let $\mathcal{G}_v$ be the graph without internal edges associated with a vertex v (see Definition 4.4). Since the boundary conditions (A, B) on $\mathcal{G}$ are assumed to be local, we can consider the Laplace operator $\Delta(A(v), B(v))$ on $L^2(\mathcal{G}_v)$ associated with the boundary conditions $(A(v), B(v))$ induced by (A, B) (see Definition 4.2). By (3.46) the scattering matrix for $\Delta(A_v, B_v)$ is given by

$$S_v(\mathsf{k}) = -(A(v) + \mathrm{i}\mathsf{k}B(v))^{-1}(A(v) - \mathrm{i}\mathsf{k}B(v)).$$

Now to each walk $\mathbf{w} = \{e', i_1, \ldots, i_N, e\}$ from $e' \in \mathcal{E}$ to $e \in \mathcal{E}$ on the graph $\mathcal{G}$ we associate a weight $W(\mathbf{w}; \mathsf{k})$ by

$$W(\mathbf{w}; \mathsf{k}) = \mathrm{e}^{\mathrm{i}\mathsf{k}\langle \underline{n}(\mathbf{w}), \underline{a}\rangle}\, \widetilde{W}(\mathbf{w}; \mathsf{k}) \tag{6.2}$$

with

$$\widetilde{W}(\mathbf{w}; \mathsf{k}) = \prod_{k=0}^{|\mathbf{w}|_{\mathrm{comb}}} [S_{v_k}(\mathsf{k})]_{e_k^{(+)}, e_k^{(-)}}. \tag{6.3}$$

Here $e_k^{(\pm)} \in \mathcal{E}_{v_k}$ are defined as

$$e_k^{(-)} = \begin{cases} \Psi_{v_k}^{-1}(i_k), & \text{if} \quad 1 \leq k \leq |\mathbf{w}|_{\mathrm{comb}}, \\ \Psi_{v_k}^{-1}(e'), & \text{if} \quad k = 0, \end{cases}$$

and

$$e_k^{(+)} = \begin{cases} \Psi_{v_k}^{-1}(i_{k+1}), & \text{if} \quad 0 \leq k \leq |\mathbf{w}|_{\mathrm{comb}} - 1, \\ \Psi_{v_k}^{-1}(e), & \text{if} \quad k = |\mathbf{w}|_{\mathrm{comb}} + 1, \end{cases}$$

where the map Ψ_v is defined in Definition 4.4. Note that $\widetilde{W}(\mathbf{w}; \mathsf{k})$ is independent of the metric properties of the graph. Obviously, $\widetilde{W}(\mathbf{w}; \mathsf{k}) = [S_{\partial(e)}(\mathsf{k})]_{e',e}$ if the walk $\mathbf{w}$ is trivial.

We write $\mathcal{W}_{e,e'}$ as an infinite union of disjoint, non-empty sets by grouping together all walks $\mathbf{w}$ with the same score $\underline{n}(\mathbf{w})$,

$$\mathcal{W}_{e,e'}(\underline{n}) = \big\{\mathbf{w} \in \mathcal{W}_{e,e'} \mid \underline{n}(\mathbf{w}) = \underline{n}\big\}$$

such that

$$\mathcal{W}_{e,e'} = \bigcup_{\underline{n} \in (\mathbb{N}_0)^{|\mathcal{I}|}} \mathcal{W}_{e,e'}(\underline{n}). \tag{6.4}$$

Note that these sets depend only on topology of the graph $\mathcal{G}$ and are independent of its metric properties. Also if $\mathbf{w} \in \mathcal{W}_{e,e'}(\underline{n})$ then $\mathbf{w}_{\mathrm{rev}} \in \mathcal{W}_{e',e}(\underline{n})$. $\mathcal{W}_{e,e'}(\underline{0}) = \emptyset$ if and only if $\partial(e) \neq \partial(e')$.

We have the following obvious result.

Lemma 6.5. *The sets $\mathcal{W}_{e,e'}(\underline{n})$ are at most finite. The number of different walks in $\mathcal{W}_{e,e'}(\underline{n})$ satisfies the bound*

$$|\mathcal{W}_{e,e'}(\underline{n})| \leq \frac{|\underline{n}|!}{\prod_{i \in \mathcal{I}} n_i!}, \tag{6.5}$$

where

$$|\underline{n}| = \sum_{i \in \mathcal{I}} n_i$$

is the combinatorial length of any walk $\mathbf{w} \in \mathcal{W}_{e,e'}(\underline{n})$.

Theorem 6.6. *For any local boundary conditions (A, B) satisfying* (3.10) *the matrix elements of the $\underline{n}$-th Fourier coefficients* (5.2) *are given by the sum over the walks with the score $\underline{n}$,*

$$[\widehat{S}_{\underline{n}}(\mathsf{k}; A, B)]_{e,e'} = \sum_{\mathbf{w}\in\mathcal{W}_{e,e'}(\underline{n})} \widetilde{W}(\mathbf{w}; \mathsf{k}) \tag{6.6}$$

whenever $\mathcal{W}_{e,e'}(\underline{n})$ is nonempty and $[\widehat{S}_{\underline{n}}(\mathsf{k}; A, B)]_{e,e'} = 0$ if $\mathcal{W}_{e,e'}(\underline{n}) = \emptyset$.

Proof. Obviously, it suffices to show that the $\underline{n}$-th coefficient of the multi-dimensional Taylor expansion of the function $F(\underline{t})$ (defined in (5.13)) with respect to $\underline{t} \in \mathbb{D}^{|\mathcal{I}|}$ coincides with the r.h.s. of (6.6). Recall that by Theorem 3.10 and Lemma 5.3 for all $\underline{a} \in \mathcal{A}$ the scattering matrix is given by

$$S(\mathsf{k}; A, B, \underline{a}) = -\begin{pmatrix}\mathbb{I} & 0 & 0\end{pmatrix} [\mathbb{I} - \mathfrak{S}(\mathsf{k}; A, B)T(\mathsf{k}; \underline{a})]^{-1}\, \mathfrak{S}(\mathsf{k}; A, B) \begin{pmatrix}\mathbb{I}\\ 0\\ 0\end{pmatrix}, \tag{6.7}$$

where $\mathfrak{S}(\mathsf{k}; A, B)$ is given by (3.46) and $T(\mathsf{k}; \underline{a})$ by (3.32). Since $\|T(\mathsf{k}; \underline{a})\| < 1$ for all $\underline{a} \in \mathcal{A}$ we obtain the series

$$\begin{aligned} S(\mathsf{k}; A, B, \underline{a}) &= \\ &= \sum_{n=0}^{\infty} \begin{pmatrix}\mathbb{I} & 0 & 0\end{pmatrix} [\mathfrak{S}(\mathsf{k}; A, B)T(\mathsf{k}; \underline{a})]^{n}\, \mathfrak{S}(\mathsf{k}; A, B) \begin{pmatrix}\mathbb{I}\\ 0\\ 0\end{pmatrix} \end{aligned} \tag{6.8}$$

converging in norm for all $\underline{a} \in \mathcal{A}$.

Recall that

$$\mathfrak{S}(\mathsf{k}; A, B) = \mathfrak{S}(\mathsf{k}; CA, CB)$$

for every invertible C. It follows directly from Definition 4.2 that

$$\mathfrak{S}(\mathsf{k}; A, B) = \bigoplus_{v\in V} S(\mathsf{k}; A(v), B(v)).$$

Plugging this equality into (6.8) proves that

$$[S(\mathsf{k}; A, B, \underline{a})]_{e,e'} = \sum_{\mathbf{w}\in\mathcal{W}_{e,e'}} W(\mathbf{w}; \mathsf{k}) \equiv \sum_{\mathbf{w}\in\mathcal{W}_{e,e'}} \widetilde{W}(\mathbf{w}; \mathsf{k})\, \mathrm{e}^{\mathrm{i}\mathsf{k}\langle \underline{n}(\mathbf{w}), \underline{a}\rangle} \tag{6.9}$$

for all $\mathsf{k} > 0$ and $\underline{a} \in \mathcal{A}$. By uniqueness of the Fourier expansion Theorem 6.6 implies the claim. □

Remark 6.7. *Theorem 6.6 implies that the scattering matrix of the metric graph $(\mathcal{G}, \underline{a})$ is determined by the scattering matrices associated with all its single vertex subgraphs. This result can also be obtained by applying the factorization formula* [43].

Since $\widetilde{W}(\mathbf{w}; \mathsf{k})$ is independent of the metric properties of the graph, it is natural to view (6.9) as a *combinatorial Fourier expansion* of the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$. We will show that (6.9) actually coincides with the Fourier expansion (5.1) in Theorem 5.2.

For given $e, e' \in \mathcal{E}$ consider the set of scores of all walks from e' to e,

$$\mathcal{N}_{e,e'} = \left\{ \underline{n} \in (\mathbb{N}_0)^{|\mathcal{I}|} \mid \text{there is a walk } \mathbf{w} \in \mathcal{W}_{e,e'}(\underline{n}) \right\}. \tag{6.10}$$

Since $\underline{n}(\mathbf{w}) = \underline{n}(\mathbf{w}_{\mathrm{rev}})$, we have $\mathcal{N}_{e,e'} = \mathcal{N}_{e',e}$. By Theorems 5.2 and 6.6 we can rewrite (5.1) as

$$[S(\mathsf{k}; A, B, \underline{a})]_{e,e'} = \sum_{\underline{n}\in\mathcal{N}_{e,e'}} [\widehat{S}_{\underline{n}}(\mathsf{k}; A, B)]_{e,e'}\, \mathrm{e}^{\mathrm{i}\mathsf{k}\langle \underline{n}, \underline{a}\rangle}. \tag{6.11}$$

By Lemma 6.5, (6.6) is a finite sum. Hence, $[\widehat{S}_{\underline{n}}(\mathsf{k}; A, B)]_{e,e'}$ is a rational function of k. This function may vanish identically even if $\mathcal{W}_{e,e'}(\underline{n}) \neq \emptyset$. This is well illustrated by the following simple example.

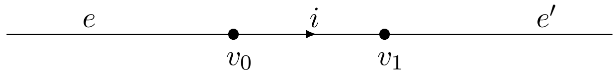

FIG. 2. The graph from Example 6.8. The length of the internal edge i is arbitrary. The arrow shows the orientation of the internal edge.

Example 6.8. *Consider the graph $\mathcal{G}$ depicted in Fig. 2. Choose the boundary conditions $A\underline{\psi} + B\underline{\psi}' = 0$ with*

$$A = \begin{pmatrix} 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \qquad B = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}$$

and

$$\underline{\psi} = \begin{pmatrix} \psi_e(0) \\ \psi_i(0) \\ \psi_i(a_i) \\ \psi_{e'}(0) \end{pmatrix}, \qquad \underline{\psi}' = \begin{pmatrix} \psi_e'(0) \\ \psi_i'(0) \\ -\psi_i'(a_i) \\ \psi_{e'}'(0) \end{pmatrix}.$$

Obviously, these boundary conditions are local on $\mathcal{G}$. It is easy to see that

$$S_{v_0}(\mathsf{k}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \text{and} \qquad S_{v_1}(\mathsf{k}) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Thus, for any walk from e to e the factor $\widetilde{W}(\mathbf{w};\mathsf{k})$ equals zero. Therefore, $S(\mathsf{k};\underline{n})_{e,e} = 0$ for all $\underline{n} \in \mathbb{N}_0$. Note that $\mathcal{W}_{e,e}(\underline{n}) \neq \emptyset$ for all $\underline{n} \in 2\mathbb{N}_0$.

Below we will show that in the generic case the matrix elements vanishes identically if and only if $\mathcal{W}_{e,e'}(\underline{n}) = \emptyset$. First we will prove this statement for a particular choice of boundary conditions. These boundary conditions will be used for the discussion of some combinatorial problems in Section 9.

Theorem 6.9. *Let $\{H(v)\}_{v\in V}$ be a collection of $\deg(v) \times \deg(v)$ self-adjoint matrices with strictly positive entries. Let $(A(v), B(v))$ be the boundary conditions associated with $H(v)$ by Lemma 3.20. Define the local boundary conditions (A, B) on the graph $\mathcal{G}$ given by*

$$A = \bigoplus_{v\in V} A(v) \qquad \text{and} \qquad B = \bigoplus_{v\in V} B(v)$$

with respect to the orthogonal decomposition (4.2). *Then for any $e, e' \in \mathcal{E}$ the matrix element $[\widehat{S}_{\underline{n}}(\mathsf{k}; A, B)]_{e,e'}$ of the Fourier coefficient* (5.2) *of the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ vanishes identically for all $\mathsf{k} > 0$ if and only if $\mathcal{W}_{e,e'}(\underline{n}) = \emptyset$.*

We introduce some notion which will be used in the proof. Consider an arbitrary nontrivial walk $\mathbf{w} = \{e', i_1, \ldots, i_N, e\}$. We say that the walk is *transmitted* at the vertex

$$v_k \in \mathbf{c}(\mathbf{w}) = \{v_0 = \partial(e'), \ldots, v_k, \ldots, v_N = \partial(e)\}$$

if either $v_k = \partial(e)$ or $v_k = \partial(e')$ or $v_k \in \partial(i_k)$, $v_k \in \partial(i_{k+1})$, and $i_k \neq i_{k+1}$. We say that a trivial walk from e' to e is transmitted at the vertex $v = \partial(e) = \partial(e')$ if $e \neq e'$. Otherwise the walk is said to be *reflected*. Let $\mathsf{T}(\mathbf{w})$ denote the ordered set of vertices of the graph $\mathcal{G}$

successively visited by the walk $\mathbf{w}$, at which the walk is transmitted. Thus, the set $\mathsf{T}(\mathbf{w})$ can be obtained from the chain $\mathbf{c}(\mathbf{w})$ by deleting all vertices, at which the walk is reflected.

Set

$$t_{e,e'}(\underline{n}) = \min_{\mathbf{w}\in\mathcal{W}_{e,e'}(\underline{n})} |\mathsf{T}(\mathbf{w})|.$$

Then

$$\mathcal{W}^{\min}_{e,e'}(\underline{n}) = \{\mathbf{w}\in\mathcal{W}_{e,e'}(\underline{n}) \mid |\mathsf{T}(\mathbf{w})| = t_{e,e'}(\underline{n})\}$$

is the set of walks from e' to e with the score $\underline{n}$ having the smallest number of transmissions.

Proof of Theorem 6.9. The "if" part of the statement follows from Theorem 6.6. To prove the "only if" part, we assume that $\mathcal{W}_{e,e'}(\underline{n}) \neq \emptyset$. For an arbitrary walk $\mathbf{w}\in\mathcal{W}_{e,e'}(\underline{n})$ consider the weight $\widetilde{W}(\mathbf{w};\mathsf{k})$ given by (6.3). For $\mathsf{k}\to+\infty$ from Lemma 3.20 we obtain the following asymptotics of this weight

$$\widetilde{W}(\mathbf{w};\mathsf{k}) = \mathsf{k}^{-|\mathsf{T}(\mathbf{w})|}\, \mathrm{i}^{|\mathsf{T}(\mathbf{w})|} \prod_{v\in\mathsf{T}(\mathbf{w})} [H(v)]_{e^{(+)}(v),e^{(-)}(v)}[1+o(1)].$$

The product is understood in the ordered sense. By assumption this product is strictly positive.

By Theorem 6.6 the matrix element $[\widehat{S}_{\underline{n}}(\mathsf{k};A,B)]_{e,e'}$ has the following asymptotics

$$[\widehat{S}_{\underline{n}}(\mathsf{k};A,B)]_{e,e'} = \mathsf{k}^{-t_{e,e'}(\underline{n})}\, \mathrm{i}^{t_{e,e'}(\underline{n})} \sum_{\mathbf{w}\in\mathcal{W}^{\min}_{e,e'}(\underline{n})} \prod_{v\in\mathsf{T}(\mathbf{w})} [H(v)]_{e^{(+)}(v),e^{(-)}(v)}[1+o(1)].$$

Noting that

$$\sum_{\mathbf{w}\in\mathcal{W}^{\min}_{e,e'}(\underline{n})} \prod_{v\in\mathsf{T}(\mathbf{w})} [H(v)]_{e^{(+)}(v),e^{(-)}(v)}$$

is a sum of strictly positive numbers proves that $[\widehat{S}_{\underline{n}}(\mathsf{k};A,B)]_{e,e'}$ does not vanish identically. □

We turn to the discussion of general local boundary conditions. The set of all local boundary conditions is isomorphic to the direct product

$$\mathsf{U}_{\mathcal{G}} := \times_{v\in V} \mathsf{U}(\deg(v))$$

of the groups of all unitary $\deg(v)\times\deg(v)$ matrices. Let μ be the probability measure on $\mathsf{U}_{\mathcal{G}}$ defined as a product measure by

$$\mu(\sigma) = \bigotimes_{v\in V} \mu_v(\sigma_v), \qquad \sigma = \times_{v\in V} \sigma_v,$$

where μ_v is the normalized Haar measure on $\mathsf{U}(\deg(v))$ and σ_v is an open subset of $\mathsf{U}(\deg(v))$.

Definition 6.10. *A property P holds for Haar almost all local boundary conditions if*

$$\mu\Big\{U\in \times_{v\in V}\mathsf{U}(\deg(v)) \mid P \text{ holds for the boundary conditions defined by the maximal isotropic subspace } \mathcal{M}(U)\Big\} = \mu\left(\times_{v\in V}\mathsf{U}(\deg(v))\right) = 1.$$

is valid.

The following theorem shows that for Haar almost all local boundary conditions the function $\widehat{S}_{\underline{n}}(\mathsf{k})_{e,e'}$ does not vanish identically whenever $\mathcal{W}_{e,e'}(\underline{n})\neq\emptyset$.

Theorem 6.11. *For Haar almost all local boundary conditions (A,B) satisfying* (3.10) *the matrix element $[\widehat{S}_{\underline{n}}(\mathsf{k};A,B)]_{e,e'}$ of the Fourier coefficient* (5.2) *of the scattering matrix $S(\mathsf{k};A,B,\underline{a})$ vanishes identically for all $\mathsf{k}>0$ if and only if $\mathcal{W}_{e,e'}(\underline{n})=\emptyset$.*

Proof. The group $\mathsf{U}_{\mathcal{G}}$ is a real-analytic manifold of real dimension $\dim_{\mathbb{R}} \mathsf{U}_{\mathcal{G}} = N_{\mathcal{G}}$ with

$$N_{\mathcal{G}} := \sum_{v\in V} [\deg(v)]^2.$$

Let $\mathsf{U}^0(\deg(v))$ be the subset of $\mathsf{U}(\deg(v))$ consisting of those unitaries which do not have -1 as an eigenvalue. By Lemma 3.22 the set $\mathsf{U}^0(\deg(v))$ is of full Haar measure. It is an open dense subset in $\mathsf{U}(\deg(v))$. Set $\mathsf{U}_{\mathcal{G}}^0 := \times_{v\in V} \mathsf{U}^0(\deg(v))$.

For any given score $\underline{n} \in \mathcal{N}_{e,e'}$ define the map $\Phi_{\underline{n}} : \mathsf{U}_{\mathcal{G}}^0 \to \mathbb{C}$ by

$$U \mapsto \Phi_{\underline{n}}(U) = \sum_{\mathbf{w}\in\mathcal{W}_{e,e'}^{\min}(\underline{n})} \prod_{v\in\mathsf{T}(\mathbf{w})} [(U(v)+\mathbb{I})^{-1}(U(v)-\mathbb{I})]_{e^{(+)}(v),e^{(-)}(v)}, \tag{6.12}$$

where

$$U = \bigoplus_{v\in V} U(v) \in \mathsf{U}_{\mathcal{G}}^0$$

with respect to the orthogonal decomposition (4.2).

Observe that by Lemma 3.20 and equation (3.59) the quantity $\Phi_{\underline{n}}(U)$ with $U \in \mathsf{U}_{\mathcal{G}}^0$ determines the asymptotics for $\mathsf{k} \to \infty$ of the Fourier coefficient $\widehat{S}_{\underline{n}}(\mathsf{k}; A_U, B_U)$ of the scattering matrix $S(\mathsf{k}; A_U, B_U, \underline{a})$,

$$[\widehat{S}_{\underline{n}}(\mathsf{k}; A_U, B_U)]_{e,e'} = \mathsf{k}^{-t_{e,e'}(\underline{n})}\, \mathrm{i}^{t_{e,e'}(\underline{n})} \Phi_{\underline{n}}(U)[1+o(1)],$$

where $A_U = -(U-\mathbb{I})/2$, $B_U = (U+\mathbb{I})/(2\mathrm{i}\mathsf{k})$ (see Proposition 3.7). Therefore, (see the proof of Theorem 6.9) the function $U \mapsto \Phi_{\underline{n}}(U)$ is not identically zero.

Let $\mathcal{U} \subset \mathsf{U}_{\mathcal{G}}^0$ be an arbitrary open set belonging to a single chart of the manifold $\mathsf{U}_{\mathcal{G}}$. Denote by $\varkappa : \mathcal{U} \to \mathbb{R}^{\mathbb{N}_{\mathcal{G}}}$ a (real-analytic) coordinate map. Let $\mathcal{Z} \subset \mathsf{U}_{\mathcal{G}}^0$ be the set of all zeroes of the function $\Phi_{\underline{n}}$. Assume that $\mathcal{Z}\cap\mathcal{U}$ has a positive Haar measure. Then the function $\Phi_{\underline{n}}\circ\varkappa^{-1}$ vanishes on a subset of $\mathbb{R}^{\mathbb{N}_{\mathcal{G}}}$ of a positive Lebesgue measure. Observe that $\operatorname{Re}\Phi_{\underline{n}}\circ\varkappa^{-1}$ and $\operatorname{Im}\Phi_{\underline{n}}\circ\varkappa^{-1}$ are real-analytic functions. Hence, by the Lojaciewicz theorem [51], the function $\Phi_{\underline{n}}\circ\varkappa^{-1}$ is identically zero on $\varkappa^{-1}(\mathcal{U}) \subset \mathbb{R}^{\mathbb{N}_{\mathcal{G}}}$. Thus, $\Phi_{\underline{n}}$ vanishes identically on $\mathsf{U}_{\mathcal{G}}^0$, a contradiction. □

7. Proof of Theorem 1

Given a finite noncompact connected graph $\mathcal{G} = \mathcal{G}(V, \mathcal{I}, \mathcal{E}, \partial)$, for arbitrary $e, e' \in \mathcal{E}$ consider the set of nonnegative real numbers

$$\mathcal{L}_{e,e'} = \left\{ \langle \underline{n}(\mathbf{w}), \underline{a}\rangle \,|\, \mathbf{w}\in\mathcal{W}_{e,e'} \right\},$$

where $\underline{n}(\mathbf{w})$ is the score of the walk $\mathbf{w}$. Obviously, $\mathcal{L}_{e,e'} = \mathcal{L}_{e',e}$. Also, $\mathcal{I} = \emptyset$ if and only if $\mathcal{L}_{e,e'} = \{0\}$ for all $e, e' \in \mathcal{E}$. Furthermore, $\mathcal{L}_{e'',e} = \mathcal{L}_{e'',e'}$ for all $e'' \in \mathcal{E}$ whenever $\partial(e) = \partial(e')$.

Lemma 7.1. *Assume that the graph $\mathcal{G} = \mathcal{G}(V, \mathcal{I}, \mathcal{E}, \partial)$ is connected, $\mathcal{E} \neq \emptyset$. Then for any metric $\underline{a}$ on $\mathcal{G}$ the set of internal edges $\mathcal{I}$ is nonempty if and only if $\mathcal{L}_{e,e'}$ is an infinite discrete set for all $e, e' \in \mathcal{E}$,*

$$\mathcal{L}_{e,e'} = \{\omega_{e,e'}(k)\}_{k\in\mathbb{N}_0}, \quad \textit{where} \quad \omega_{e,e'}(k) < \omega_{e,e'}(k+1) \quad \textit{for all} \quad k\in\mathbb{N}_0.$$

Proof. The "if" part is obvious. For the "only if" part assume that $\mathcal{I} \neq \emptyset$. Then the set $\mathcal{L}_{e,e'}$ is infinite. Choose an arbitrary $w \in \mathcal{L}_{e,e'}$. Observe that for any $\epsilon > 0$ the set

$$\{\underline{x} \in (\mathbb{R}_+)^{|\mathcal{I}|} \,|\, |\langle \underline{x}, \underline{a}\rangle - w| < \epsilon\}$$

is bounded. Therefore, the set

$$\{\underline{n} \in (\mathbb{N}_0)^{|\mathcal{I}|} \,|\, |\langle \underline{n}, \underline{a}\rangle - w| < \epsilon\}$$

is at most finite. Thus, $\mathcal{L}_{e,e'}$ has no finite accumulation points. □

The following uniqueness result is a key technical tool to determine the topology of the graph from its scattering matrix. In contrast to Theorem 5.2 which implies the uniqueness of the Fourier expansion (5.1) for fixed $\mathsf{k} > 0$, this result corresponds to the case, where $\underline{a} \in (\mathbb{R}_+)^{|\mathcal{I}|}$ is kept fixed.

Theorem 7.2. *Assume that the graph $\mathcal{G} = \mathcal{G}(V, \mathcal{I}, \mathcal{E}, \partial)$ is connected, $\mathcal{E} \neq \emptyset$. For any fixed $\underline{a} \in (\mathbb{R}_+)^{|\mathcal{I}|}$ satisfying Assumption 2 the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ has a unique absolutely converging expansion*

$$S(\mathsf{k}; A, B, \underline{a}) = \sum_{\underline{n} \in (\mathbb{N}_0)^{|\mathcal{I}|}} \widehat{S}_{\underline{n}}(\mathsf{k}; A, B)\, \mathrm{e}^{\mathrm{i}\mathsf{k}\langle \underline{n}, \underline{a}\rangle}, \qquad \mathsf{k} \in \mathbb{R}_+. \tag{7.1}$$

In particular, for any $e, e' \in \mathcal{E}$ the Fourier coefficients $\left[\widehat{S}_{\underline{n}}(\mathsf{k}; A, B)\right]_{e,e'}$ and the set

$$\widetilde{\mathcal{L}}_{e,e'} := \left\{ \langle \underline{n}, \underline{a}\rangle \,\middle|\, \underline{n} \in (\mathbb{N}_0)^{|\mathcal{I}|} \text{ and } \left[\widehat{S}_{\underline{n}}(\mathsf{k}; A, B)\right]_{e,e'} \text{ does not vanish identically} \right\} \subset \mathcal{L}_{e,e'}$$

are uniquely determined by the map $\mathbb{R}_+ \ni \mathsf{k} \mapsto [S(\mathsf{k}; A, B, \underline{a})]_{e,e'}$.

Note that for local boundary conditions leading to k-independent single vertex scattering matrices (like standard boundary conditions considered in Example 4.5 or more general boundary conditions discussed in Remark 3.9) the statement follows from the uniqueness theorem for almost periodic functions. For general boundary conditions Theorem 5.2 implies that the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ admits an expansion of the form (7.1). However, it does not imply that $\mathbb{R}_+ \ni \mathsf{k} \mapsto S(\mathsf{k}; A, B, \underline{a})$ uniquely determines the coefficients $\widehat{S}_{\underline{n}}(\mathsf{k}; A, B)$ in (7.1).

Remark 7.3. *By Theorem 6.11 the sets $\widetilde{\mathcal{L}}_{e,e'}$ and $\mathcal{L}_{e,e'}$ agree for Haar almost all local boundary conditions. Similarly, $\widetilde{\mathcal{L}}_{e,e'} = \mathcal{L}_{e,e'}$ for the boundary conditions referred to in Theorem 6.9.*

Proof of Theorem 7.2. Fix $\underline{a} \in (\mathbb{R}_+)^{|\mathcal{I}|}$ and boundary conditions (A, B). Set for brevity $S(\mathsf{k}) := S(\mathsf{k}; A, B, \underline{a})$ and $\widehat{S}_{\underline{n}}(\mathsf{k}) := \widehat{S}_{\underline{n}}(\mathsf{k}; A, B)$. By Lemma 7.1 the set $\widetilde{\mathcal{L}}_{e,e'}$ is discrete, $\widetilde{\mathcal{L}}_{e,e'} = \{\widetilde{w}_{e,e'}(k)\}_{k\in\mathbb{N}_0}$ with $\widetilde{w}_{e,e'}(k) < \widetilde{w}_{e,e'}(k+1)$.

From Corollary 3.18 and Theorem 6.6 it follows that for all sufficiently large $\mathsf{k} \in \mathbb{C}$ the Fourier coefficients $\widehat{S}_{\underline{n}}(\mathsf{k})$ admit an absolutely converging expansion of the form

$$\widehat{S}_{\underline{n}}(\mathsf{k}) = \sum_{m=0}^{\infty} \widehat{S}_{\underline{n}}^{(m)} \mathsf{k}^{-m}. \tag{7.2}$$

By Assumption 2 there is a unique $\underline{n}_0 \in (\mathbb{N}_0)^{|\mathcal{I}|}$ such that $\langle \underline{n}_0, \underline{a}\rangle = w_{e,e'}(0)$.

Obviously,

$$\lim_{\operatorname{Im}\mathsf{k}\to+\infty} \mathsf{k}^{-1} \log[S(\mathsf{k})]_{e,e'} = \mathrm{i}\widetilde{w}_{e,e'}(0)$$

and

$$\lim_{\operatorname{Im}\mathsf{k}\to+\infty} \mathrm{e}^{-\mathrm{i}\mathsf{k}\widetilde{w}_{e,e'}(0)}[S(\mathsf{k})]_{e,e'} = [\widehat{S}_{\underline{n}_0}^{(0)}]_{e,e'}.$$

Successively we can determine all coefficients of the series (7.2) with $\underline{n} = \underline{n}_0$,

$$\lim_{\operatorname{Im}\mathsf{k}\to+\infty} \mathsf{k}^{m+1} \left(\mathrm{e}^{-\mathrm{i}\mathsf{k}\widetilde{w}_{e,e'}(0)}[S(\mathsf{k})]_{e,e'} - \sum_{s=0}^{m} [\widehat{S}_{\underline{n}_0}^{(s)}]_{e,e'} \mathsf{k}^{-s} \right) = [\widehat{S}_{\underline{n}_0}^{(m+1)}]_{e,e'}, \qquad m \in \mathbb{N}_0.$$

Further, we observe that

$$\lim_{\operatorname{Im}\mathsf{k}\to+\infty} \mathsf{k}^{-1} \log\left([S(\mathsf{k})]_{e,e'} - [\widehat{S}_{\underline{n}_0}(\mathsf{k})]_{e,e'} \mathrm{e}^{\mathrm{i}\mathsf{k}w_{e,e'}(0)} \right) = \mathrm{i}\widetilde{w}_{e,e'}(1).$$

Since $\widetilde{\mathcal{L}}_{e,e'}$ is discrete, proceeding inductively as above we can determine this set and all non-vanishing Fourier coefficients in (7.1). □

The number $\omega_{e,e'}(0) \in \mathcal{L}_{e,e'}$ is the metric length of a geodesic walk from e' to e, that is a walk with the shortest metric length. Under Assumption 2 the geodesic walk is unique. Obviously, $\omega_{e,e'}(0) = 0$ if and only if $\partial(e) = \partial(e')$.

For any subsets M_1 and M_2 of $\mathbb{R}_+$ define $M_1 + M_2$ to be the set $\{a+b|\ a \in M_1,\ b \in M_2\} \subset \mathbb{R}_+$. With this notation we have the following result:

Lemma 7.4. *For any $e, e' \in \mathcal{E}$ the set $\mathcal{L}_{e,e'}$ is invariant under the additive action of both $\mathcal{L}_{e,e}$ and $\mathcal{L}_{e',e'}$ in the sense that*

$$\mathcal{L}_{e,e'} + \mathcal{L}_{e,e} = \mathcal{L}_{e,e'} + \mathcal{L}_{e',e'} = \mathcal{L}_{e,e'} \tag{7.3}$$

holds.

Equation (7.3) implies that for every $e \in \mathcal{E}$ the set $\mathcal{L}_{e,e}$ is an Abelian monoid (that is, a commutative semigroup with identity $w_{e,e}(0) = 0$) with respect to the arithmetic addition. Below this observation will be used extensively.

Let $\mathfrak{T}(\mathbf{w})$ be the tour associated with a walk $\mathbf{w}$. Given a tour $\mathfrak{T}$ we set

$$\mathcal{L}_{e,e'}^{\mathfrak{T}} := \left\{ \langle \underline{n}(\mathbf{w}), \underline{a} \rangle |\, \mathbf{w} \in \mathcal{W}_{e,e'} \quad \text{such that} \quad \mathfrak{T}(\mathbf{w}) = \mathfrak{T} \right\} \tag{7.4}$$

if $\mathfrak{T}$ is associated with at least one walk from e' to e and $\mathcal{L}_{e,e'}^{\mathfrak{T}} = \emptyset$ otherwise.

Obviously, $\mathcal{L}_{e,e'}^{\mathfrak{T}} = \mathcal{L}_{e',e}^{\mathfrak{T}}$. By $w_{\mathfrak{T}} = \min \mathcal{L}_{e,e'}^{\mathfrak{T}}$ we denote the smallest number in the set $\mathcal{L}_{e,e'}^{\mathfrak{T}}$. Clearly, $w_{\mathfrak{T}}$ is the metric length of a shortest walk $\mathbf{w}$ from $e' \in \mathcal{E}$ to $e \in \mathcal{E}$ traversing each $i \in \mathfrak{T}$ at least once,

$$w_{\mathfrak{T}} = \sum_{i \in \mathfrak{T}} a_i n_i(\mathbf{w}).$$

In general, even under Assumption 2 such walk need not be unique.

Let $\mathcal{G}_{\mathfrak{T}}$ be a compact subgraph of $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ associated with the tour $\mathfrak{T}$, that is, $\mathcal{G}_{\mathfrak{T}} = (V_{\mathfrak{T}}, \mathfrak{T}, \emptyset, \partial|_{\mathfrak{T}})$ with $V_{\mathfrak{T}} \subset V$ the set of vertices incident with the internal edges $i \in \mathfrak{T}$.

Given $\mathfrak{T}$ we consider the (additive) Abelian groups $\mathcal{C}_1$ and $\mathcal{C}_0$ generated by the (oriented) 1-simplices σ_i, $i \in \mathfrak{T}$ and the 0-simplices σ_v, $v \in V_{\mathfrak{T}}$, respectively, i.e.,

$$\mathcal{C}_1 = \left\{ \sum_{i \in \mathfrak{T}} n_i \sigma_i \Big| n_i \in \mathbb{Z} \right\} \cong \mathbb{Z}^{|\mathfrak{T}|}, \qquad \mathcal{C}_0 = \left\{ \sum_{v \in \partial(\mathfrak{T})} n_v \sigma_v \Big| n_v \in \mathbb{Z} \right\} \cong \mathbb{Z}^{|V_{\mathfrak{T}}|}.$$

Define the boundary operator $\delta_1 : \mathcal{C}_1 \to \mathcal{C}_0$

$$\delta_1 : \quad c = \sum_{i \in \mathfrak{T}} n_i \sigma_i \quad \longmapsto \quad \delta_1 c = \sum_{i \in \mathfrak{T}} n_i (\sigma_{\partial^+(i)} - \sigma_{\partial^-(i)}).$$

Obviously, δ_1 is a group homomorphism and we have

$$\delta_1 c = 0 \quad \Longleftrightarrow \quad \sum_{i:\, \partial^+(i) = v} n_i = \sum_{i:\, \partial^-(i) = v} n_i \quad \text{for all} \quad v \in V_{\mathfrak{T}}. \tag{7.5}$$

We extend the map $\mathcal{C}_1 \xrightarrow{\delta_1} \mathcal{C}_0$ to a chain complex

$$0 \longleftarrow \mathbb{Z} \xleftarrow{\delta_0} \mathcal{C}_0 \xleftarrow{\delta_1} \mathcal{C}_1$$

with

$$\delta_0 c = \sum_{v \in V_{\mathfrak{T}}} n_v \quad \text{for} \quad c = \sum_{v \in V_{\mathfrak{T}}} n_v \sigma_v \in \mathcal{C}_0.$$

Obviously, $\delta_0 \delta_1 = 0$. We call $\operatorname{Ker} \delta_1$ the first homology group $H_1(\mathfrak{T}, \mathbb{Z})$ of the graph $\mathcal{G}_{\mathfrak{T}}$ and we set $H_0(\mathfrak{T}, \mathbb{Z}) = \operatorname{Ker}\ \delta_0 / \operatorname{Ran}\ \delta_1$ to be the zeroth homology group of $\mathcal{G}_{\mathfrak{T}}$. The dimension of $H_1(\mathfrak{T}, \mathbb{Z})$ is equal to $|\mathfrak{T}| - |V_{\mathfrak{T}}| + 1$ (see [45, Section 3]).

We say that the walks $\mathbf{w}_1 \in \mathcal{W}_{e,e'}$ and $\mathbf{w}_2 \in \mathcal{W}_{e,e'}$ are equivalent ($\mathbf{w}_1 \sim \mathbf{w}_2$) if $\mathfrak{T}(\mathbf{w}_1) = \mathfrak{T}(\mathbf{w}_2)$. The factor set $\mathcal{T}_{e,e'} = \mathcal{W}_{e,e'} / \sim$ is the set of all different tours associated with the walks from $e' \in \mathcal{E}$ to $e \in \mathcal{E}$. Obviously, the number of such tours is bounded by $2^{|\mathcal{I}|}+1$. If $\partial(e) = \partial(e')$, then the empty tour $\mathfrak{T}^{(0)}$ corresponding to the trivial walk $\{e, e'\}$ is contained in $\mathcal{T}_{e,e}$.

Lemma 7.5. *Assume that the metric graph $(\mathcal{G}, \underline{a})$ satisfies conditions (i), (ii) of Assumption 1 as well as Assumption 2. If $\mathcal{I} \neq \emptyset$, then for arbitrary $e, e' \in \mathcal{E}$ the set $\mathcal{L}_{e,e'}$ has the following decomposition into disjoint subsets*

$$\mathcal{L}_{e,e'} = \bigsqcup_{\mathfrak{T} \in \mathcal{T}_{e,e'}} \mathcal{L}_{e,e'}^{\mathfrak{T}}. \tag{7.6}$$

Every set $\mathcal{L}_{e,e'}^{\mathfrak{T}}$ has the form

$$\begin{aligned} \mathcal{L}_{e,e'}^{\mathfrak{T}} = \Big\{ w_{\mathfrak{T}} + 2\sum_{i\in\mathfrak{T}} n_i a_i + \sum_{i\in\mathfrak{T}} |m_i|\, a_i \Big| \; & n_i \in \mathbb{N}_0, \\ m_i \in \mathbb{Z} \quad \textit{such that} \quad & \sum_{i\in\mathfrak{T}} m_i \sigma_i \in H_1(\mathfrak{T}, \mathbb{Z}) \Big\}, \end{aligned} \tag{7.7}$$

where $w_{\mathfrak{T}}$ is the length of a shortest walk from e' to e traversing each edge $i \in \mathfrak{T}$ at least once.

In particular, (7.7) implies that for any tour $\mathfrak{T} \in \mathcal{T}_{e,e}$ the set $\mathcal{L}_{e,e}^{\mathfrak{T}}$ is a semigroup with respect to the arithmetic addition.

Proof. The inclusion

$$\begin{aligned} \mathcal{L}_{e,e'}^{\mathfrak{T}} \supset \Big\{ w_{\mathfrak{T}} + 2\sum_{i\in\mathfrak{T}} n_i a_i + \sum_{i\in\mathfrak{T}} |m_i|\, a_i \Big| \; & n_i \in \mathbb{N}_0, \\ m_i \in \mathbb{Z} \quad \text{such that} \quad & \sum_{i\in\mathfrak{T}} m_i \sigma_i \in H_1(\mathfrak{T}, \mathbb{Z}) \Big\} \end{aligned}$$

is obvious. To prove the opposite inclusion choose an arbitrary number $w > w_{\mathfrak{T}}$ belonging to $\mathcal{L}_{e,e'}^{\mathfrak{T}}$. By (7.4) there is a walk

$$\mathbf{w} = \{e', i_1, \ldots, i_N, e\}$$

from $e' \in \mathcal{E}$ to $e \in \mathcal{E}$ associated with the tour $\mathfrak{T}$ such that $|\mathbf{w}| = w$. Let $\widehat{\mathbf{w}} = \{e', \widehat{i}_1, \ldots, \widehat{i}_N, e\}$ be a shortest walk from $e' \in \mathcal{E}$ to $e \in \mathcal{E}$ associated with the tour $\mathfrak{T}$, $|\widehat{\mathbf{w}}| = w_{\mathfrak{T}}$. Obviously,

$$w = w_{\mathfrak{T}} + \sum_{i\in\mathfrak{T}} n_i a_i \tag{7.8}$$

with some $n_i \in \mathbb{N}_0$.

Consider the 1-chain associated with a walk $\mathbf{w}$

$$\sigma_{\mathbf{w}} = \sum_{p=1}^{|\mathbf{w}|_{\mathrm{comb}}} \sigma_{i_p} \operatorname{sign}(i_p),$$

where $\operatorname{sign}(i_p) = +1$ if the p-th element v_p of the sequence $\mathbf{c}(\mathbf{w}) = \{v_0, \ldots, v_p, \ldots, v_N\}$ is the terminal vertex of the internal edge i_p and $\operatorname{sign}(i_p) = -1$ otherwise. Similarly, consider the 1-chain

$$\sigma_{\widehat{\mathbf{w}}} = \sum_{p=1}^{|\widehat{\mathbf{w}}|_{\mathrm{comb}}} \sigma_{\widehat{i}_p} \operatorname{sign}(\widehat{i}_p)$$

associated with the shortest walk $\widehat{\mathbf{w}}$. Consider the walk from e' to e' which follows the walk $\mathbf{w}$ from e' to e and then the reversed walk $\widehat{\mathbf{w}}_{\mathrm{rev}}$ from e to e'. Obviously, we have

$$\sigma_{\mathbf{w}} - \sigma_{\widehat{\mathbf{w}}} \in H_1(\mathfrak{T}, \mathbb{Z}). \tag{7.9}$$

Observe that if $\mathbf{w}$ is such that the equality $\sigma_{\mathbf{w}} = \sigma_{\widehat{\mathbf{w}}}$ holds, then the numbers n_i in (7.8) satisfy $n_i \in 2\mathbb{N}_0$ for all $i \in \mathfrak{T}$. This observation combined with (7.9) completes the proof of the equality (7.7).

To prove (7.6) it suffices to show that $\mathcal{L}_{e,e'}^{\mathfrak{T}_1} \cap \mathcal{L}_{e,e'}^{\mathfrak{T}_2} = \emptyset$ if $\mathfrak{T}_1 \neq \mathfrak{T}_2$. Assume that there exists a number $w \geq 0$ such that $w \in \mathcal{L}_{e,e'}^{\mathfrak{T}_1} \cap \mathcal{L}_{e,e'}^{\mathfrak{T}_2}$. Thus,

$$w = \sum_{i\in\mathcal{I}} n_i^{(1)} a_i \qquad \text{and} \qquad w = \sum_{i\in\mathcal{I}} n_i^{(2)} a_i$$

for some $n_i^{(1)} \in \mathbb{N}_0$ and $n_i^{(2)} \in \mathbb{N}_0$. Thus, by Assumption 2, we have $n_i^{(1)} = n_i^{(2)}$ for all $i \in \mathcal{I}$. Noting that

$$\mathfrak{T}_k = \{i \in \mathcal{I} |\ n_i^{(k)} \neq 0\}, \qquad k = 1, 2,$$

we obtain the equality $\mathfrak{T}_1 = \mathfrak{T}_2$, a contradiction. □

Further we will be mainly interested in the case $e = e'$ for an arbitrary external edge $e \in \mathcal{E}$. However, the case $e \neq e'$ will be of importance in Section 9. Recall that the empty tour $\mathfrak{T}^{(0)}$ (with $w_{\mathfrak{T}^{(0)}} = 0$) is contained in $\mathcal{T}_{e,e}$. Lemma 7.5 implies that $w_{\mathfrak{T}_1} \neq w_{\mathfrak{T}_2}$ whenever $\mathfrak{T}_1 \neq \mathfrak{T}_2$. Therefore, $\mathcal{T}_{e,e}$ is a totally ordered set with respect to the order relation $\mathfrak{T}_1 \lhd \mathfrak{T}_2$ defined by $w_{\mathfrak{T}_1} \leq w_{\mathfrak{T}_2}$. Hence, the elements of the set $\mathcal{T}_{e,e}$ can be written in increasing order $\mathfrak{T}^{(0)} \lhd \mathfrak{T}^{(1)} \lhd \ldots \lhd \mathfrak{T}^{(q)}$ such that $w_{\mathfrak{T}^{(l)}} < w_{\mathfrak{T}^{(m)}}$ for any $1 \leq l < m \leq q$, where $q = |\mathcal{T}_{e,e}| - 1$.

Define an integer valued function $\eta : \{0, 1, \ldots, q\} \to \mathbb{N}_0$ recursively by $\eta(0) = 0$, $\eta(1) = 1$, and

$$\eta(k) := \begin{cases} \eta(k-1) & \text{if} \quad \mathfrak{T}^{(k)} \subset \displaystyle\bigcup_{l=1}^{k-1} \mathfrak{T}^{(l)}, \\ \eta(k-1)+1 & \text{if} \quad \mathfrak{T}^{(k)} \not\subset \displaystyle\bigcup_{l=1}^{k-1} \mathfrak{T}^{(l)} \end{cases} \qquad \text{for all} \quad 2 \leq k \leq q.$$

For any $0 \leq k \leq q$ we set

$$\mathcal{I}^{(\eta(k))} := \bigcup_{l=0}^{k} \mathfrak{T}^{(l)} \tag{7.10}$$

such that $\mathcal{I}^{(0)} = \emptyset$ and $\mathcal{I}^{(\eta(q))} = \mathcal{I}$. Further, for any $p \in \{0, 1, \ldots, \eta(q)\}$ we set

$$\mathcal{L}_{e,e}^{(p)} := \bigsqcup_{\substack{0\leq k\leq q\\ \eta(k)\geq p}} \mathcal{L}_{e,e}^{(\mathfrak{T}^{(k)})}, \tag{7.11}$$

where the sets $\mathcal{L}_{e,e}^{(\mathfrak{T}^{(k)})}$ are defined by (7.7). In particular, $\mathcal{L}_{e,e}^{(0)} = \mathcal{L}_{e,e}$ and $\mathcal{L}_{e,e}^{(\eta(q))} = \emptyset$.

Let $v_0 := \partial(e)$. For any $p \in \{0, 1, \ldots, \eta(q)\}$ we set

$$V^{(p)} := \{v_0\} \cup \bigcup_{i\in\mathcal{I}^{(p)}} \{\partial^-(i)\} \cup \{\partial^+(i)\}. \tag{7.12}$$

By construction, the set $\mathcal{L}_{e,e}^{(p)}$ consists of the metric lengths of all walks on the graph $\mathcal{G}$ from e to e traversing at least one edge not belonging to $\mathcal{I}^{(p)}$. The number

$$w^{(p)} := \min \mathcal{L}_{e,e}^{(p)}$$

is the metric length of a shortest walk from e to e on the graph $\mathcal{G}$ traversing at least one edge not belonging to $\mathcal{I}^{(p)}$. The next result shows that this walk traverses *precisely* one edge not belonging to $\mathcal{I}^{(p)}$, that is, $\mathcal{I}^{(p+1)} \setminus \mathcal{I}^{(p)}$ consists of precisely one element. Along with Theorem 7.2 this constitutes the second tool to determine the topology of the graph from its scattering matrix.

Theorem 7.6. *Under Assumptions 1 and 2 the walk from e to e on the graph $\mathcal{G}$ having the metric length $w^{(p)}$ traverses precisely one internal edge $i \notin \mathcal{I}^{(p)}$.*

Proof. Let $\mathbf{w}$ be a shortest walk (with the metric length w_p) from e to e traversing at least one edge not belonging to $\mathcal{I}^{(p)}$. Assume to the contrary that the walk $\mathbf{w}$ traverses at least two different internal edges not belonging to $\mathcal{I}^{(p)}$, that is, there are $\widehat{i}_1, \ldots, \widehat{i}_q \in \mathcal{I} \setminus \mathcal{I}^{(p)}$, $q \geq 2$, such that $\widehat{i}_k \in \mathfrak{I}(\mathbf{w})$ for all $k \in \{1, \ldots, q\}$. Obviously, $\mathbf{w}$ visits $v_0 = \partial(e)$ precisely twice.

Claim 1: The set

$$V^{(p)} \cap \Big(\{\partial^-(\widehat{i}_1)\} \cup \ldots \cup \{\partial^-(\widehat{i}_q)\} \cup \{\partial^+(\widehat{i}_1)\} \cup \ldots \cup \{\partial^+(\widehat{i}_q)\}\Big)$$

consists of at least two elements. Assume to the contrary that this set consists of a single vertex $\widehat{v} \in V^{(p)}$. Assume first that $\widehat{v} \neq v_0$. Let

$$\mathbf{w}' = \{e, i^{(1)}, \ldots, i^{(r)}, i^{(r)}, \ldots, i^{(1)}, e\},$$

where $i^{(1)}, \ldots, i^{(r)} \in \mathcal{I}^{(p)}$, $\widehat{v} \in \partial(i^{(r)})$, be a shortest walk visiting the vertex $\widehat{v}$. Obviously, $n_i(\mathbf{w}) = n_i(\mathbf{w}')$ for all $i \in \mathcal{I}^{(p)}$.

If there is only one edge $\widehat{i} \in \{\widehat{i}_1, \ldots, \widehat{i}_q\}$ incident with the vertex $\widehat{v}$, then the walk $\mathbf{w}$ traverses $\widehat{i}$ twice. Therefore, the walk

$$\mathbf{w}'' = \{e, i^{(1)}, \ldots, i^{(r)}, \widehat{i}, \widehat{i}, i^{(r)}, \ldots, i^{(1)}, e\}, \tag{7.13}$$

traverses precisely one edge $\widehat{i} \notin \mathcal{I}^{(p)}$ and its metric length is, obviously, smaller than $|\mathbf{w}|$, which is a contradiction. Assume that the edges $\widehat{i}_1, \ldots, \widehat{i}_k \notin \mathcal{I}^{(p)}$, $2 \leq k \leq q$ are incident with the vertex $\widehat{v}$. Let $\widehat{i}_1$ be the edge with the shortest length among $\widehat{i}_1, \ldots, \widehat{i}_k$. Then,

$$\begin{aligned} |\mathbf{w}| &\geq |\mathbf{w}'| + a_{\widehat{i}_1} + \ldots + a_{\widehat{i}_k} \\ &> |\mathbf{w}'| + k a_{\widehat{i}_1} \geq |\mathbf{w}'| + 2a_{\widehat{i}_1} = |\mathbf{w}''|. \end{aligned}$$

Thus, the walk $\mathbf{w}''$ traverses precisely one edge $\widehat{i}_1 \notin \mathcal{I}^{(p)}$ and its length is smaller than $|\mathbf{w}|$, again a contradiction.

If $\widehat{v} = v_0$, the same arguments show that the walk $\{e, \widehat{i}_1, \widehat{i}_1, e\}$ traverses precisely one edge $\widehat{i}_1 \notin \mathcal{I}^{(p)}$ and its metric length is smaller than $|\mathbf{w}|$. This completes the proof of Claim 1.

Claim 2: $v_0 \notin \{\partial^-(\widehat{i}_1)\} \cup \ldots \cup \{\partial^-(\widehat{i}_q)\} \cup \{\partial^+(\widehat{i}_1)\} \cup \ldots \cup \{\partial^+(\widehat{i}_q)\}$. Assume to the contrary that $v_0 \in \{\partial^-(\widehat{i}_1)\} \cup \ldots \cup \{\partial^-(\widehat{i}_q)\} \cup \{\partial^+(\widehat{i}_1)\} \cup \ldots \cup \{\partial^+(\widehat{i}_q)\}$. Since $\mathbf{w}$ visits v_0 precisely twice, there are at most two different edges (say $\widehat{i}_1$ and $\widehat{i}_2$) incident with v_0. Without loss of generality we can assume that $a_{\widehat{i}_1} < a_{\widehat{i}_2}$. The walk $\{e, \widehat{i}_1, \widehat{i}_1, e\}$ traverses precisely one edge $\widehat{i}_1 \notin \mathcal{I}^{(p)}$ and its metric length is smaller than $|\mathbf{w}|$,

$$2a_{\widehat{i}_1} < a_{\widehat{i}_1} + a_{\widehat{i}_2} \leq |\mathbf{w}|.$$

Thus, $\widehat{i}_1$ is the only edge among $\widehat{i}_1, \ldots, \widehat{i}_q$ incident with the vertex v_0.

By the Claim 1 there is a vertex $\widehat{v} \in V^{(p)}$, $\widehat{v} \neq v_0$ such that

$$\widehat{v} \in V^{(p)} \cap \Big(\{\partial^-(\widehat{i}_1)\} \cup \ldots \cup \{\partial^-(\widehat{i}_q)\} \cup \{\partial^+(\widehat{i}_1)\} \cup \ldots \cup \{\partial^+(\widehat{i}_q)\}\Big)$$

and either the walk $\mathbf{w}$ or its reversed $\mathbf{w}_{\mathrm{rev}}$ does not leave $\mathcal{I}^{(p)}$ after visiting the vertex $\widehat{v}$. Let

$$\mathbf{w}' = \{e, i^{(1)}, \ldots, i^{(r)}, i^{(r)}, \ldots, i^{(1)}, e\},$$

where $i^{(1)}, \ldots, i^{(r)} \in \mathcal{I}^{(p)}$, $\widehat{v} \in \partial(i^{(r)})$, be a shortest walk visiting the vertex $\widehat{v}$. It is unique up to reversing. Obviously, after visiting the vertex $\widehat{v}$ the remainder of the walk $\mathbf{w}$ (or its reversed) agrees with the remainder $(i^{(r)}, \ldots, i^{(r)}, e)$ of the walk $\mathbf{w}'$.

Assume that $\partial(\widehat{i}_1) \doteq \{v_0, \widehat{v}\}$, that is, either $\partial(\widehat{i}_1) = \{v_0, \widehat{v}\}$ or $\partial(\widehat{i}_1) = \{\widehat{v}, v_0\}$. Then the walk

$$\{e, i^{(1)}, \ldots, i^{(r)}, \widehat{i}_1, e\}$$

traverses precisely one edge $\widehat{i}_1 \in \mathcal{I}_p$ and its metric length is smaller than that of the walk $\mathbf{w}$. Thus, $\partial(\widehat{i}_1) \neq \{v_0, \widehat{v}\}$ and, hence, there is an edge $\widehat{i} \in \{\widehat{i}_2, \ldots, \widehat{i}_q\}$ incident with the vertex $\widehat{v}$.

Let $\widehat{i} \in \{\widehat{i}_2, \ldots, \widehat{i}_q\}$ be an edge incident with the vertex $\widehat{v}$. The metric length of the walk $\mathbf{w}$ is given by

$$|\mathbf{w}| = a_{\widehat{i}_1} + a_{\widehat{i}} + |\mathbf{w}'|/2 + \xi,$$

where ξ is a nonnegative number. From the assumption $|\mathbf{w}| < 2a_{\widehat{i}_1}$ it follows that

$$a_{\widehat{i}} + |\mathbf{w}'|/2 + \xi < a_{\widehat{i}_1}. \tag{7.14}$$

On the other hand, $|\mathbf{w}| < |\mathbf{w}''| = |\mathbf{w}'| + 2a_{\widehat{i}}$, where $\mathbf{w}''$ is defined by (7.13). Thus,

$$a_{\widehat{i}_1} + \xi < a_{\widehat{i}} + |\mathbf{w}'|/2 \leq a_{\widehat{i}} + |\mathbf{w}'|/2 + 2\xi,$$

which implies the inequality

$$a_{\widehat{i}} + |\mathbf{w}'|/2 + \xi > a_{\widehat{i}_1}$$

contradicting to (7.14) and, thus, completing the proof of Claim 2.

Claim 3: The walk $\mathbf{w}$ traverses precisely one edge $\widehat{i} \notin \mathcal{I}^{(p)}$. We continue to assume that $\mathbf{w}$ visits at least two edges not belonging to $\mathcal{I}^{(p)}$. From the Claims 1 and 2 it follows that there are two different vertices $\widehat{v}, \widetilde{v} \in V^{(p)}$ such that the walk $\mathbf{w}$ does not leave $\mathcal{I}^{(p)}$ before visiting $\widehat{v}$ and after visiting $\widetilde{v}$. Let $\widehat{i} \notin \mathcal{I}^{(p)}$ and $\widetilde{i} \notin \mathcal{I}^{(p)}$ be edges incident with $\widehat{v}$ and $\widetilde{v}$, respectively. It is easy to show that $\widehat{i} \neq \widetilde{i}$, $\partial(\widehat{i}) \neq \{\widehat{v}, \widetilde{v}\}$, and $\partial(\widetilde{i}) \neq \{\widehat{v}, \widetilde{v}\}$.

Set

$$\widehat{\mathbf{w}} = \{e, i^{(1)}, \ldots, i^{(r)}, i^{(r)}, \ldots, i^{(1)}, e\}$$

and

$$\widetilde{\mathbf{w}} = \{e, i^{(r+1)}, \ldots, i^{(r+s)}, i^{(r+s)}, \ldots, i^{(r+1)}, e\},$$

where $i^{(1)}, \ldots, i^{(r+s)} \in \mathcal{I}^{(p)}$, $\widehat{v} \in \partial(i^{(r)})$, $\widetilde{v} \in \partial(i^{(r+s)})$, be shortest walks visiting the vertices $\widehat{v}$ and $\widetilde{v}$, respectively. Consider the walks

$$\mathbf{w}' = \{e, i^{(1)}, \ldots, i^{(r)}, \widehat{i}, \widehat{i}, i^{(r)}, \ldots, i^{(1)}, e\},$$

and

$$\mathbf{w}'' = \{e, i^{(r+1)}, \ldots, i^{(r+s)}, \widetilde{i}, \widetilde{i}, i^{(r+s)}, \ldots, i^{(r+1)}, e\}.$$

The metric length of the walk $\mathbf{w}$ satisfies

$$|\mathbf{w}| \geq |\widehat{\mathbf{w}}|/2 + |\widetilde{\mathbf{w}}|/2 + a_{\widehat{i}} + a_{\widetilde{i}}.$$

By Assumption 2 either

$$a_{\widehat{i}} + \sum_{k=1}^{r} a_{i^{(k)}} < a_{\widetilde{i}} + \sum_{k=1}^{s} a_{i^{(r+k)}}$$

or

$$a_{\widehat{i}} + \sum_{k=1}^{r} a_{i^{(k)}} > a_{\widetilde{i}} + \sum_{k=1}^{s} a_{i^{(r+k)}}.$$

Thus, either the walk $\mathbf{w}'$ of length $2(a_{\widehat{i}} + \sum_{k=1}^{r} a_{i^{(k)}})$, or the walk $\mathbf{w}''$ of length $2(a_{\widetilde{i}} + \sum_{k=1}^{s} a_{i^{(r+k)}})$ is shorter than the walk $\mathbf{w}$. Since both these walks traverse precisely one edge not belonging to $\mathcal{I}_p$, we arrive at a contradiction. The theorem is proven. □

As an immediate consequence of Theorem 7.6 we obtain the following result.

Corollary 7.7. *Under Assumptions 1 and 2 for any $v \in V^{(p)}$ there is a unique $k \in \{0, 1, \ldots, p\}$ such that $w^{(k)}$ is the length of the shortest walk on the graph $\mathcal{G}$ from e to e visiting the vertex v precisely once. The number $w^{(k)}$ is necessarily of the form*

$$w^{(k)} = \sum_{i \in \mathcal{I}} n_i a_i \qquad \text{with} \qquad n_i \in \{0, 2\}.$$

For an arbitrary $e \in \mathcal{E}$ let $\mathcal{G}_e$ denote the graph obtained from $\mathcal{G} = (V, \mathcal{E}, \mathcal{I}, \partial)$ by removing all external edges $e' \neq e$, $\mathcal{G}_e = (V, \mathcal{I}, \{e\}, \partial|_{\{e\}\cup\mathcal{I}})$. So $\mathcal{G}_e$ has only one external edge e. The graphs $\mathcal{G}_e$ and $\mathcal{G}$ have the same interior.

The strategy to prove the first part of Theorem 1 is to construct the graph $\mathcal{G}_e$. The following result combined with Theorem 7.2 and Remark 7.3 implies the first part of Theorem 1.

Theorem 7.8. *Assume that the metric graph $(\mathcal{G}, \underline{a})$, $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ satisfies Assumptions 1 and 2. Let $e \in \mathcal{E}$ be arbitrary. The set $\mathcal{L}_{e,e}$ determines the graph $\mathcal{G}_{\rm int} = (V, \mathcal{I}, \emptyset, \partial|_{\mathcal{I}})$, the vertex $v_0 = \partial(e)$ and the metric $\underline{a}$ uniquely.*

We start the proof with the following simple observation: $\mathcal{L}_{e,e} = \{0\}$ if and only if $\mathcal{G}_e$ is a single vertex graph with no internal edges such that $\mathcal{G}_e = (\{v\}, \emptyset, \{e\}, \partial)$. Therefore, from now on we assume that the graph $\mathcal{G}_e$ contains at least one internal edge. Thus, by Lemma 7.1 the set $\mathcal{L}_{e,e}$ is infinite.

To prove Theorem 7.8 we construct a sequence of metric graphs $(\mathcal{G}_e^{(p)}, \underline{a}^{(p)})$ with $\mathcal{G}_e^{(p)} := (V^{(p)}, \mathcal{I}^{(p)}, \{e\}, \partial^{(p)})$ and $\underline{a}^{(p)} = \{a_i\}_{i \in \mathcal{I}^{(p)}}$, where $\partial^{(p)} = \partial|_{\mathcal{I}^{(p)} \cup \{e\}}$, and the sets $\mathcal{I}^{(p)}$ and $V^{(p)}$ are given by (7.10) and (7.12), respectively. The set of lengths of all walks on the graph $\mathcal{G}_e^{(p)}$ from e to e agrees with $\mathcal{L}_{e,e} \setminus \mathcal{L}_{e,e}^{(p)}$. By Theorem 7.6 the graph $\mathcal{G}_e^{(p+1)}$ can be constructed by adding an internal edge i_{p+1} to the graph $\mathcal{G}_e^{(p)}$. By the discussion above, $\mathcal{L}_{e,e}^{(r)} = \emptyset$ for a sufficiently large $r \in \mathbb{N}$ and, therefore, $\mathcal{G}_e^{(r)} = \mathcal{G}_e$ with $|\mathcal{I}| = r$. Below we will prove that this sequence can be constructed in a unique way.

Before we turn to the general case, we will treat in detail the construction of the graphs $\mathcal{G}_e^{(1)}$ and $\mathcal{G}_e^{(2)}$. Since $V^{(0)} = \{v_0\}$, we have $\mathcal{G}_e^{(0)} = (\{v_0\}, \emptyset, \{e\}, \partial^{(0)})$ such that $\partial^{(0)}(e) = v$. Now we construct $\mathcal{G}_e^{(1)} = (\{v_0, v_1\}, \{i_1\}, \{e\}, \partial^{(1)})$ from $\mathcal{G}_e^{(0)}$. Here $\partial^{(1)}(e) = v_0$ and $\partial^{(1)}(i_1) \doteq \{v_0, v_1\}$ (see Fig. 3). Since the shortest nontrivial walk from e to e on $\mathcal{G}_e^{(1)}$ is $\{e, i_1, i_1, e\}$ we necessarily

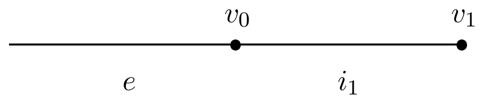

FIG. 3. The graph $\mathcal{G}_e^{(1)}$. It has one external edge e, one boundary vertex v, one internal vertex v_1, and one internal edge i_1 with length a_{i_1}.

have that the length of the internal edge i_1 is equal to $a_{i_1} = w_{e,e}(1)/2 > 0$.

We turn to the construction of the graph $\mathcal{G}_e^{(2)}$. By Lemma 7.4 the set $\{2na_{i_1}\}_{n\in\mathbb{N}_0}$ is contained in $\mathcal{L}_{e,e}$. From (7.11) it follows that

$$\mathcal{L}_{e,e}^{(1)} = \mathcal{L}_{e,e} \setminus \{2na_{i_1}\}_{n\in\mathbb{N}_0}. \tag{7.15}$$

If the set $\mathcal{L}_{e,e}^{(1)}$ is empty, then we are finished: $\mathcal{G}_e = \mathcal{G}_e^{(1)}$, $|V^{(1)}| = 2$, and $|\mathcal{I}^{(1)}| = 1$.

Assume now that $\mathcal{L}_{e,e}^{(1)}$ is nonempty and let $w^{(1)} > w_{e,e}(1)$ be the smallest number in $\mathcal{L}_{e,e}^{(1)}$. By Lemma 7.5 from Assumption 2 it follows that $w^{(1)}$ and $w_{e,e}(1)$ are rationally independent.

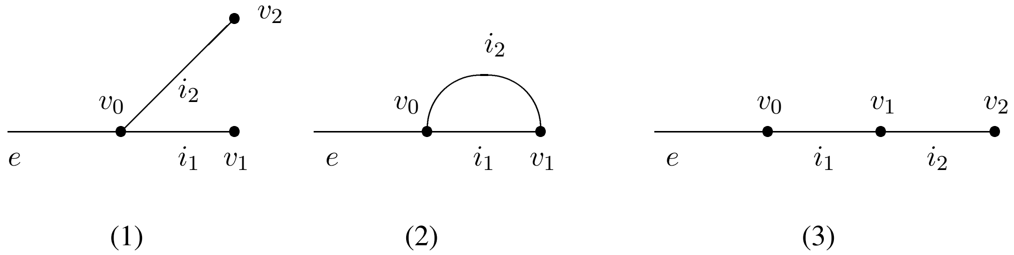

FIG. 4. Three topologically different possibilities to construct the graph $\mathcal{G}_e^{(2)}$ from $\mathcal{G}_e^{(1)}$.

The graph $\mathcal{G}_e^{(2)}$ will be constructed from $\mathcal{G}_e^{(1)}$ by adding an internal edge i_2. Ignoring the orientation of internal edges, there are three topologically different possibilities to add this edge (see Fig. 4):

(1) The edge i_2 has v_0 as the initial vertex. Its terminal vertex v_2 coincides neither with v_0 nor with v_1. Thus, $V^{(2)} = \{v_0, v_1, v_2\}$.
(2) The edge i_2 has v_0 as the initial vertex and v_1 as the terminal one. Thus, $V(\mathcal{G}_e^{(2)}) = \{v_0, v_1\}$.
(3) The edge i_2 has v_1 as the initial vertex. Its terminal vertex v_2 coincides neither with v_0 nor with v_1. Thus, $V^{(2)} = \{v_0, v_1, v_2\}$.

There is only one choice of the length a_{i_2} of the internal edge i_2 guaranteeing that the shortest walk from e to e traversing the edge i_2 has the metric length $w^{(1)}$:

Case (1): $a_{i_2} = w^{(1)}/2$,
Case (2): $a_{i_2} = w^{(1)} - a_{i_1}$,
Case (3): $a_{i_2} = w^{(1)}/2 - a_{i_1}$.

Note that in all three cases the lengths a_{i_1} and a_{i_2} of the internal edges i_2 and i_1 are not only different but also rationally independent.

Observe that the structure of the set $\mathcal{L}_{e,e}^{(1)}$ uniquely fixes the possibility to add the internal edge i_2 to the graph $\mathcal{G}_e^{(1)}$. Indeed, with the integer-valued function

$$\nu(m) := \min\left\{n \in \mathbb{Z} \,\middle|\, n a_{i_1} + m w^{(1)} \in \mathcal{L}_{e,e}^{(1)}\right\}, \qquad m \in \mathbb{N}. \tag{7.16}$$

we have the following proposition.

Proposition 7.9. $\nu(m) = 0$ *for all* $m \in \mathbb{N}$ *if and only if the Case (1) holds.*

$$\nu(m) = \begin{cases} -m & \textit{for all} \quad m \in 2\mathbb{N}, \\ 1-m & \textit{for all} \quad m \in 2\mathbb{N}-1 \end{cases} \quad \textit{if and only if the Case (2) holds.}$$

$\nu(m) = 2(1-m)$ *for all* $m \in \mathbb{N}$ *if and only if the Case (3) holds.*

Proof. The "if" parts of all statements can be verified by direct calculations. This immediately implies that the "only if" part of each statement holds. □

The construction of the graph $\mathcal{G}_e^{(p+1)}$ from $\mathcal{G}_e^{(p)}$ for general $p \in \mathbb{N}$ is similar to the case $p = 1$ already discussed. By Theorem 7.6 the graph $\mathcal{G}_e^{(p+1)}$ can be constructed by adding an internal edge i_{p+1} to the graph $\mathcal{G}_e^{(p)}$. Ignoring the orientation of internal edges, there are four topologically different possibilities to add this edge (see Fig. 5):

(1) The edge i_{p+1} has v_0 as the initial vertex. Its terminal vertex v' does not belong to $V^{(p)}$. Thus, $V^{(p+1)} = V^{(p)} \cup \{v'\}$.

(2) The edge i_{p+1} has v_0 as the initial vertex. Its terminal vertex $v' \neq v_0$ belongs to $V^{(p)}$. Thus, $V^{(p+1)} = V^{(p)}$.
(3) The edge i_{p+1} has $v' \in V^{(p)}$, $v' \neq v_0$ as the initial vertex. Its terminal vertex v'' does not belong to $V^{(p)}$. Thus, $V^{(p+1)} = V^{(p)} \cup \{v''\}$.
(4) The edge i_{p+1} has $v' \in V^{(p)}$, $v' \neq v_0$ as the initial vertex. Its terminal vertex $v'' \neq v'$, $v'' \neq v_0$ belongs to $V^{(p)}$. Thus, $V^{(p+1)} = V^{(p)}$.

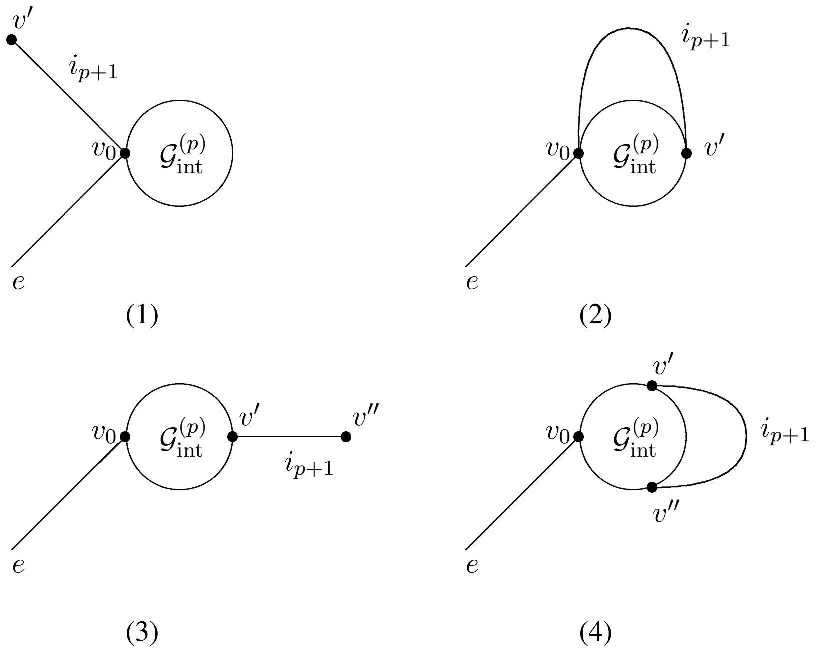

FIG. 5. Four topologically different possibilities to construct the graph $\mathcal{G}_e^{(p+1)}$ from $\mathcal{G}_e^{(p)}$. The Case (4) may occur only if $|V^{(p)}| \geq 3$.

For every $m \in \mathbb{N}$ we define

$$\nu^{(p)}(m) := \min\left\{n \in \mathbb{Z} \,\middle|\, \exists\, w \in \mathcal{L}_{e,e} \setminus \mathcal{L}_{e,e}^{(p)} \quad \text{such that} \quad mw^{(p)} + nw/2 \in \mathcal{L}_{e,e}^{(p)}\right\}.$$

For $p = 1$ this definition agrees with (7.16).

Lemma 7.10. *Assume that the Case (2) holds. Then the shortest walk from e to e traversing the edge i_{p+1} also traverses at least one edge $i \in \mathcal{I}^{(p)}$.*

Proof. Assume to the contrary that the shortest walk from e to e traversing the edge i_{p+1} traverses none of the edges $i \in \mathcal{I}^{(p)}$. By Lemma 7.6 it is of the form

$$\mathbf{w} = \{e, i_{p+1}, i_{p+1}, e\}.$$

Let $v' \neq v_0$ be the other vertex incident with i_{p+1}. By Corollary 7.7 there is a walk

$$\mathbf{w}_0 = \{e, j_1, \ldots, j_k, j_k, \ldots, j_1, e\}, \qquad v' \in \partial(j_k)$$

from e to e visiting the vertex v' with $j_1, \ldots, j_k \in \mathcal{I}^{(p)}$. Its metric length is strictly smaller than $|\mathbf{w}| = 2a_{i_{p+1}}$. But then the walk

$$\mathbf{w}' = \{e, j_1, \ldots, j_k, i_{p+1}, e\}$$

traversing the edge i_{p+1} also traverses at least one edge in $\mathcal{I}^{(p)}$. Its metric length satisfies the inequality

$$|\mathbf{w}'| = \frac{1}{2}(|\mathbf{w}| + |\mathbf{w}_0|) < |\mathbf{w}_0|,$$

which is a contradiction. □

Lemma 7.11. *Assume that the Case (4) holds. Let* $\mathbf{w}$ *be the shortest walk from* e *to* e *on the graph* $\mathcal{G}$ *traversing the edge* i_{p+1} *at least once. Let* $\mathbf{w}'$ *be the shortest walk from* e *to* e *on the graph* $\mathcal{G}_e^{(p)}$ *visiting the vertex* v' *and* $\mathbf{w}''$ *be the shortest walk from* e *to* e *on the graph* $\mathcal{G}_e^{(p)}$ *visiting the vertex* v''. *Then*

$$\mathfrak{T}(\mathbf{w}) = \mathfrak{T}(\mathbf{w}') \cup \mathfrak{T}(\mathbf{w}'') \cup \{i_{p+1}\}. \tag{7.17}$$

Proof. A priori there are three possibilities:

$$\begin{aligned} &(\alpha) \qquad |\mathbf{w}'|/2 > |\mathbf{w}''|/2 + a_{i_{p+1}},\\ &(\beta) \qquad |\mathbf{w}'|/2 = |\mathbf{w}''|/2 + a_{i_{p+1}},\\ &(\gamma) \qquad |\mathbf{w}'|/2 < |\mathbf{w}''|/2 + a_{i_{p+1}}. \end{aligned}$$

Without loss of generality, by Assumption 2 we may assume $|\mathbf{w}'| < |\mathbf{w}''|$. Then, inequality (α) contradicts Corollary 7.7 for the vertex v'. Equality (β) contradicts Assumption 2. Thus, inequality (γ) holds, which implies (7.17). □

Remark 7.12. *Lemma 7.11 does not exclude the possibilities* $\mathfrak{T}(\mathbf{w}') \subset \mathfrak{T}(\mathbf{w}'')$ *and* $\mathfrak{T}(\mathbf{w}'') \subset \mathfrak{T}(\mathbf{w}')$.

Proposition 7.13. *(i) The Case (1) holds if and only if* $\nu^{(p)}(m) = 0$ *for all* $m \in \mathbb{N}$.

(ii) The Case (2) holds if and only if the following two conditions hold simultaneously

$$\nu^{(p)}(m) = \begin{cases} -m & \textit{for all} \quad m \in 2\mathbb{N}, \\ 1-m & \textit{for all} \quad m \in 2\mathbb{N}-1, \end{cases} \tag{7.18}$$

and

$$\begin{cases} \textit{For every} \quad w = \sum_{i\in\mathcal{I}} n_i a_i \in \mathcal{L}_{e,e} \setminus \mathcal{L}_{e,e}^{(p)} \quad \textit{with} \quad n_i \in \{0,2\} \quad \textit{satisfying} \\ m w^{(p)} + \nu^{(p)}(m) w/2 \in \mathcal{L}_{e,e}^{(p)} \quad \textit{for all} \quad m \in \mathbb{N} \\ \textit{the equality} \quad w = w^{(k)} \quad \textit{holds for some} \quad k \in \{1,\ldots,p-1\}. \end{cases} \tag{7.19}$$

(iii) The Case (3) holds if and only if the following two conditions hold simultaneously

$$\nu^{(p)}(m) = 2(1-m) \quad \textit{for all} \quad m \in \mathbb{N} \tag{7.20}$$

and

$$\begin{cases} \textit{For every} \quad w = \sum_{i\in\mathcal{I}} n_i a_i \in \mathcal{L}_{e,e} \setminus \mathcal{L}_{e,e}^{(p)} \quad \textit{satisfying} \\ m w^{(p)} + \nu^{(p)}(m) w/2 \in \mathcal{L}_{e,e}^{(p)} \quad \textit{for all} \quad m \in \mathbb{N} \\ \textit{the number} \quad w' := \sum_{i\in\mathcal{I}} n_i' a_i \quad \textit{with} \quad n_i' = \begin{cases} 2 & \textit{if} \quad n_i \neq 0 \\ 0 & \textit{if} \quad n_i = 0 \end{cases} \\ \textit{satisfies} \quad m w^{(p)} + \nu^{(p)}(m) w'/2 \in \mathcal{L}_{e,e}^{(p)} \quad \textit{for all} \quad m \in \mathbb{N}. \end{cases} \tag{7.21}$$

Note that if the Case (4) holds, then either

$$\nu^{(p)}(m) = \begin{cases} -m & \text{for all} \quad m \in 2\mathbb{N} \\ 1-m & \text{for all} \quad m \in 2\mathbb{N}-1 \end{cases}$$

or $\nu^{(p)}(m) = 2(1-m)$ for all $m \in \mathbb{N}$ depending on whether the shortest walk traversing the edge $i_{p+1} \notin \mathcal{I}^{(p)}$ traverses any edge $i \in \mathcal{I}^{(p)}$ at most once or there is an edge $i' \in \mathcal{I}^{(p)}$ traversed by this walk twice.

Proof of Proposition 7.13. Observe that by Theorem 7.6 the number $w^{(p)}$ is the length of the shortest walk from e to e traversing the edge i_{p+1} at least once and not traversing any edge $i \in \mathcal{I} \setminus (\mathcal{I}^{(p)} \cup \{i_{p+1}\})$. With this observation the "only if" parts of all three statements can be verified by direct calculations.

To prove the "if" part of the claim (i) we assume that $\nu^{(p)}(m) = 0$ for all $m \in \mathbb{N}$. Then

$$mw^{(p)} - nw/2 \notin \mathcal{L}_{e,e}^{(p)} \text{ for any } w \in \mathcal{L}_{e,e} \setminus \mathcal{L}_{e,e}^{(p)} \text{ and for all } m, n \in \mathbb{N}. \tag{7.22}$$

Assume that the Case (2) holds. Let $\mathbf{w}$ be a shortest walk from e to e on the graph $\mathcal{G}_e^{(p)}$ visiting the vertex v'. Therefore, $|\mathbf{w}| \in \mathcal{L}_{e,e} \setminus \mathcal{L}_{e,e}^{(p)}$. Then for arbitrary even $m \in \mathbb{N}$

$$mw^{(p)} - \frac{m}{2}|\mathbf{w}| \in \mathcal{L}_{e,e}^{(p)},$$

which contradicts (7.22).

Assume that the Case (3) holds. Let $\mathbf{w}$ be a shortest walk from e to e on the graph $\mathcal{G}_e^{(p)}$ visiting the vertex v'. Then for any $m \in \mathbb{N}$

$$mw^{(p)} - (m-1)|\mathbf{w}| \in \mathcal{L}_{e,e}^{(p)},$$

which again contradicts (7.22).

Assume next that the Case (4) holds. Let $\mathbf{w}$ be a shortest walk from e to e on the graph $\mathcal{G}$ traversing the edge i_{p+1} at least once. Let $\mathbf{w}'$ be the shortest walk from e to e on the graph $\mathcal{G}_e^{(p)}$ visiting the vertex v' and let $\mathbf{w}''$ be the shortest walk from e to e on the graph $\mathcal{G}_e^{(p)}$ visiting the vertex v''. Observe that

$$|\mathbf{w}'| + |\mathbf{w}''| \in \mathcal{L}_{e,e} \setminus \mathcal{L}_{e,e}^{(p)}.$$

By Lemma 7.11

$$\mathfrak{T}(\mathbf{w}) = \mathfrak{T}(\mathbf{w}') \cup \mathfrak{T}(\mathbf{w}'') \cup \{i_{p+1}\}.$$

Therefore, for any odd $m > 1$,

$$mw^{(p)} - \frac{m-1}{2}(|\mathbf{w}'| + |\mathbf{w}''|) \in \mathcal{L}_{e,e}^{(p)},$$

which once more contradicts (7.22). Thus, the claim (i) is proven.

We turn to the proof of the "if" part of the claim (ii). By (i) and by the "only if" part of (iii) the condition (7.18) implies that either the Case (2) or the Case (4) holds. Assume that the Case (4) holds. Let $v', v'' \in V(\mathcal{G}_e^{(p)})$, $v' \neq v''$ be vertices incident with the edge i_{p+1}. Let $\mathbf{w}'$ and $\mathbf{w}''$ be the shortest walks on the graph $\mathcal{G}_e^{(p)}$ from e to e visiting the vertices v' and v'', respectively. There are no edges in $\mathcal{I}^{(p)}$ traversed by both walks $\mathbf{w}'$ and $\mathbf{w}''$. Indeed, assume to the contrary that there is an edge $\widetilde{i} \in \mathcal{I}^{(p)}$ traversed by both walks. Then, the shortest walk from e to e on the graph $\mathcal{G}_e^{(p+1)}$ traversing the edge i_{p+1} traverses the edge $\widetilde{i}$ twice. Therefore, $\nu^{(p)}(m) = 2(1-m)$ for all $m \in \mathbb{N}$, which contradicts (7.18). Further, the scores of the walks $\mathbf{w}'$ and $\mathbf{w}''$ contain only 0's and 2's.

With these observations we obtain that the shortest walk from e to e traversing the edge i_{p+1} (and, thus, visiting the vertices v' and v'') traverses every edge $i \in \mathcal{I}^{(p)}$ at most once. By Lemma 7.11 the number $w = |\mathbf{w}'| + |\mathbf{w}''| \in \mathcal{L}_{e,e} \setminus \mathcal{L}_{e,e}^{(p)}$ satisfies

$$mw^{(p)} + \nu^{(p)}(m)w/2 \in \mathcal{L}_{e,e}^{(p)}.$$

in particular for $m = 3$ with $\nu^{(p)}(m) = -2$. By Corollary 7.7 the equalities $|\mathbf{w}'| = w^{(k_1)}$ and $|\mathbf{w}'| = w^{(k_2)}$ hold for some $k_1, k_2 \in \{1, \ldots, p\}$. Therefore, $w \neq w^{(k)}$ for all $k \in \{1, \ldots, p\}$. Thus, (7.19) does not hold, which is a contradiction. This proves the "if" part of the claim (ii).

Now we turn to the proof of the "if" part of the claim (iii). By what we already proved only the Cases (3) or (4) may occur. Assume that the Case (4) holds. Let $\mathbf{w}$ be a shortest walk from e to e on the graph $\mathcal{G}$ traversing the edge i_{p+1} at least once. Recall that by Theorem 7.6 this walk does not traverse any edge $i \in \mathcal{I} \setminus (\mathcal{I}^{(p)} \cup \{i_{p+1}\})$. Let $v', v'' \in V(\mathcal{G}_e^{(p)})$, $v' \neq v''$ be vertices incident with the edge i_{p+1}. Let $\mathbf{w}'$ and $\mathbf{w}''$ be the shortest walks on the graph $\mathcal{G}_e^{(p)}$ from e to e visiting the vertices v' and v'', respectively. Recall (see Remark 7.12) that it is possible that either $\mathfrak{T}(\mathbf{w}') \subset \mathfrak{T}(\mathbf{w}'')$ or $\mathfrak{T}(\mathbf{w}'') \subset \mathfrak{T}(\mathbf{w}')$.

The number $w = |\mathbf{w}'| + |\mathbf{w}''|$ satisfies

$$mw^{(p)} + \nu^{(p)}(m)w/2 \in \mathcal{L}_{e,e}^{(p)} \quad \text{for all} \quad m \in \mathbb{N}.$$

Let

$$n_i' := \begin{cases} 2 & \text{if} \quad n_i(\mathbf{w}) \neq 0, \\ 0 & \text{if} \quad n_i(\mathbf{w}) = 0. \end{cases}$$

Obviously, $\{n_i'\}_{i\in\mathcal{I}}$ is the score of a walk on graph $\mathcal{G}_e^{(p)}$ visiting both vertices v' and v''.

Choose $m = 3$ for which $\nu^{(p)}(m) = -4$. The walk $\mathbf{w}$ traverses at least one edge $\widehat{i} \in \mathcal{I}^{(p)}$ precisely once and at least one edge in $\mathcal{I}^{(p)}$ twice. Let

$$w' := \sum_{i\in\mathcal{I}} n_i' a_i.$$

Therefore,

$$mw^{(p)} + \nu^{(p)}(m)w'/2 = \sum_{i\in\mathcal{I}} \widetilde{n}_i a_i$$

with $\widetilde{n}_{\widehat{i}} = -1$. Hence, the condition

$$mw^{(p)} + \nu^{(p)}(m)w'/2 \in \mathcal{L}_{e,e}^{(p)}$$

is not satisfied for $m = 3$, which contradicts (7.21). □

The following proposition ensures the uniqueness of the graph $\mathcal{G}_e^{(p+1)}$.

Proposition 7.14. *In Cases (2), (3), and (4) there is a unique possibility to construct the graph* $\mathcal{G}_e^{(p+1)} = (V^{(p+1)}, \mathcal{I}^{(p+1)}, \{e\}, \partial^{(p+1)})$ *from* $\mathcal{G}_e^{(p)} = (V^{(p)}, \mathcal{I}^{(p)}, \{e\}, \partial^{(p)})$. *More precisely:*

(i) Assume that the Case (2) or (3) holds. Then there is a unique vertex $v' \in V^{(p)}$, $v' \neq v_0$ *such that*

(a) *the set of lengths of all walks from e to e on the graph $\mathcal{G}_e^{(p+1)}$ obtained from $\mathcal{G}_e^{(p)}$ by adding the edge i_{p+1} with $v' \in \partial(i_{p+1})$, is contained in $\mathcal{L}_{e,e}$,*

(b) *the metric graph $\mathcal{G}_e^{(p+1)}$ satisfies Assumptions 1 and 2.*

The metric length of the edge i_{p+1} is given by

$$a_{i_{p+1}} = \begin{cases} w^{(p)} - |\mathbf{w}'|/2 & \textit{if the Case (2) holds}, \\ (w^{(p)} - |\mathbf{w}'|)/2 & \textit{if the Case (3) holds}, \end{cases}$$

where $\mathbf{w}'$ is a shortest walk on the graph $\mathcal{G}_e^{(p)}$ from e to e visiting the vertex v' precisely once.

(ii) Assume that the Case (4) holds. Then there is a unique pair of vertices $v' \neq v'' \in V^{(p)}$ *such that*

(a) *the set of lengths of all walks from e to e on the graph $\mathcal{G}_e^{(p+1)}$ obtained from $\mathcal{G}_e^{(p)}$ by adding the edge i_{p+1} with $\partial(i_{p+1}) \simeq \{v', v''\}$, is contained in $\mathcal{L}_{e,e}$,*

(b) *the metric graph $\mathcal{G}_e^{(p+1)}$ satisfies Assumptions 1 and 2.*

The metric length of the edge i_{p+1} is given by

$$a_{i_{p+1}} = w^{(p)} - (|\mathbf{w}'| + |\mathbf{w}''|)/2,$$

where $\mathbf{w}'$ and $\mathbf{w}''$ are the shortest walks on the graph $\mathcal{G}_e^{(p)}$ from e to e visiting the vertices v' and v'', respectively.

Proof. The proofs in all three cases are rather similar. Therefore, we will deal with the Case (4) only.

Let $v' \neq v''$ and $\widetilde{v}' \neq \widetilde{v}''$ belong to $V^{(p)}$. Let $\mathbf{w}'$, $\mathbf{w}''$, $\widetilde{\mathbf{w}}'$, and $\widetilde{\mathbf{w}}''$ be the shortest walks from e to e visiting the vertices v', v'', $\widetilde{v}'$, and $\widetilde{v}''$, respectively. Set

$$a_{i_{p+1}} = w^{(p)} - (|\mathbf{w}'| + |\mathbf{w}''|)/2 \quad \text{and} \quad a_{\widetilde{i}_{p+1}} = w^{(p)} - (|\widetilde{\mathbf{w}}'| + |\widetilde{\mathbf{w}}''|)/2.$$

Assume that at least one of the inequalities $v' \neq \widetilde{v}'$ and $v'' \neq \widetilde{v}''$ holds. Then $a_{i_{p+1}} \neq a_{\widetilde{i}_{p+1}}$. Without loss of generality we can assume that $a_{\widetilde{i}_{p+1}} < a_{i_{p+1}}$.

Let $\mathcal{G}_e^{(p+1)}$ be obtained from $\mathcal{G}_e^{(p)}$ by adding the edge i_{p+1} such that $\partial(i_{p+1}) \doteq \{v', v''\}$ and correspondingly the graph $\widetilde{\mathcal{G}}_e^{(p+1)}$ – by adding the edge $\widetilde{i}_{p+1}$ such that $\partial(\widetilde{i}_{p+1}) \doteq \{\widetilde{v}', \widetilde{v}''\}$. Let ℓ be the set of lengths of all walks from e to e on the graph $\mathcal{G}_e^{(p+1)}$, and correspondingly $\widetilde{\ell}$ – on the graph $\widetilde{\mathcal{G}}_e^{(p+1)}$.

Assume that both sets ℓ and $\widetilde{\ell}$ are contained in $\mathcal{L}_{e,e}$. In particular, we have that $2w^{(p)} \in \ell \cap \widetilde{\ell}$, which implies

$$a_{i_{p+1}} + a_{\widetilde{i}_{p+1}} + (|\mathbf{w}'| + |\mathbf{w}''|)/2 + (|\widetilde{\mathbf{w}}'| + |\widetilde{\mathbf{w}}''|)/2 \in \ell.$$

Since $\widetilde{i}_{p+1} \notin \mathcal{I}^{(p+1)}$, from this equation it follows that

$$a_{\widetilde{i}_{p+1}} = \sum_{i \in \mathcal{I}^{(p+1)}} n_i a_i$$

with some $n_i \in \mathbb{N}_0$. Since by assumption $a_{\widetilde{i}_{p+1}} < a_{i_{p+1}}$, the coefficient $n_{i_{p+1}}$ has to be zero. Thus, the set $\{a_{i_1}, \ldots, a_{i_p}, a_{\widetilde{i}_{p+1}}\}$ is not rationally independent. Hence, the metric graph $\widetilde{\mathcal{G}}_e^{(p+1)}$ does not satisfy Assumption 2. □

Now we proceed by induction. By Lemma 7.5 after a finite number of induction steps we get $\mathcal{L}_{e,e}^{(r)} = \varnothing$ and, thus, $\mathcal{G}_e^{(r)} = \mathcal{G}_e$. This completes the proof of Theorem 7.8.

Proof of the second part of Theorem 1. It suffices to show that whenever the interior $\mathcal{G}_{\mathrm{int}}$ of the graph $\mathcal{G}$, the vertex $\partial(e)$, and the metric $\underline{a}$ are known, the transmission amplitude $[S(\mathsf{k}; A, B, \underline{a})]_{e,e'}$, $e \neq e'$ determines the boundary vertex $\partial(e')$.

By Theorem 7.2 and Remark 7.3 the transmission amplitude determines the set $\mathcal{L}_{e,e'} = \{w_{e,e'}(k)\}_{k \in \mathbb{N}_0}$ uniquely. Since $e \neq e'$ we have that $w_{e,e'}(0) > 0$ is the metric length of the geodesic walk $\mathbf{w}$ from e' to e. By Assumption 2 the score $\underline{n}(\mathbf{w})$ of this walk is uniquely determined. Since $\mathbf{w}$ is geodesic either $n_i = 1$ or $n_i = 0$ for all $i \in \mathcal{I}$. Since the geodesic walk is unique, the score determines the walk $\mathbf{w}$ uniquely (up to reversal). Thus, the vertex $\partial(e')$ is determined uniquely. □

8. PROOF OF THEOREM 2

In this section we will study local boundary conditions on a given metric graph $\mathcal{G}$ which lead to the same scattering matrix. More precisely, we consider the following problem: Given local boundary conditions (A, B) on the metric graph $(\mathcal{G}, \underline{a})$ find all local boundary conditions (A', B') on $\mathcal{G}$ not equivalent to (A, B) for which the Laplace operators $\Delta(A', B'; \underline{a})$ are isoscattering with $\Delta(A, B; \underline{a})$, that is,

$$S(\mathsf{k}; A', B', \underline{a}) = S(\mathsf{k}; A, B, \underline{a})$$

holds for all $\mathsf{k} > 0$. Recall (see Definition 3.5) that the boundary conditions (A, B) and (A', B') are equivalent if the corresponding maximal isotropic subspaces $\mathcal{M}(A, B)$ and $\mathcal{M}(A', B')$ of ${}^d\mathcal{K}$ coincide. The solution of this problem is given by Theorem 8.4 below. This result immediately implies Theorem 2.

Let ϕ denote an arbitrary family $\{\phi_j\}_{j\in\mathcal{I}\cup\mathcal{E}}$ of real numbers. To such ϕ we associate a unitary map $G(\phi)$ in $\mathcal{H}$ defined by

$$(G(\phi)\psi)_j(x) = \mathrm{e}^{\mathrm{i}\phi_j}\psi_j(x), \qquad j \in \mathcal{I}\cup\mathcal{E}.$$

It is easy to verify that

$$G(\phi)^\dagger \Delta(A, B; \underline{a}) G(\phi) = \Delta(AU_\phi, BU_\phi; \underline{a}),$$

where

$$U_\phi = \left(\bigoplus_{e\in\mathcal{E}} \mathrm{e}^{\mathrm{i}\phi_e}\right) \oplus \left(\bigoplus_{i\in\mathcal{I}} \mathrm{e}^{\mathrm{i}\phi_i}\right) \oplus \left(\bigoplus_{i\in\mathcal{I}} \mathrm{e}^{\mathrm{i}\phi_i}\right) \tag{8.1}$$

is a unitary transformation on $\mathcal{K} = \mathcal{K}_\mathcal{E} \oplus \mathcal{K}_\mathcal{I}^{(-)} \oplus \mathcal{K}_\mathcal{I}^{(+)}$. Motivated by our study [45] of magnetic Laplace operators on graphs we call such transformations *gauge transformations*. Transformations of the type (8.1) correspond to the case of vanishing magnetic fields.

Definition 8.1. *A unitary transformation on $\mathcal{K}$ of the form* (8.1) *is called a* trivial gauge transformation *if $\phi_e = 0$ for all $e \in \mathcal{E}$, that is, if $U_\phi|_{\mathcal{K}_\mathcal{E}} = \mathbb{I}|_{\mathcal{K}_\mathcal{E}}$.*

The set of all trivial gauge transformations will be denoted by U_0. Obviously, U_0 is an Abelian group isomorphic to the torus $\mathbb{T}^{|\mathcal{I}|}$.

Proposition 8.2. *Trivial gauge transformations do not change the scattering matrix, that is, for arbitrary boundary conditions (A, B) satisfying* (3.10)

$$S(\mathsf{k}; AU, BU, \underline{a}) = S(\mathsf{k}; A, B, \underline{a}) \quad \textit{for all} \quad \mathsf{k} > 0 \tag{8.2}$$

whenever $U \in \mathsf{U}_0$.

Proof. Observe that

$$\mathfrak{S}(\mathsf{k}; AU, BU) = U^\dagger \mathfrak{S}(\mathsf{k}; A, B) U$$

for all unitary $U \in \mathsf{U}(|\mathcal{E}| + 2|\mathcal{I}|)$, where $\mathfrak{S}(\mathsf{k}; A, B)$ is defined in (3.14). Any gauge transformation U commutes with $T(\mathsf{k}; \underline{a})$ defined in (3.32). Thus,

$$K(\mathsf{k}; AU, BU, \underline{a}) = U^\dagger K(\mathsf{k}; A, B, \underline{a}) U.$$

Now relation (3.36) in Theorem 3.10 implies equality (8.2) for any $U \in \mathsf{U}_0$. □

We note that from the proof it follows that the transmission probabilities $|[S(\mathsf{k}; A, B, \underline{a})]_{e,e'}|^2$, $(e \neq e')$ as well as the reflection amplitudes $[S(\mathsf{k}; A, B, \underline{a})]_{e,e}$ are invariant under *any* gauge transformation.

The following proposition shows that generically trivial gauge transformations do not leave the Laplace operator unchanged.

Proposition 8.3. *For Haar almost all local boundary conditions (A, B) the equality*

$$\mathcal{M}(A, B) = \mathcal{M}(AU, BU) \tag{8.3}$$

for some $U \in \mathsf{U}_0$ implies that $U = \mathbb{I}$.

Using (3.20) we can rephrase this result as follows: For Haar almost all local boundary conditions (A, B) the invariance of the subspace $\mathcal{M}(A, B) \subset {}^d\mathcal{K}$ with respect to ${}^dU := \begin{pmatrix} U & 0 \\ 0 & U \end{pmatrix}$ for some $U \in \mathsf{U}_0$, that is, the equality

$${}^dU\mathcal{M}(A, B) = \mathcal{M}(A, B),$$

implies that $U = \mathbb{I}$.

Proof. From Proposition 3.23 and Definition 4.1 it follows that A and B are invertible for Haar almost all local boundary conditions (A, B). By Theorem 1 in [45] equality (8.3) implies that U commutes with $A^{-1}B$. Recall that $A^{-1}B$ is self-adjoint since $AB^\dagger$ is (see the proof of Proposition 3.19). Therefore, U and $\mathfrak{S}(\mathsf{k}; A, B)$ (defined by (3.14)) are commuting for all $\mathsf{k} > 0$.

Assume now that for some boundary conditions (A, B) equality (8.3) holds for some $U \neq \mathbb{I}$, $U \in \mathsf{U}_0$. Then there are two elements $\chi_1 \neq \chi_2$ of the standard basis in $\mathcal{K} \cong \mathbb{C}^{|\mathcal{E}|+2|\mathcal{I}|}$, which are eigenvectors of U corresponding to different eigenvalues. Thus, $\langle \chi_1, \mathfrak{S}(\mathsf{k}; A, B)\chi_2\rangle = 0$ for all $\mathsf{k} > 0$. But by Lemma 3.22 this can only hold for a set of boundary conditions, which is of zero Haar measure. □

Let $\mathsf{F}(A, B)$ be the set of all local boundary conditions which are isoscattering with (A, B). From Proposition 8.2 it follows that $\mathsf{U}_0 \subset \mathsf{F}(A, B)$. Under additional assumptions also the opposite inclusion holds for Haar almost all boundary conditions. The following result implies Theorem 2.

Theorem 8.4. *Under Assumptions 1 and 2 the equality* $\mathsf{F}(A, B) = \mathsf{U}_0$ *holds for Haar almost all local boundary conditions.*

The remainder of this section is devoted to the proof of this theorem. Given local boundary conditions (A, B) satisfying (3.10) assume that there are local boundary conditions (A', B') such that

$$S(\mathsf{k}; A, B, \underline{a}) = S(\mathsf{k}; A', B', \underline{a}) \qquad \text{for all} \quad \mathsf{k} > 0. \tag{8.4}$$

By Proposition 4.2 due to equation (3.46) the unitary matrices $\mathfrak{S}(\mathsf{k}; A, B)$ and $\mathfrak{S}(\mathsf{k}; A', B')$ possess the orthogonal decompositions

$$\mathfrak{S}(\mathsf{k}; A, B) = \bigoplus_{v\in V} S_v(\mathsf{k}; A_v, B_v) \qquad \text{and} \qquad \mathfrak{S}(\mathsf{k}; A', B') = \bigoplus_{v\in V} S_v(\mathsf{k}; A'_v, B'_v) \tag{8.5}$$

with respect to decomposition (4.2).

We start the proof of Theorem 8.4 with the following proposition. Fix an arbitrary boundary vertex $v \in \partial V$ and consider the graph $\mathcal{G}_v = (\{v\}, \mathcal{I}_v = \emptyset, \mathcal{E}_v, \partial_v)$ associated with the vertex v (see Definition 4.4).

Set $\mathsf{U}_v = \{U \in \mathsf{U}_0 | \, U\chi = \chi \text{ for all } \chi \in \mathcal{K} \ominus \mathcal{L}_v\}$ such that

$$\mathsf{U}_0 = \mathop{\times}_{v\in V} \mathsf{U}_v.$$

Note that any $U \in \mathsf{U}_v$ leaves all subspaces $\mathcal{L}_v \subset \mathcal{K}$ (see Section 4) invariant.

Proposition 8.5. *Under Assumptions 1 and 2 for Haar almost all local boundary conditions the scattering matrix* $S(\mathsf{k}; A, B, \underline{a})$ *determines the maximal isotropic subspaces* $\mathcal{M}(A_v, B_v) \subset {}^d\mathcal{L}_v$, $v \in \partial V$ *uniquely up to trivial gauge transformations* $U \in \mathsf{U}_v$.

In other words, the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ determines the family of maximal isotropic subspaces $\{\mathcal{M}(A_vU, B_vU)\}_{U\in\mathsf{U}_v}$ uniquely.

We split the proof into several lemmas.

By Theorem 7.2 and Remark 7.3 the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ on the metric graph $(\mathcal{G}, \underline{a})$ uniquely determines all Fourier coefficients $\widehat{S}_{\underline{n}}(\mathsf{k}; A, B)$ in the Fourier expansion (5.1).

Lemma 8.6. *Let* $e \in \mathcal{E}$ *be arbitrary,* $v := \partial(e)$. *For Haar almost all boundary conditions* (A, B) *the matrix element* $[\widehat{S}_{\underline{n}}(\mathsf{k}; A, B)]_{e,e}$ *with* $\underline{n} = \underline{0}$ *determines the scattering matrix* $S_v(\mathsf{k}) \equiv S(\mathsf{k}; A_v, B_v)$ *up to unitary transformation. Moreover, the matrix elements* $[S_v(\mathsf{k})]_{e_1,e_2}$, $e_1, e_2 \in \mathcal{E}_v$ *with* $\Psi_v(e_1), \Psi_v(e_2) \in \mathcal{E}$ *are determined uniquely.*

Proof. By Theorem 6.6 the matrix elements $[\widehat{S}_{\underline{n}}(\mathsf{k}; A, B)]_{e,e'}$, $\partial(e) = \partial(e') = v$ with $\underline{n} = \underline{0}$ equals $[S_v(\mathsf{k})]_{\Psi_v^{-1}(e),\Psi_v^{-1}(e')}$, where the map Ψ_v is defined in Definition 4.4. Thus, the matrix elements $[S_v(\mathsf{k})]_{e_1,e_2}$ with $\Psi_v(e_1), \Psi_v(e_2) \in \mathcal{E}$ are determined uniquely. Recall that by Theorem 3.24 for Haar almost all boundary conditions the scattering matrix $S_v(\mathsf{k})$ has the form

$$S_v(\mathsf{k}) = \frac{\mathsf{k} + \mathrm{i}H_v/2}{\mathsf{k} - \mathrm{i}H_v/2} \tag{8.6}$$

with some Hermitian H_v. For any $e' \in \mathcal{E}_v$ the matrix element $[S_v(\mathsf{k})]_{e',e'}$ can be represented as the scalar product $\langle \chi, S_v(\mathsf{k})\, \chi\rangle$ with χ an element of the canonical basis in the subspace $\mathcal{L}_v$ defined by (4.3).

By Theorem 3.24 for almost all boundary conditions (A_v, B_v) the vector χ is not orthogonal to any eigenvector of the matrix H_v. Thus, the analytic continuation in k of $[S_v(\mathsf{k})]_{e',e'}$ with $e' \in \mathcal{E}_v$, $\Psi_v(e') \in \mathcal{E}$ determines all poles of $S_v(\mathsf{k})$. In turn, this determines all eigenvalues of the matrix H_v and, therefore, the matrix H_v up to unitary equivalence. By (8.6) this determines the scattering matrix $S_v(\mathsf{k})$ up to unitary equivalence. □

The orthogonal decomposition $\mathcal{K} = \mathcal{K}_{\mathcal{E}} \oplus \mathcal{K}_{\mathcal{I}}$ with $\mathcal{K}_{\mathcal{I}} = \mathcal{K}_{\mathcal{I}}^{(-)} \oplus \mathcal{K}_{\mathcal{I}}^{(+)}$ (see (3.3)) induces the orthogonal decomposition of the subspace $\mathcal{L}_v$ into the orthogonal sum $\mathcal{L}_v^{(\mathcal{E})} \oplus \mathcal{L}_v^{(\mathcal{I})}$, where $\mathcal{L}_v^{(\mathcal{E})} = \mathcal{L}_v \cap \mathcal{K}_{\mathcal{E}}$ and $\mathcal{L}_v^{(\mathcal{I})} = \mathcal{L}_v \cap \mathcal{K}_{\mathcal{I}}$. Set $p = \dim \mathcal{L}_v^{(\mathcal{E})}$ and $q = \dim \mathcal{L}_v^{(\mathcal{I})}$ such that $p + q = \deg(v)$.

Denote $S_v'(\mathsf{k}) := S_v(\mathsf{k}; A_v', B_v')$, where (A_v, B_v) corresponds to the local boundary conditions (A', B') satisfying (8.4). Lemma 8.6 implies that if the k-independent matrix

$$H_v = -\mathrm{i}\mathsf{k}\frac{S_v(\mathsf{k}) - \mathbb{I}}{S_v(\mathsf{k}) + \mathbb{I}}$$

is represented in a block form

$$H_v = \begin{pmatrix} K_{00} & K_{01} \\ K_{10} & K_{11} \end{pmatrix} \tag{8.7}$$

with respect to the orthogonal decomposition $\mathcal{L}_v = \mathcal{L}_v^{(\mathcal{E})} \oplus \mathcal{L}_v^{(\mathcal{I})}$, then the matrix

$$H_v' := -\mathrm{i}\mathsf{k}\frac{S_v'(\mathsf{k}) - \mathbb{I}}{S_v'(\mathsf{k}) + \mathbb{I}}$$

has a block form

$$H_v' = \begin{pmatrix} K_{00} & K_{01}U \\ U^\dagger K_{10} & U^\dagger K_{11} U \end{pmatrix},$$

where U is a unitary transformation on $\mathcal{L}_v^{(\mathcal{I})}$. To prove Proposition 8.5 it suffices to show that U is necessarily diagonal with respect to the canonical basis in $\mathcal{L}_v^{(\mathcal{I})}$ such that $\mathbb{I} \oplus U \in \mathsf{U}_v$ for Haar almost all local boundary conditions.

For brevity we will set $H_{e',i} := [H_v]_{\Psi_v(e'),\Psi_v(i)}$ and $H'_{e',i} := [H'_v]_{\Psi_v(e'),\Psi_v(i)}$. A similar shorthand notation will be used for the scattering matrices.

Lemma 8.7. *Equation* (8.4) *implies that for all $e \in \mathcal{E} \cap \mathcal{S}(v)$ and all $i \in \mathcal{I} \cap \mathcal{S}(v)$*

$$H'_{e,i} = H_{e,i}\mathrm{e}^{\mathrm{i}\gamma_i}$$

with some real numbers γ_i independent of e.

Proof. For arbitrary external edges $e, e' \in \mathcal{E} \cap \mathcal{S}(v)$ consider the Fourier expansion (6.6) of the scattering matrix element $[S(\mathsf{k}; A, B, \underline{a})]_{e,e'}$. The coefficients associated to the exponents $\mathrm{e}^{2\mathrm{i}\mathsf{k}a_i}$, $i \in \mathcal{I} \cap \mathcal{S}(v)$ are equal to

$$[S_v(\mathsf{k})]_{e,i}[S_{v_i}(\mathsf{k})]_{i,i}[S_v(\mathsf{k})]_{i,e'},$$

where $v_i \in \partial(i)$, $v_i \neq v$. By Lemma 3.20 the leading term of these products for $\mathsf{k} \to +\infty$ equals $H_{e,i}H_{i,e'}$. This implies that

$$H_{e,i}H_{i,e'} = H'_{e,i}H'_{i,e'} \tag{8.8}$$

for all $e, e' \in \mathcal{E} \cap \mathcal{S}(v)$ and all $i \in \mathcal{I} \cap \mathcal{S}(v)$. In particular, if $e = e'$ we have $|H_{e,i}| = |H'_{e,i}|$. Thus,

$$H'_{e,i} = H_{e,i}\mathrm{e}^{\mathrm{i}\gamma_{e,i}}, \qquad H'_{i,e} = H_{i,e}\mathrm{e}^{-\mathrm{i}\gamma_{e,i}} \tag{8.9}$$

with some real numbers $\gamma_{e,i}$. If $|\mathcal{E} \cap \mathcal{S}(v)| = 1$ the claim is proven. Assume now that $|\mathcal{E} \cap \mathcal{S}(v)| > 1$. Plugging (8.9) into (8.8) for $e \neq e'$ we obtain that $\gamma_{e,i} = \gamma_{e',i}$ modulo 2π, which completes the proof. □

To proceed further we need the following result.

Lemma 8.8. *Let $\{x_k\}_{k=1}^p$ and $\{y_j\}_{j=1}^q$ be orthonormal bases in $\mathcal{L}_v^{(\mathcal{E})}$ and $\mathcal{L}_v^{(\mathcal{I})}$, respectively. If for some unitary transformation $U : \mathcal{L}_v^{(\mathcal{I})} \to \mathcal{L}_v^{(\mathcal{I})}$ the relations*

$$\langle x_k, K_{01}Uy_j\rangle = \langle x_k, K_{01}y_j\rangle \mathrm{e}^{\mathrm{i}\gamma_j} \tag{8.10}$$

hold for all $j \in \mathcal{I} \cap \mathcal{S}(v)$ and all $k \in \mathcal{E} \cap \mathcal{S}(v)$ with some real numbers γ_j independent of k, then

$$U^\dagger|_{\operatorname{Ran} K_{10}} = \Lambda^\dagger|_{\operatorname{Ran} K_{10}}, \tag{8.11}$$

where Λ is a unitary map defined by

$$\langle y_k, \Lambda y_j\rangle = \delta_{jk}\mathrm{e}^{\mathrm{i}\gamma_j}.$$

Proof. From (8.10) it follows that

$$\langle y_j, U^\dagger K_{10}x_k\rangle = \langle y_j, K_{10}x_k\rangle \mathrm{e}^{-\mathrm{i}\gamma_j}$$

for all $j \in \mathcal{I} \cap \mathcal{S}(v)$ and all $k \in \mathcal{E} \cap \mathcal{S}(v)$. This implies that

$$U^\dagger K_{10}x_k = \Lambda^\dagger K_{10}x_k.$$

Noting that the linear span of $\{K_{10}x_k\}_{k=1}^p$ is the whole $\operatorname{Ran} K_{10}$ we obtain the claim. □

Remark 8.9. *Lemma 8.8 implies that under the conditions of this lemma*

$$U = W\Lambda, \tag{8.12}$$

where W is a unitary transformation leaving $\operatorname{Ran} K_{10}$ invariant and which satisfies $W|_{\operatorname{Ran} K_{10}} = \mathbb{I}|_{\operatorname{Ran} K_{10}}$. To prove this fact we note that from (8.11) it follows that

$$U^\dagger = \Lambda^\dagger P_{\operatorname{Ran} K_{10}} + V^\dagger P^\perp_{\operatorname{Ran} K_{10}}$$

with some linear map V.

Without loss of generality the map V can be chosen to be unitary. Indeed, from the unitarity of U it follows that $V^\dagger P^\perp_{\operatorname{Ran} K_{10}} V$ is an orthogonal projection such that on $(\operatorname{Ran} K_{10})^\perp$ the map $V^\dagger$ must coincide with some unitary operator.

From the unitarity of U we also obtain

$$P_{\operatorname{Ran} K_{10}} \Lambda V^\dagger P^\perp_{\operatorname{Ran} K_{10}} = 0.$$

Thus, $(\operatorname{Ran} K_{10})^\perp$ is invariant for $\Lambda V^\dagger$. Since $\Lambda V^\dagger$ is unitary, this implies that $\operatorname{Ran} K_{10}$ is invariant for $\Lambda V^\dagger$. Thus, $\Lambda V^\dagger = W_0 \oplus W_1$ with respect to the orthogonal decomposition $\mathcal{L}_v^{(\mathcal{I})} = \operatorname{Ran} K_{10} \oplus (\operatorname{Ran} K_{10})^\perp$. Therefore, $V^\dagger = \Lambda^\dagger(W_0 \oplus W_1)$. Hence, we obtain

$$\begin{aligned} U &= P_{\operatorname{Ran} K_{10}}\Lambda + P^\perp_{\operatorname{Ran} K_{10}}(W_0 \oplus W_1)\Lambda \\ &= (\mathbb{I} \oplus W_1)\Lambda, \end{aligned}$$

which proves the claim.

Note that if $p \geq q$, then for Haar almost all boundary conditions $\operatorname{Ran} K_{10} = \mathcal{L}_v^{(\mathcal{I})}$. Hence, by Lemma 8.8 $U = \Lambda$ such that $(\mathbb{I} \oplus U) \in \mathsf{U}_v$. In this case the proof of Proposition 8.5 is complete.

Now we assume that $p < q$ which implies that $q \geq 2$.

Lemma 8.10. *Equation* (8.4) *implies that for all* $i_1, i_2 \in \mathcal{I} \cap \mathcal{S}(v)$, $i_1 \neq i_2$ *either*

$$H'_{i_1,i_2} = H_{i_1,i_2} \mathrm{e}^{\mathrm{i}(\gamma_{i_2}-\gamma_{i_1})}$$

or

$$H'_{i_1,i_2} = \overline{H_{i_1,i_2}} \mathrm{e}^{\mathrm{i}(\gamma_{i_2}-\gamma_{i_1})} \mathrm{e}^{\mathrm{i}\varphi_{i_1,i_2}}, \qquad \mathrm{e}^{\mathrm{i}\varphi_{i_1,i_2}} = \mathrm{e}^{-\mathrm{i}\varphi_{i_2,i_1}} := \frac{\overline{H_{e,i_1} H_{i_2,e}}}{H_{e,i_1} H_{i_2,e}} \tag{8.13}$$

with the same numbers γ_i *as in Lemma 8.7.*

Proof. We split the proof into several steps.

Step 1. For an arbitrary external edge $e \in \mathcal{E} \cap \mathcal{S}(v)$ consider the Fourier expansion (6.6) of the scattering matrix element $[S(\mathsf{k}; A, B, \underline{a})]_{e,e}$. The quotient of the coefficients associated to the exponents $\mathrm{e}^{4\mathrm{i}\mathsf{k}a_i}$ and $\mathrm{e}^{2\mathrm{i}\mathsf{k}a_i}$, $i \in \mathcal{I} \cap \mathcal{S}(v)$ equals

$$[S_v(\mathsf{k})]_{ii} [S_{v_i}(\mathsf{k})]_{ii},$$

where $v_i \in \partial(i)$, $v_i \neq v$. Thus,

$$[S_v(\mathsf{k})]_{ii} [S_{v_i}(\mathsf{k})]_{ii} = [S'_v(\mathsf{k})]_{ii} [S'_{v_i}(\mathsf{k})]_{ii}$$

for all $i \in \mathcal{I} \cap \mathcal{S}(v)$.

Step 2. For arbitrary $i_1, i_2 \in \mathcal{I} \cap \mathcal{S}(v)$, $i_1 \neq i_2$ the coefficient associated to the exponent $\mathrm{e}^{2\mathrm{i}\mathsf{k}(a_{i_1}+a_{i_2})}$ of the Fourier expansion (6.6) of the scattering matrix element $[S(\mathsf{k}; A, B, \underline{a})]_{e,e}$ equals

$$\begin{aligned} &[S_v(\mathsf{k})]_{e,i_2} [S_{v_2}(\mathsf{k})]_{i_2,i_2} [S_v(\mathsf{k})]_{i_2,i_1} [S_{v_1}(\mathsf{k})]_{i_1,i_1} [S_v(\mathsf{k})]_{i_1,e} \\ &+ [S_v(\mathsf{k})]_{e,i_1} [S_{v_1}(\mathsf{k})]_{i_1,i_1} [S_v(\mathsf{k})]_{i_1,i_2} [S_{v_2}(\mathsf{k})]_{i_2,i_2} [S_v(\mathsf{k})]_{i_2,e}. \end{aligned} \tag{8.14}$$

By Lemma 3.20 the leading term of this expression for $\mathsf{k} \to +\infty$ equals

$$-\frac{\mathrm{i}}{\mathsf{k}^3} (H_{e,i_2} H_{i_2,i_1} H_{i_1,e} + H_{e,i_1} H_{i_1,i_2} H_{i_2,e}).$$

Thus,

$$\operatorname{Re}(H_{e,i_2} H_{i_2,i_1} H_{i_1,e}) = \operatorname{Re}(H'_{e,i_2} H'_{i_2,i_1} H'_{i_1,e}) \tag{8.15}$$

for all $i_1, i_2 \in \mathcal{I} \cap \mathcal{S}(v)$, $i_1 \neq i_2$.

Step 3. For arbitrary $i_1, i_2 \in \mathcal{I} \cap \mathcal{S}(v)$, $i_1 \neq i_2$ the coefficient associated to the exponent $\mathrm{e}^{\mathrm{i}\mathsf{k}(4a_{i_1}+2a_{i_2})}$ of the Fourier expansion (6.6) of the scattering matrix element $[S(\mathsf{k}; A, B, \underline{a})]_{e,e}$ equals

$$\begin{aligned} &[S_v(\mathsf{k})]_{e,i_1} [S_{v_1}(\mathsf{k})]_{i_1,i_1} [S_v(\mathsf{k})]_{i_1,i_2} [S_{v_2}(\mathsf{k})]_{i_2,i_2} [S_v(\mathsf{k})]_{i_2,i_1} [S_{v_1}(\mathsf{k})]_{i_1,i_1} [S_v(\mathsf{k})]_{i_1,e} \\ &+ [S_v(\mathsf{k})]_{e,i_2} [S_{v_2}(\mathsf{k})]_{i_2,i_2} [S_v(\mathsf{k})]_{i_2,i_1} [S_{v_1}(\mathsf{k})]_{i_1,i_1} [S_v(\mathsf{k})]_{i_1,i_1} [S_{v_1}(\mathsf{k})]_{i_1,i_1} [S_v(\mathsf{k})]_{i_1,e} \\ &+ [S_v(\mathsf{k})]_{e,i_1} [S_{v_1}(\mathsf{k})]_{i_1,i_1} [S_v(\mathsf{k})]_{i_1,i_1} [S_{v_1}(\mathsf{k})]_{i_1,i_1} [S_v(\mathsf{k})]_{i_1,i_2} [S_{v_2}(\mathsf{k})]_{i_2,i_2} [S_v(\mathsf{k})]_{i_2,e}. \end{aligned} \tag{8.16}$$

Observe that the sum of two last terms equals

$$\begin{aligned} \alpha(\mathsf{k}) \Big\{ &[S_v(\mathsf{k})]_{e,i_2} [S_{v_2}(\mathsf{k})]_{i_2,i_2} [S_v(\mathsf{k})]_{i_2,i_1} [S_{v_1}(\mathsf{k})]_{i_1,i_1} [S_v(\mathsf{k})]_{i_1,e} \\ &+ [S_v(\mathsf{k})]_{e,i_1} [S_{v_1}(\mathsf{k})]_{i_1,i_1} [S_v(\mathsf{k})]_{i_1,i_2} [S_{v_2}(\mathsf{k})]_{i_2,i_2} [S_v(\mathsf{k})]_{i_2,e} \Big\}, \end{aligned}$$

where $\alpha(\mathsf{k}) := [S_{v_1}(\mathsf{k})]_{i_1,i_1} [S_v(\mathsf{k})]_{i_1,i_1}$ has been determined in Step 1. The sum in the braces coincides with (8.14) and is uniquely determined in Step 2. Thus, the first term in (8.16) is uniquely determined by the Fourier coefficient with the exponent $e^{ik(4a_{i_1}+2a_{i_2})}$. For $k \to +\infty$ by Lemma 3.20 this term has the asymptotics

$$\frac{1}{k^4}|H_{e,i_1}|^2|H_{i_1,i_2}|^2.$$

Thus,

$$|H_{i_1,i_2}| = |H'_{i_1,i_2}|$$

and, in particular,

$$|H_{e,i_2}H_{i_2,i_1}H_{i_1,e}| = |H'_{e,i_2}H'_{i_2,i_1}H'_{i_1,e}| \tag{8.17}$$

for all $i_1, i_2 \in \mathcal{I} \cap \mathcal{S}(v)$, $i_1 \neq i_2$.

Comparing (8.15) and (8.17) we conclude that either

$$\operatorname{Im}(H_{e,i_2}H_{i_2,i_1}H_{i_1,e}) = \operatorname{Im}(H'_{e,i_2}H'_{i_2,i_1}H'_{i_1,e}) \tag{8.18}$$

or

$$\operatorname{Im}(H_{e,i_2}H_{i_2,i_1}H_{i_1,e}) = -\operatorname{Im}(H'_{e,i_2}H'_{i_2,i_1}H'_{i_1,e}). \tag{8.19}$$

From (8.15) and (8.19) it follows that either

$$H_{e,i_2}H_{i_2,i_1}H_{i_1,e} = H'_{e,i_2}H'_{i_2,i_1}H'_{i_1,e}$$

or

$$H_{e,i_2}H_{i_2,i_1}H_{i_1,e} = \overline{H'_{e,i_2}H'_{i_2,i_1}H'_{i_1,e}}.$$

Applying Lemma 8.7 proves the claim. □

We will need the following result due to Friedland [18], [19] (see also [2]) on Hermitian matrices with prescribed off-diagonal entries.

Lemma 8.11. *Let K be a Hermitian $q \times q$ matrix. There are at most $q!$ different matrices L unitarily equivalent to K and satisfying*

$$L_{jk} = K_{jk} \qquad \text{for all} \quad j \neq k.$$

By this result we obtain that if equality (8.4) is satisfied, then for Haar almost all boundary conditions (A, B) up to trivial gauge transformations from U_v there is at most a finite number (depending on $q = \dim \mathcal{L}_v^{(\mathcal{I})}$ only) of unitary matrices $U \in \mathsf{U}(q)$ such that

$$H'_v = \begin{pmatrix} \mathbb{I} & 0 \\ 0 & U \end{pmatrix}^\dagger H_v \begin{pmatrix} \mathbb{I} & 0 \\ 0 & U \end{pmatrix}, \qquad H_v = \begin{pmatrix} K_{00} & K_{01} \\ K_{10} & K_{11} \end{pmatrix},$$

where H_v and H'_v are Hermitian matrices associated with the boundary conditions (A_v, B_v) and (A'_v, B'_v) via

$$\mathfrak{S}(k; A_v, B_v) = \frac{k + iH_v/2}{k - iH_v/2}, \qquad \mathfrak{S}(k; A'_v, B'_v) = \frac{k + iH'_v/2}{k - iH'_v/2}$$

for an arbitrary $k > 0$.

Lemmas 8.10 and 8.11 imply that these unitary matrices U are determined only by K_{11} and by the complex arguments of the entries of K_{10}. On the other hand, Lemma 8.8 and Remark 8.9 state that they have a special structure (8.12) which is determined by the matrix K_{10} and, in particular, only by the absolute values of its entries. Intuitively, it is clear that these two conditions on U are independent and, therefore, can be satisfied simultaneously in exceptional cases only. This observation will allow us to prove the uniqueness of U.

We return to the proof of Proposition 8.5. Without loss of generality we can choose all numbers γ_i, $i \in \mathcal{I} \cap \mathcal{S}(v)$ referred to in Lemma 8.7 to be zero. Note that equation (8.12) implies in this case that U leaves $\operatorname{Ran} K_{10}$ invariant and $U|_{\operatorname{Ran} K_{10}} = \mathbb{I}|_{\operatorname{Ran} K_{10}}$.

Let
$$\begin{pmatrix} \widetilde{K}_{00} & \widetilde{K}_{01} \\ \widetilde{K}_{10} & \widetilde{K}_{11} \end{pmatrix}$$
be an arbitrary $(p+q)\times(p+q)$ Hermitian matrix written in the block form with respect to the orthogonal decomposition $\mathcal{L}_v = \mathcal{L}_v^{(\mathcal{E})} \oplus \mathcal{L}_v^{(\mathcal{I})}$. Denote by $\mathfrak{N}(\widetilde{K}_{00}, \widetilde{K}_{01}, \widetilde{K}_{11})$ the set of all Hermitian matrices H of the form
$$H = \begin{pmatrix} \widetilde{K}_{00} & K_{01} \\ K_{10} & \widetilde{K}_{11} \end{pmatrix} \tag{8.20}$$
such that complex arguments of the entries of K_{01} agree with those of $\widetilde{K}_{01}$, that is,
$$\arg\bigl([K_{01}]_{e,i}\bigr) = \arg\bigl([\widetilde{K}_{01}]_{e,i}\bigr) \quad \text{for all} \quad e \in \mathcal{E}\cap\mathcal{S}(v) \quad \text{and} \quad i \in \mathcal{I}\cap\mathcal{S}(v).$$
On this set we define the measure
$$d\widetilde{\nu} = \prod_{\substack{e\in\mathcal{E}\cap\mathcal{S}(v)\\ i\in\mathcal{I}\cap\mathcal{S}(v)}} d\,|[K_{01}]_{e,i}|.$$

Let $\mathfrak{U}(H)$ be the set of all unitary matrices $U \in \mathsf{U}(q)$ with the property that for every $i_1, i_2 \in \mathcal{I}\cap\mathcal{S}(v)$, $i_1 \neq i_2$ either
$$[U^\dagger \widetilde{K}_{11} U]_{i_1,i_2} = [\widetilde{K}_{11}]_{i_1,i_2}, \qquad [U^\dagger \widetilde{K}_{11} U]_{i_2,i_1} = [\widetilde{K}_{11}]_{i_2,i_1}$$
or
$$[U^\dagger \widetilde{K}_{11} U]_{i_1,i_2} = [\widetilde{K}_{11}]_{i_1,i_2} \mathrm{e}^{\mathrm{i}\varphi_{i_1,i_2}}, \qquad [U^\dagger \widetilde{K}_{11} U]_{i_2,i_1} = [\widetilde{K}_{11}]_{i_2,i_1} \mathrm{e}^{-\mathrm{i}\varphi_{i_1,i_2}}$$
holds, where φ_{i_1,i_2} is defined in (8.13). By Lemmas 8.10 and 8.11 this set is finite and $\mathfrak{U}(H_1) = \mathfrak{U}(H_2)$ for all $H_1, H_2 \in \mathfrak{N}(\widetilde{K}_{00}, \widetilde{K}_{01}, \widetilde{K}_{11})$.

Lemma 8.12. *Assume that $p < q$. For $\widetilde{\nu}$-almost all $H \in \mathfrak{N}(\widetilde{K}_{00}, \widetilde{K}_{01}, \widetilde{K}_{11})$ no $U \in \mathfrak{U}(H)\setminus\{\mathbb{I}\}$ satisfies the condition*
$$U|_{\operatorname{Ran} K_{10}} = \mathbb{I}|_{\operatorname{Ran} K_{10}}, \tag{8.21}$$
where K_{10} is the off-diagonal block of the matrix H in the representation (8.20).

Proof. Assume that condition (8.21) is satisfied for some unitary matrix $U \in \mathfrak{U}(H)$, $U \neq \mathbb{I}$. Thus, U has 1 as an eigenvalue. Its multiplicity is not less than $\dim \operatorname{Ran} K_{10}$. Since $U \neq \mathbb{I}$, there is at least one eigenvalue $\lambda \neq 1$ of U. The corresponding eigenvector $y \in \mathcal{L}_v^{(\mathcal{I})}$ is orthogonal to $\operatorname{Ran} K_{10}$. By assumption we have
$$0 = \langle y, UK_{10}x\rangle = \langle U^\dagger y, K_{10}x\rangle = \lambda\langle y, K_{10}x\rangle$$
for any $x \in \mathcal{L}_v^{(\mathcal{E})}$. Thus, $y \in \operatorname{Ker} K_{10}^\dagger = \operatorname{Ker} K_{01}$. The subspace $\operatorname{Ker} K_{01}$ is nontrivial, since $p < q$.

Observe that for $\widetilde{\nu}$-almost all $H \in \mathfrak{N}(\widetilde{K}_{00}, \widetilde{K}_{01}, \widetilde{K}_{11})$ the matrix K_{01} has a rank $p \geq 1$. Recall that the complex arguments of the entries of K_{10} are fixed. Therefore, the equation $K_{01}y = 0$ represents p linearly independent relations for the numbers $|[K_{01}]_{e,i}|$, $e \in \mathcal{E}\cap\mathcal{S}(v)$, $i \in \mathcal{I}\cap\mathcal{S}(v)$. Hence, the set of all Hermitian matrices $H \in \mathfrak{N}(\widetilde{K}_{00}, \widetilde{K}_{01}, \widetilde{K}_{11})$ satisfying (8.21) is of zero $\widetilde{\nu}$-measure. $\square$

Now we are in position to complete the proof of Proposition 8.5. Observe that the measure ν defined in (3.61) is a product measure containing $\widetilde{\nu}$ as a factor. Lemma 8.12 immediately implies that the set of all Hermitian matrices H satisfying $\mathfrak{U}(H) \neq \{\mathbb{I}\}$ is of zero ν-measure. Hence, by Lemma 3.25,
$$\varkappa\bigl(\{H \,|\, \mathfrak{U}(H) \neq \{\mathbb{I}\}\}\bigr) = 0.$$

By definition (3.60) of the measure $\varkappa$, this implies that

$$\mu\bigl(\{\mathfrak{S}|\,\mathfrak{U}(H(\mathfrak{S}))\neq\{\mathbb{I}\}\}\bigr)=0,$$

where μ is the Haar measure on $\mathsf{U}(\deg(v))$ and $H(\mathfrak{S})$ is given by

$$H(\mathfrak{S})=-\mathrm{i}\frac{\mathfrak{S}-\mathbb{I}}{\mathfrak{S}+\mathbb{I}}.$$

This completes the proof of Proposition 8.5.

We turn to the proof of Theorem 8.4.

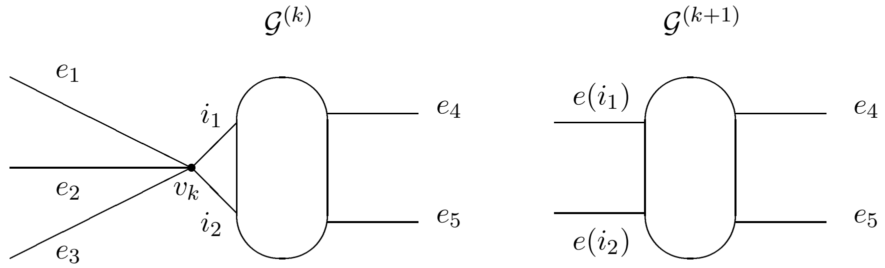

FIG. 6. The construction of the graph $\mathcal{G}^{(k+1)}$ from the graph $\mathcal{G}^{(k)}$. Inside the ovals the graphs are not specified but agree there.

With the graph $\mathcal{G}=(V,\mathcal{I},\mathcal{E},\partial)$ we associate a sequence of graphs $\{\mathcal{G}^{(k)}\}_{k=1}^{|V|}$, $\mathcal{G}^{(k)}=(V_k,\mathcal{I}_k,\mathcal{E}_k,\partial_k)$ such that $\mathcal{G}^{(1)}=\mathcal{G}$ and $\mathcal{G}^{(k+1)}$ is constructed from $\mathcal{G}^{(k)}$ in the following way (see Fig. 6):

(i) The vertex set V_{k+1} of the graph $\mathcal{G}^{(k+1)}$ is obtained from the vertex set V_k by removing a boundary vertex v_k of V_k, $v_k\in\partial V_k$;

(ii) The set of internal edges $\mathcal{I}_{k+1}$ of the graph $\mathcal{G}^{(k)}$ is obtained from $\mathcal{I}_k$ by removing all internal edges $i\in\mathcal{I}_k$ incident with the vertex v_k, that is,

$$\mathcal{I}_{k+1}=\mathcal{I}_k\setminus\mathcal{S}(v_k);$$

(iii) The set of external edges $\mathcal{E}_{k+1}$ of the graph $\mathcal{G}^{(k)}$ is obtained from $\mathcal{E}_k$ by adding $|\mathcal{I}_k|-|\mathcal{I}_{k+1}|$ external edges to $\mathcal{E}_k$. The set $\mathcal{E}_{k+1}\setminus\mathcal{E}_k$ is in one-to-one correspondence with the set $\mathcal{I}_k\setminus\mathcal{I}_{k+1}$, that is, for any $e\in\mathcal{E}_{k+1}\setminus\mathcal{E}_k$ there is a unique $i(e)\in\mathcal{I}_k\setminus\mathcal{I}_{k+1}$ and for any $i\in\mathcal{I}_k\setminus\mathcal{I}_{k+1}$ there is a unique $e(i)\in\mathcal{E}_{k+1}\setminus\mathcal{E}_k$;

(iv) The boundary operator ∂_{k+1} coincides with ∂_k on $\mathcal{E}_k\cap\mathcal{E}_{k+1}$ and $\mathcal{I}_k\cap\mathcal{I}_{k+1}$. On $\mathcal{E}_{k+1}\setminus\mathcal{E}_k$ the boundary operator is defined as $\partial_{k+1}(e)=v$, where v is the vertex adjacent to v_k in the graph $\mathcal{G}^{(k)}$ by the internal edge $i(e)\in\mathcal{I}_k\setminus\mathcal{I}_{k+1}$.

Note that the graphs $\mathcal{G}^{(k)}$ with $k>1$ are not necessarily connected and the graph $\mathcal{G}^{(|V|)}$ is a graph with no internal edges.

Given local boundary conditions

$$A=\bigoplus_{v\in V}A_v,\qquad B=\bigoplus_{v\in V}B_v$$

on the graph $\mathcal{G}$, let $S^{(k)}(\mathsf{k})$ denote the scattering matrix of the Laplace operator on the graph $\mathcal{G}_k$ associated with local boundary conditions defined by

$$A_k:=\bigoplus_{v\in V_k}A_v,\qquad B_k:=\bigoplus_{v\in V_k}B_v.$$

In particular, we have $S^{(1)}(\mathsf{k}):=S(\mathsf{k};A,B,\underline{a})$. Let $v_k\in V_k\setminus V_{k+1}$.

Proposition 8.13. *Given the scattering matrices $S_{v_k}(\mathsf{k})$ on the graph $\mathcal{G}_{v_k}$ and $S^{(k)}(\mathsf{k})$ on the graph $\mathcal{G}^{(k)}$, respectively, the scattering matrix $S^{(k+1)}(\mathsf{k})$ on the graph $\mathcal{G}^{(k+1)}$ is defined uniquely.*

Proof. Let $e, e' \in \mathcal{E}_k \cap \mathcal{E}_{k+1}$. The sum of all terms of the Fourier expansion (6.6) of the scattering matrix element $[S^{(k)}(\mathsf{k})]_{e,e'}$ containing none of the factors $\mathrm{e}^{\mathrm{i}\mathsf{k}a_i}$ with $i \in \mathcal{I}_k \setminus \mathcal{I}_{k+1}$ gives, obviously, the scattering matrix element $[S^{(k+1)}(\mathsf{k})]_{e,e'}$.

To determine $[S^{(k+1)}(\mathsf{k})]_{e(i),e'}$ for $e' \in \mathcal{E}_k \cap \mathcal{E}_{k+1}$ and $i \in \mathcal{I}_k \setminus \mathcal{I}_{k+1}$ consider the sum of all terms of the Fourier expansion (6.6) of the scattering matrix element $[S^{(k)}(\mathsf{k})]_{e,e'}$ with arbitrary $e \in \mathcal{E}_k \setminus \mathcal{E}_{k+1}$ which contain the factor $\mathrm{e}^{\mathrm{i}\mathsf{k}a_i}$ precisely once and none of the factors $\mathrm{e}^{\mathrm{i}\mathsf{k}a_{i'}}$, $i' \in \mathcal{I}_k \setminus \mathcal{I}_{k+1}$, $i' \neq i$. This sum is of the form

$$[S_{v_k}(\mathsf{k})]_{e,i}[S^{(k+1)}(\mathsf{k})]_{e(i),e'}\mathrm{e}^{\mathrm{i}\mathsf{k}a_i}$$

and, thus, determines $[S^{(k+1)}(\mathsf{k})]_{e(i),e'}$ uniquely. The matrix elements $[S^{(k+1)}(\mathsf{k})]_{e,e(i)}$ can be determined similarly.

To determine $[S^{(k+1)}(\mathsf{k})]_{e(i),e(i)}$ for $i \in \mathcal{I}_k \setminus \mathcal{I}_{k+1}$ we consider a scattering matrix element $[S^{(k)}(\mathsf{k})]_{e,e}$ with $e \in \mathcal{E}_k \setminus \mathcal{E}_{k+1}$. Consider the sum of all terms of the Fourier expansion (6.6) of this matrix element containing the factor $\mathrm{e}^{2\mathrm{i}\mathsf{k}a_i}$ exactly once and none of the factors $\mathrm{e}^{\mathrm{i}\mathsf{k}a_{i'}}$, $i' \in \mathcal{I}_k \setminus \mathcal{I}_{k+1}$, $i' \neq i$. This sum is of the form

$$[S_{v_k}(\mathsf{k})]_{e,i}[S^{(k+1)}(\mathsf{k})]_{e(i),e(i)}[S_{v_k}(\mathsf{k})]_{i,e}\mathrm{e}^{2\mathrm{i}\mathsf{k}a_i}$$

and, thus, determines $[S^{(k+1)}(\mathsf{k})]_{e(i),e(i)}$ uniquely.

If $|\mathcal{I}_k \setminus \mathcal{I}_{k+1}| = 1$, the proof is completed. Assume now that $|\mathcal{I}_k \setminus \mathcal{I}_{k+1}| > 1$. To complete the proof it suffices to show that the matrix elements $[S^{(k+1)}(\mathsf{k})]_{e(i_1),e(i_2)}$ for all $i_1 \neq i_2$, $i_1, i_2 \in \mathcal{I}_k \setminus \mathcal{I}_{k+1}$ are defined uniquely.

If the vertices $v^{(1)} \in \partial_k(i_1)$, $v^{(1)} \neq v_k$ and $v^{(2)} \in \partial_k(i_2)$, $v^{(2)} \neq v_k$ belong to different connected components of the graph $\mathcal{G}^{(k+1)}$, then $[S^{(k+1)}(\mathsf{k})]_{e(i_1),e(i_2)}$ is identically zero. Therefore, we may assume that $v^{(1)}$ and $v^{(2)}$ belong to the same connected component of the graph $\mathcal{G}^{(k+1)}$.

The coefficient associated to the exponent $\mathrm{e}^{\mathrm{i}\mathsf{k}(a_{i_1}+a_{i_2})}$ of the Fourier expansion (6.6) of the scattering matrix element $[S^{(k+1)}(\mathsf{k})]_{e,e}$ equals

$$\begin{aligned}&[S_{v_k}(\mathsf{k})]_{e,e(i_2)}[S^{(k)}(\mathsf{k})]_{e(i_2),e(i_1)}[S_{v_k}(\mathsf{k})]_{e(i_1),e}\\ &+[S_{v_k}(\mathsf{k})]_{e,e(i_1)}[S^{(k)}(\mathsf{k})]_{e(i_1),e(i_2)}[S_{v_k}(\mathsf{k})]_{e(i_2),e}.\end{aligned} \tag{8.22}$$

The sum of all terms of the Fourier expansion (6.6) of the scattering matrix element $[S^{(k+1)}(\mathsf{k})]_{e,e}$ containing the factor $\mathrm{e}^{\mathrm{i}\mathsf{k}(3a_{i_1}+a_{i_2})}$ is given by

$$\begin{aligned}&[S_{v_k}(\mathsf{k})]_{e,e(i_2)}[S^{(k)}(\mathsf{k})]_{e(i_2),e(i_2)}[S_{v_k}(\mathsf{k})]_{e(i_2),e(i_2)}[S^{(k)}(\mathsf{k})]_{e(i_2),e(i_1)}[S_{v_k}(\mathsf{k})]_{e(i_2),e}\\ &+[S_{v_k}(\mathsf{k})]_{e,e(i_2)}[S^{(k)}(\mathsf{k})]_{e(i_2),e(i_1)}[S_{v_k}(\mathsf{k})]_{e(i_1),e(i_2)}[S^{(k)}(\mathsf{k})]_{e(i_2),e(i_2)}[S_{v_k}(\mathsf{k})]_{e(i_2),e}\\ &+[S_{v_k}(\mathsf{k})]_{e,e(i_1)}[S^{(k)}(\mathsf{k})]_{e(i_1),e(i_2)}[S_{v_k}(\mathsf{k})]_{e(i_2),e(i_2)}[S^{(k)}(\mathsf{k})]_{e(i_2),e(i_2)}[S_{v_k}(\mathsf{k})]_{e(i_2),e}.\end{aligned} \tag{8.23}$$

Observe that the only unknown factors in (8.22) and (8.23) are

$$[S^{(k)}(\mathsf{k})]_{e(i_1),e(i_2)} \qquad \text{and} \qquad [S^{(k)}(\mathsf{k})]_{e(i_2),e(i_1)}.$$

It is easy to see that (8.22) and (8.23) considered as linear combinations of the variables $[S^{(k)}(\mathsf{k})]_{e(i_1),e(i_2)}$ and $[S^{(k)}(\mathsf{k})]_{e(i_2),e(i_1)}$, are linearly independent. Thus, (8.22) and (8.23) determine $[S^{(k)}(\mathsf{k})]_{e(i_1),e(i_2)}$ and $[S^{(k)}(\mathsf{k})]_{e(i_2),e(i_1)}$ uniquely. □

Combining Propositions 8.5 and 8.13 concludes the proof of Theorem 8.4.

9. The Traveling Salesman Problem

In this section we will present applications of the theory of Laplace operators on non-compact graphs developed in the present work to some well-known combinatorial problems. In particular, we provide a new approach to solving the Traveling Salesman Problem (TSP) as well as some other combinatorial problems. The graph $\mathcal{G} = \mathcal{G}(V, \mathcal{I}, \mathcal{E}, \partial)$ with $\mathcal{I} \neq \emptyset$ and $\mathcal{E} \neq \emptyset$ is now assumed to satisfy Assumption 1.

We start with a formulation of these problems adapted to the context of walks on noncompact graphs.

The Königsberger Brücken Problem (KBP). *For given $e, e' \in \mathcal{E}$ determine whether there is a walk $\mathbf{w}$ (called Euler path) from e' to e which traverses each internal edge $i \in \mathcal{I}$ exactly once, i.e. $n_i(\mathbf{w}) = 1$ for all $i \in \mathcal{I}$. There is no limitation on the number of times a vertex $v \in V$ may be visited.*

Recall that the solution of KBP for $e = e'$ is given by the celebrated Euler theorem (see, e.g., [14]): An Euler path $\mathbf{w} \in \mathcal{W}_{e,e}$ exists if and only if $\deg_{\mathcal{G}_{\mathrm{int}}}(v)$ is even for all $v \in V$. Here $\deg_{\mathcal{G}_{\mathrm{int}}}(v)$ is the degree of the vertex $v \in V$ in the interior $\mathcal{G}_{\mathrm{int}}$ of the graph $\mathcal{G}$. If the graph $\mathcal{G}_{\mathrm{int}}$ has more than two vertices of odd degree, then there is no Euler path for all $e, e' \in \mathcal{E}$. If the graph $\mathcal{G}_{\mathrm{int}}$ has exactly two vertices of odd degree, then the Euler path exists if and only if $\partial(e) \neq \partial(e')$ and both vertices $\partial(e)$ and $\partial(e')$ in the interior $\mathcal{G}_{\mathrm{int}}$ of the graph $\mathcal{G}$ have an odd degree.

The Hamiltonian Path Problem (HPP). *For given $e, e' \in \mathcal{E}$ determine whether there is a walk $\mathbf{w}$ from e' to e such that*

(a) *it visits each vertex $v \in V$ exactly once if $\partial(e) \neq \partial(e')$,*
(b) *it visits each vertex $v \neq \partial(e)$ exactly once and the vertex $v = \partial(e)$ exactly twice if $\partial(e) = \partial(e')$.*

There are no known simple necessary and sufficient conditions for the existence of Hamiltonian paths. Some sufficient conditions can be found, e.g., in [14]. The HPP is NP-complete.

In contrast to KBP and HPP, the TSP involves the metric structure on the graph $\mathcal{G}$. This problem is also NP-complete. There are several slightly different versions considered in the literature. Here we give three formulations suited for the present context.

Assume that a metric $\underline{a}_0 \in (\mathbb{R}_+)^{|\mathcal{I}|}$ on the graph $\mathcal{G}$ is given.

The Traveling Salesman Problem (TSP I). *For given $e, e' \in \mathcal{E}$ find a walk $\mathbf{w}$ from e' to e with minimal metric length $|\mathbf{w}|$ which visits each vertex $v \in V$ of the graph $\mathcal{G}$ at least once.*

The reader is referred to [3], [59] and the references quoted therein for known combinatorial solutions of TSP I. The second version of TSP is HPP extended by a metric length condition.

The Traveling Salesman Problem (TSP II). *For given $e, e' \in \mathcal{E}$ determine whether there is a walk $\mathbf{w}$ from e' to e satisfying the same conditions as in HPP and which, in addition, is of shortest metric length.*

The third version is the same as TSP I but formulated as a decision problem involving an additional length condition.

The Traveling Salesman Problem (TSP III). *For given $e, e' \in \mathcal{E}$ and a given number $L > 0$ decide whether there is a walk $\mathbf{w}$ from e' to e which visits each vertex $v \in V$ of the graph $\mathcal{G}$ at least once and $|\mathbf{w}| \leq L$.*

Recall that the definition of walks on the graph $\mathcal{G}$ is independent of the particular choice of the orientation of the edges (see Remark 6.1). Therefore, we deal with *symmetric* versions of the combinatorial problems listed above, where the length of an edge is independent of the direction in which this edge is traversed.

9.1. **Solution of KBP.** Choose any of the boundary conditions (A, B) referred to in Theorem 6.9. For an arbitrary metric structure $\underline{a} \in (\mathbb{R}_+)^{|\mathcal{I}|}$ they define a self-adjoint Laplace operator $\Delta(A, B; \underline{a})$. The associated scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ we will denote for brevity by $S(\mathsf{k}; \underline{a})$. Set

$$\underline{1} := \{1\}_{i\in\mathcal{I}} \in (\mathbb{N}_0)^{|\mathcal{I}|}.$$

By Theorem 6.9 to solve KBP, we only have to see whether the matrix element of the Fourier coefficient $[\widehat{S}_{\underline{1}}(\mathsf{k})]_{e,e'}$ defined in (5.2) of the scattering matrix $S(\mathsf{k}; \underline{a})$ vanishes identically or not. In particular, evaluating integrals in (5.2), one can give a purely analytic proof of the Euler theorem.

9.2. **Solution of HPP.** First, assume that the graph $\mathcal{G}$ has a vertex v with $\deg(v) = 1$. Let $i \in \mathcal{I}$ be the unique internal edge incident with this vertex. Then, HPP has a solution if and only if $|\mathcal{I}| = 1$, $|V| = 2$, and $\partial(e) \in \partial(i)$ for all $e \in \mathcal{E}$. Indeed, assume that for some graph $\mathcal{G}$ with minimum degree 1 there exists a walk $\mathbf{w}$ satisfying the conditions of HPP. Let $\deg(v) = 1$, $v \in \partial(i)$. Denote by v' the vertex adjacent to v by the edge i. Thus, the walk $\mathbf{w}$ visits v' twice. If v' is not a boundary vertex, this is a contradiction. If not, there are external edges $e, e' \in \mathcal{E}$ (possibly $e = e'$) such that $\mathbf{w} = \{e', i, i, e\}$. Thus, if $|V| > 2$ the walk $\mathbf{w}$ does not visit any other vertex different from v and v'.

By this observation, we may assume that $\deg(v) > 1$ for all $v \in V$. Obviously, any solution $\mathbf{w}$ of HPP traverses any internal edge at most once. We call a score $\underline{n} = \{n_i\}_{i\in\mathcal{I}}$ *simple* if $n_i \in \{0, 1\}$ for all $i \in \mathcal{I}$. Let $\mathcal{N}_{e,e'}^{\mathrm{simple}}$ be the (possibly empty) set of simple scores in the set $\mathcal{N}_{e,e'}$ defined in (6.10). Obviously, $|\mathcal{N}_{e,e'}^{\mathrm{simple}}| \leq 2^{|\mathcal{I}|}$.

Lemma 9.1. *If a walk* $\mathbf{w}$ *solves HPP, then its score* $\underline{n}(\mathbf{w})$ *satisfies*

$$|\underline{n}(\mathbf{w})| = \begin{cases} |V| & \text{if} \quad \partial(e) = \partial(e') \\ |V| - 1 & \text{if} \quad \partial(e) \neq \partial(e'). \end{cases} \tag{9.1}$$

Proof. Assume $\mathbf{w} \in \mathcal{W}_{e,e'}(\underline{n})$ is a walk solving HPP. Then the score $\underline{n} \equiv \{n_i\}_{i\in\mathcal{I}} := \underline{n}(\mathbf{w})$ is simple. Let $\mathcal{G}' = (V', \mathcal{I}', \mathcal{E}', \partial')$ be the (noncompact) graph obtained from $\mathcal{G} = (V, \mathcal{I}, \mathcal{E}, \partial)$ by removing the internal edges $i \in \mathcal{I}$ with $n_i = 0$. Obviously, $V' = V$ and $\mathcal{E}' = \mathcal{E}$. If $\partial(e) \neq \partial(e')$, then the degree $\deg_{\mathcal{G}'_{\mathrm{int}}}(v)$ of any vertex $v \notin \{\partial(e), \partial(e')\}$ in the interior $\mathcal{G}'_{\mathrm{int}}$ of the graph $\mathcal{G}'$ equals 2. The degree of the vertices $\partial(e)$ and $\partial(e')$ in $\mathcal{G}'_{\mathrm{int}}$ equals 1. Thus, applying the First Theorem of Graph Theory to $\mathcal{G}'_{\mathrm{int}}$ we obtain

$$|\underline{n}| = |\mathcal{I}'| = \frac{1}{2} \sum_{v\in V} \deg_{\mathcal{G}'_{\mathrm{int}}}(v) = |V| - 1.$$

If $\partial(e) = \partial(e')$, then $\deg_{\mathcal{G}'_{\mathrm{int}}}(v) = 2$ for all $v \in V$. Therefore, we get

$$|\underline{n}| = |\mathcal{I}'| = \frac{1}{2} \sum_{v\in V} \deg_{\mathcal{G}'_{\mathrm{int}}}(v) = |V|.$$

This proves (9.1). □

Let

$$\mathcal{N}_{e,e'}^{(\mathrm{HPP})} = \{\underline{n} \in \mathcal{N}_{e,e'}^{\mathrm{simple}} \mid |\underline{n}| \quad \text{satisfies (9.1)}\}.$$

Obviously,

$$|\mathcal{N}_{e,e'}^{(\mathrm{HPP})}| \leq \begin{cases} \frac{|\mathcal{I}|!}{|V|!(|\mathcal{I}|-|V|)!} & \text{if} \quad \partial(e) = \partial(e'), \\ \frac{|\mathcal{I}|!}{(|V|-1)!(|\mathcal{I}|-|V|+1)!} & \text{if} \quad \partial(e) \neq \partial(e'). \end{cases}$$

Note that to determine the number of elements in the set $\mathcal{N}_{e,e'}^{(\mathrm{HPP})}$ there are simple procedures based on the calculation of the generating function. Some counting problems of this type are considered in [46].

We emphasize that $\underline{n} \in \mathcal{N}_{e,e'}^{(\mathrm{HPP})}$ in general does not imply that a walk $\mathbf{w}$ from e' to e with the score $\underline{n}$ solves HPP.

Let $\mathbf{w}$ be an arbitrary walk from $e' \in \mathcal{E}$ to $e \in \mathcal{E}$, $\underline{n} = \underline{n}(\mathbf{w})$ its score. For any vertex $v \in V$ define

$$N_{e,e'}(v;\underline{n}) = \frac{1}{2} \sum_{i\in\mathcal{I}: v\in\partial(i)} n_i + \frac{n_{e,e'}(v)}{2}, \qquad \underline{n} = \{n_i\}_{i\in\mathcal{I}}, \tag{9.2}$$

where

$$n_{e,e'}(v) = \begin{cases} 2 & \text{if} \quad v = \partial(e) = \partial(e'), \\ 1 & \text{if} \quad \partial(e) \neq \partial(e') \quad \text{and} \quad v = \partial(e) \quad \text{or} \quad v = \partial(e'), \\ 0 & \text{otherwise.} \end{cases} \tag{9.3}$$

It is easy to check that $N_{e,e'}(v;\underline{n})$ is the number of times a walk $\mathbf{w} \in \mathcal{W}_{e,e'}$ visits the vertex $v \in V$.

Theorem 9.2. *Assume that the minimum degree of the graph $\mathcal{G}$ is bigger than 1. The HPP has a solution if and only if there is $\underline{n} \in \mathcal{N}_{e,e'}^{(\mathrm{HPP})}$ such that $N_{e,e'}(v;\underline{n}) \neq 0$ for all $v \in V$.*

Proof. It remains to prove the "if" part of the statement. Assume that there is $\underline{n} \equiv \{n_i\}_{i\in\mathcal{I}} \in \mathcal{N}_{e,e'}^{(\mathrm{HPP})}$. Therefore, there is a walk $\mathbf{w} \in \mathcal{W}_{e,e'}(\underline{n})$ from e' to e traversing any internal edge of the graph $\mathcal{G}$ at most once. By the assumption $N_{e,e'}(v;\underline{n}) \neq 0$ this walk visits any vertex of the graph at least once. Again, let $\mathcal{G}'$ be the graph obtained from $\mathcal{G}$ by removing the internal edges $i \in \mathcal{I}$ with $n_i = 0$.

If $\partial(e) = \partial(e')$, then the minimum degree of the graph $\mathcal{G}'_{\mathrm{int}}$ is not less than 2. Indeed, $\deg_{\mathcal{G}'_{\mathrm{int}}}(v) \geq 2$ for any vertex $v \neq \partial(e)$ by assumption. On the other hand for $v = \partial(e)$, the walk $\mathbf{w}$ visits $\partial(e)$ at least twice and, hence, there must be at least two internal edges $i \in \mathcal{I}$ incident with $\partial(e)$. Condition (9.1) and the First Theorem of Graph Theory imply that

$$\sum_{v\in V} \deg_{\mathcal{G}'_{\mathrm{int}}}(v) = 2|\mathcal{I}'| = 2|V|.$$

Therefore, $\deg_{\mathcal{G}'_{\mathrm{int}}}(v) = 2$ for all $v \in V$. This implies that the walk $\mathbf{w}$ visits every vertex $v \neq \partial(e)$ exactly once and the vertex $\partial(e)$ twice.

If $\partial(e) \neq \partial(e')$, then

$$\deg_{\mathcal{G}'_{\mathrm{int}}}(v) \geq 2 \quad \text{for all} \quad v \in V \setminus \{\partial(e), \partial(e')\},$$

and

$$\deg_{\mathcal{G}'_{\mathrm{int}}}(v) \geq 1 \quad \text{if} \quad v \in \{\partial(e), \partial(e')\}.$$

Again by (9.1) and the First Theorem of Graph Theory we have that

$$\sum_{v\in V} \deg_{\mathcal{G}'_{\mathrm{int}}}(v) = 2|\mathcal{I}'| = 2|V| - 2.$$

Therefore, $\deg_{\mathcal{G}'_{\mathrm{int}}}(v) = 2$ for all $v \in V \setminus \{\partial(e), \partial(e')\}$ and $\deg_{\mathcal{G}'_{\mathrm{int}}}(v) = 1$ for $v \in \{\partial(e), \partial(e')\}$. This implies that the walk $\mathbf{w}$ visits every vertex $v \in V$ exactly once. $\square$

Note that the condition of Theorem 9.2 can be verified by computing the Fourier coefficients of the scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ for the Laplace operator associated with any of the boundary conditions (A, B) referred to in Theorem 6.9. However, one is still faced with the combinatorial problem for scores $\underline{n} \in \mathcal{N}_{e,e'}^{\mathrm{HPP}}$. Our next aim is to solve this problem by purely analytic means.

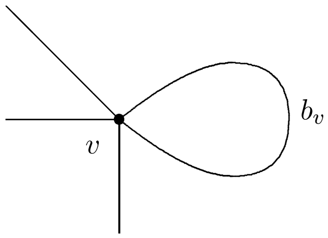

FIG. 7. A tadpole (penalty lap) attached to a vertex v which was originally incident with three edges.

At each vertex $v \in V \setminus \{\partial(e), \partial(e')\}$ of the graph $\mathcal{G}$ we attach a tadpole of metric length $b_v > 0$ (see Fig. 7). Having in mind some similarity with biathlon competition, we will call these tadpoles *penalty laps*. The resulting graph $\widetilde{\mathcal{G}} = (V, \widetilde{\mathcal{I}}, \mathcal{E}, \widetilde{\partial})$ has the same vertex set V and the same set of the external edges $\mathcal{E}$. The degree of any vertex $v \notin \{\partial(e), \partial(e')\}$ in the graph $\widetilde{\mathcal{G}}$ is given by $\deg_{\widetilde{\mathcal{G}}}(v) = \deg_{\mathcal{G}}(v) + 2$. The set of the internal edges $\widetilde{\mathcal{I}}$ is the union $\mathcal{I} \cup \mathcal{J}$ of the set $\mathcal{I}$ of the internal edges of the graph $\mathcal{G}$ and the set $\mathcal{J}$ of the penalty laps. By construction, there is a bijective mapping $\phi : V \setminus \{\partial(e), \partial(e')\} \to \mathcal{J}$. The boundary operator $\widetilde{\partial}$ is defined as follows

$$\widetilde{\partial}(i) = \begin{cases} \partial(e) & \text{if} \quad e \in \mathcal{E}, \\ \partial(i) & \text{if} \quad i \in \mathcal{I}, \\ \{\phi^{-1}(i), \phi^{-1}(i)\} & \text{if} \quad i \in \mathcal{J}. \end{cases}$$

The metric structure on the graph $\widetilde{\mathcal{G}}$ is given by $(\underline{a}, \underline{b})$, where $\underline{a} = \{a_i\}_{i \in \mathcal{I}}$, $\underline{b} = \{b_j\}_{j \in \mathcal{J}}$.

Choose any boundary conditions on the graph $\widetilde{\mathcal{G}}$ of the type referred to in Theorem 6.9. These boundary conditions define a self-adjoint Laplace operator. For brevity we denote by $\widetilde{S}(\mathsf{k}; \underline{a}, \underline{b})$ the associated scattering matrix. Let $\widetilde{\mathcal{N}}_{e,e'}$ be the set of scores of all walks from e' to e defined similarly to (6.10),

$$\widetilde{\mathcal{N}}_{e,e'} = \{(\underline{n}, \underline{m}) \mid \text{there is walk } \mathbf{w} \in \widetilde{\mathcal{W}}_{e,e'}(\underline{n}, \underline{m})\},$$

where $\widetilde{\mathcal{W}}_{e,e'}(\underline{n}, \underline{m})$ is a subset of all walks on the graph $\widetilde{\mathcal{G}}$ from e' to e having the score $(\underline{n}, \underline{m})$. Recall that $\underline{n} = \{n_i\}_{i \in \mathcal{I}}$ and $\underline{m} = \{m_j\}_{j \in \mathcal{J}}$, where $n_i \in \mathbb{N}_0$ is the number of times a walk $\mathbf{w}$ traverses the edge $i \in \mathcal{I}$ and $m_j \in \mathbb{N}_0$ is the number of times a walk $\mathbf{w}$ traverses the penalty lap $j \in \mathcal{J}$.

Theorems 5.2 and 6.6 immediately imply that the scattering matrix $\widetilde{S}(\mathsf{k}; \underline{a}, \underline{b})$ is given by the absolutely converging Fourier series

$$[\widetilde{S}(\mathsf{k}; \underline{a}, \underline{b})]_{e,e'} = \sum_{(\underline{n},\underline{m}) \in \widetilde{\mathcal{N}}_{e,e'}} [\widehat{\widetilde{S}}_{\underline{n},\underline{m}}(\mathsf{k})]_{e,e'} \, \mathrm{e}^{\mathrm{i}\mathsf{k}\langle \underline{n}, \underline{a}\rangle} \mathrm{e}^{\mathrm{i}\mathsf{k}\langle \underline{m}, \underline{b}\rangle}, \tag{9.4}$$

where

$$[\widehat{\widetilde{S}}_{\underline{n},\underline{m}}(\mathsf{k})]_{e,e'} = \left(\frac{\mathsf{k}}{2\pi}\right)^{|\mathcal{I}|+|\mathcal{J}|} \int_{[0,2\pi/\mathsf{k}]^{|\mathcal{I}|}} d\underline{a} \int_{[0,2\pi/\mathsf{k}]^{|\mathcal{J}|}} d\underline{b} \; [\widetilde{S}(\mathsf{k}; \underline{a}, \underline{b})]_{e,e'} \mathrm{e}^{-\mathrm{i}\mathsf{k}\langle \underline{n}, \underline{a}\rangle} \mathrm{e}^{-\mathrm{i}\mathsf{k}\langle \underline{m}, \underline{b}\rangle}.$$

By Theorem 6.9 none of the Fourier coefficients $\widehat{\widetilde{S}}_{\underline{n},\underline{m}}(\mathsf{k})_{e,e'}$ vanishes identically whenever $(\underline{n}, \underline{m}) \in \widetilde{\mathcal{N}}_{e,e'}$.

We are interested in the terms with $\underline{m} = \underline{1} \equiv \{1\}_{j \in \mathcal{J}}$, i.e., walks traversing each penalty lap exactly once. Such walks visit each vertex of the graph at least once.

Theorem 9.3. *Assume that the minimum degree of the graph $\mathcal{G}$ is bigger than 1. The HPP has a solution if and only if the Fourier coefficient $[\widehat{\widetilde{S}}_{\underline{n}^{(0)},\underline{1}}(\mathsf{k})]_{e,e'}$ does not vanish identically for some $\underline{n}^{(0)} \in (\mathbb{N}_0)^{|\mathcal{I}|}$ with*

$$|\underline{n}^{(0)}| = \begin{cases} |V| & \text{if} \quad \partial(e) = \partial(e'), \\ |V| - 1 & \text{if} \quad \partial(e) \neq \partial(e'). \end{cases} \tag{9.5}$$

In this case the Fourier coefficients $[\widehat{\widetilde{S}}_{\underline{n},\underline{1}}(\mathsf{k})]_{e,e'}$ vanish identically for all $\underline{n} \in (\mathbb{N}_0)^{|\mathcal{I}|}$ with $|\underline{n}| < |\underline{n}^{(0)}|$.

Remark 9.4. *By Remark 5.10 the natural number $|\underline{n}_0|$ is the order of the first nontrivial coefficient in the Taylor expansion of a function holomorphic in a polydisc. Once the existence of a solution of HPP is established, one can uniquely reconstruct the walk from its score $\underline{n}^{(0)}$.*

Proof. The "only if" part follows from Lemma 9.1 and Theorem 9.2. We turn to the proof of the "if" part. Assume there is $\underline{n}^{(0)} \equiv \{n_i^{(0)}\}_{i\in\mathcal{I}} \in (\mathbb{N}_0)^{|\mathcal{I}|}$ satisfying (9.5) such that $\widehat{S}_{\underline{n}^{(0)},\underline{1}}(\mathsf{k})$ does not vanish identically. Then by Theorem 6.9 there is walk $\widetilde{\mathbf{w}}$ on the graph $\widetilde{\mathcal{G}}$ with the score $(\underline{n}^{(0)}, \underline{1}) \in (\mathbb{N}_0)^{|\mathcal{I}|+|\mathcal{J}|}$ visiting every vertex $v \in V$ at least once. Erasing the "penalty laps" in this walk we obtain a walk $\mathbf{w}$ from e' to e on the graph $\mathcal{G}$ with a score $\underline{n}^{(0)}$ visiting every vertex $v \in V$ at least once. Thus, $N_{e,e'}(v, \underline{n}^{(0)}) \neq 0$ for all $v \in V$.

Let $\mathcal{G}'$ be the graph obtained from $\mathcal{G}$ by removing the internal edges $i \in \mathcal{I}$ with $n_i = 0$.

Claim 1: $\deg_{\mathcal{G}'_{\text{int}}}(v) \geq 2$ holds for all $v \in V$ if $\partial(e) = \partial(e')$ and for all $v \in V \setminus \{\partial(e), \partial(e')\}$ if $\partial(e) \neq \partial(e')$. Consider the case $\partial(e) = \partial(e')$. Assume to the contrary that there is at least one vertex with $\deg_{\mathcal{G}'_{\text{int}}}(v) = 1$. Let $i' \in \mathcal{I}'$ be the edge incident with v. Obviously, the walk $\mathbf{w}$ traverses i' at least twice, that is, $n_{i'}^{(0)} \geq 2$. Therefore,

$$\begin{aligned} |\underline{n}^{(0)}| &\geq |\mathcal{I}'| + |\{v \in V |\, \deg_{\mathcal{G}'_{\text{int}}}(v) = 1\}| \\ &= \frac{1}{2} \sum_{v\in V} \deg_{\mathcal{G}'_{\text{int}}}(v) + |\{v \in V |\, \deg_{\mathcal{G}'_{\text{int}}}(v) = 1\}| \\ &= \frac{1}{2} \sum_{v\in V} \max\{\deg_{\mathcal{G}'_{\text{int}}}(v), 2\} + \frac{1}{2} |\{v \in V |\, \deg_{\mathcal{G}'_{\text{int}}}(v) = 1\}| > |V|, \end{aligned}$$

which contradicts the assumption $|\underline{n}^{(0)}| = |V|$. Similarly, if $\partial(e) \neq \partial(e')$ we obtain the inequality $|\underline{n}^{(0)}| > |V| - 1$ which contradicts the assumption $|\underline{n}^{(0)}| = |V| - 1$. The claim is proven.

Claim 2: $\underline{n}^{(0)}$ is simple. Assume not, that is, there is $i' \in \mathcal{I}'$ with $n_{i'}^{(0)} \geq 2$. Using Claim 1 we obtain the inequality

$$|\underline{n}^{(0)}| > |\mathcal{I}'| = \frac{1}{2} \sum_{v\in V} \deg_{\mathcal{G}'_{\text{int}}}(v) \geq \begin{cases} |V| & \text{if} \quad \partial(e) = \partial(e'), \\ |V| - 1 & \text{if} \quad \partial(e) \neq \partial(e'), \end{cases}$$

which contradicts the assumption of the theorem.

Applying Theorem 9.2 we obtain the first assertion of the theorem. Assume now that there is $\underline{n} \in (\mathbb{N}_0)^{|\mathcal{I}|}$ with $|\underline{n}| < |\underline{n}^{(0)}|$ such that $[\widehat{\widetilde{S}}_{\underline{n},\underline{1}}(\mathsf{k})]_{e,e'}$ does not vanish identically. Then there is a walk from $e' \in \mathcal{E}$ to $e \in \mathcal{E}$ on the graph $\mathcal{G}$ with the score $\underline{n} = \{n_i\}_{i\in\mathcal{I}}$ visiting every vertex of the graph at least once.

Again by $\mathcal{G}'$ we denote the graph obtained from $\mathcal{G}$ by removing the internal edges $i \in \mathcal{I}$ with $n_i = 0$. Repeating the arguments used to prove Claim 1 we obtain that $\deg_{\mathcal{G}'_{\text{int}}}(v) \geq 2$ holds for all $v \in V$ if $\partial(e) = \partial(e')$ and for all $v \in V \setminus \{\partial(e), \partial(e')\}$ if $\partial(e) \neq \partial(e')$. But this immediately leads to the inequality

$$|\underline{n}| \geq |\mathcal{I}'| = \frac{1}{2}\sum_{v\in V} \deg_{\mathcal{G}'_{\mathrm{int}}}(v) \geq |\underline{n}^{(0)}|,$$

which is a contradiction. □

9.3. **Solution of TSP.** Recall that the metric $\underline{a}_0 \in (\mathbb{R}_+)^{|\mathcal{I}|}$ on the graph $\mathcal{G}$ is given. Choose arbitrary boundary conditions (A, B) referred to in Theorem 6.9. For an arbitrary metric structure $\underline{a} \in (\mathbb{R}_+)^{|\mathcal{I}|}$ they define a self-adjoint Laplace operator $\Delta(A, B; \underline{a})$. The associated scattering matrix $S(\mathsf{k}; A, B, \underline{a})$ we will denote for brevity by $S(\mathsf{k}; \underline{a})$.

For arbitrary $e, e' \in \mathcal{E}$ let $\mathcal{N}^{(\mathrm{I})}_{e,e'}$ be the set of all vectors $\underline{n} \equiv \{n_i\}_{i\in\mathcal{I}} \in (\mathbb{N}_0)^{|\mathcal{I}|}$ satisfying the following conditions:

(i) the matrix element $\widehat{S}_{\underline{n}}(\mathsf{k})_{e,e'}$ of the Fourier coefficient (5.2) of the scattering matrix $S(\mathsf{k}; \underline{a})$ does not vanish identically for all $\mathsf{k} > 0$,

(ii) $n_i \in \{0, 1, 2\}$ for all $i \in \mathcal{I}$,

(iii) $N_{e,e'}(v; \underline{n}) \neq 0$ for all $v \in V$.

Note that by Theorem 6.9 condition (i) implies that $\underline{n}$ is the score of some walk from e' to e. Therefore, the quantity $N_{e,e'}(v; \underline{n})$ in condition (iii) is well-defined. Obviously,

$$\mathcal{N}^{(\mathrm{I})}_{e,e'} \neq \varnothing \qquad \text{and} \qquad |\mathcal{N}^{(\mathrm{I})}_{e,e'}| \leq 3^{|\mathcal{I}|}.$$

Theorem 9.5. *A vector $\underline{n} \in \mathcal{N}^{(\mathrm{I})}_{e,e'}$ satisfying*

$$\langle \underline{n}, \underline{a}_0\rangle \leq \langle \underline{n}', \underline{a}_0\rangle \tag{9.6}$$

for all $\underline{n}' \in \mathcal{N}^{(\mathrm{I})}_{e,e'}$ is the score of a walk from e' to e solving TSP I. Conversely, if a walk $\mathbf{w}$ from e' to e solves TSP I, its score $\underline{n}(\mathbf{w})$ belongs to $\mathcal{N}^{(\mathrm{I})}_{e,e'}$ and satisfies (9.6).

The solution of TSP I is unique if the lengths of internal edges are rationally independent.

We expect the following result to be known.

Lemma 9.6. *The score $\underline{n}(\mathbf{w})$ of any solution $\mathbf{w}$ of TSP I is in $\mathcal{N}^{(\mathrm{I})}_{e,e'}$.*

Proof. It suffices to prove that the score $\underline{n}(\mathbf{w}) \equiv \{n_i\}_{i\in\mathcal{I}}$ of any solution $\mathbf{w}$ of TSP I satisfies $n_i \leq 2$ for all $i \in \mathcal{I}$. To show this we will assume on the contrary that there is at least one internal edge of the graph $\mathcal{G}$ which is traversed by the walk $\mathbf{w}$ at least three times. Obviously, this edge is traversed at least twice in the same direction. We will construct another walk $\mathbf{w}'$ from e' to e with metric length $|\mathbf{w}'| < |\mathbf{w}|$ which visits every vertex at least once.

By assumption the walk $\mathbf{w}$ is of the form

$$\mathbf{w} = \{e', i_1, \ldots, i_p, \ldots, i_q, \ldots, i_N, e\},$$

where $i_p = i_q$ for some $p < q$ and either

$$\partial^-(i_p) \in \partial(i_{p-1}), \quad \partial^+(i_p) \in \partial(i_{p+1}), \quad \partial^-(i_q) \in \partial(i_{q-1}), \quad \partial^+(i_q) \in \partial(i_{q+1})$$

or

$$\partial^-(i_p) \in \partial(i_{p+1}), \quad \partial^+(i_p) \in \partial(i_{p-1}), \quad \partial^-(i_q) \in \partial(i_{q+1}), \quad \partial^+(i_q) \in \partial(i_{q-1}).$$

Consider the walk from e' to e

$$\mathbf{w}' = \{e', i_1, \ldots, i_{p-1}, i_{q-1}, \ldots, i_{p+1}, i_{q+1}, \ldots, i_N\},$$

where the sequence $i_{q-1}, \ldots, i_{p+1}$ is the part $i_{p+1}, \ldots, i_{q-1}$ of the walk $\mathbf{w}$ taken in the reversed order. Obviously, the metric length of the walk $\mathbf{w}'$ is given by

$$|\mathbf{w}'| = |\mathbf{w}| - 2a_{i_p} < |\mathbf{w}|.$$

This completes the proof. □

Proof of Theorem 9.5. Let $\underline{n} \in \mathcal{N}_{e,e'}^{(\mathrm{I})}$ satisfy (9.6). Then there is a walk $\mathbf{w}$ from e' to e with the score $\underline{n}$ having the shortest length among all walks from e' to e with scores in $\mathcal{N}_{e,e'}^{(\mathrm{I})}$. By Lemma 9.6 the walk $\mathbf{w}$ is a solution of TSP I. □

The *solutions of TSP II and III* are similar. We formulate the final results.

Theorem 9.7. *A walk* $\mathbf{w}$ *from* e' *to* e *solving TSP II exists if and only if there is a solution of HPP. Among the solutions of HPP it is one with shortest metric length. The corresponding score* $\underline{n}(\mathbf{w})$ *is unique whenever the metric lengths* $\underline{a}_0$ *of internal edges are rationally independent.*

Theorem 9.8. *A walk* $\mathbf{w}$ *from* e' *to* e *solving TSP III exists if and only if there is a score* $\underline{n} \in \mathcal{N}_{e,e'}^{(\mathrm{I})}$ *such that* $\langle \underline{n}, \underline{a}_0 \rangle \leq L$.

As in the case of HPP one can solve the optimization problems referred to in Theorems 9.5, 9.7, and 9.8 in an analytic way. In what follows we assume that the metric lengths $\underline{a}_0$ of internal edges satisfy Assumption 2. Obviously, given $\underline{a} \in (\mathbb{R}_+)^{|\mathcal{I}|}$, this assumption can always be satisfied by changing the lengths by arbitrarily small amount. Consider the graph $\widetilde{\mathcal{G}}$ obtained from $\mathcal{G}$ by adding penalty laps at each vertex $v \in V \setminus \{\partial(e), \partial(e')\}$ and the scattering matrix $\widetilde{S}(\mathsf{k}; \underline{a}, \underline{b})$ associated with some boundary conditions referred to in Theorem 6.9 (see the previous subsection).

We consider the partial Fourier transform of the scattering matrix (9.4) with respect to the variables $\underline{b}$

$$\widetilde{S}_\sharp(\mathsf{k}; \underline{a}) = \left(\frac{\mathsf{k}}{2\pi}\right)^{|\mathcal{J}|} \int_{[0,2\pi/\mathsf{k}]^{|\mathcal{J}|}} d\underline{b}\, \widetilde{S}(\mathsf{k}; \underline{a}, \underline{b})\, \mathrm{e}^{-\mathrm{i}\mathsf{k}\langle \underline{1}, \underline{b}\rangle}$$

such that

$$\widehat{\widetilde{S}}_{\underline{n},\underline{1}}(\mathsf{k}) = \left(\frac{\mathsf{k}}{2\pi}\right)^{|\mathcal{I}|} \int_{[0,2\pi/\mathsf{k}]^{|\mathcal{I}|}} d\underline{a}\, \widetilde{S}_\sharp(\mathsf{k}; \underline{a})\, \mathrm{e}^{-\mathrm{i}\mathsf{k}\langle \underline{n}, \underline{a}\rangle}$$

and the series

$$[\widetilde{S}_\sharp(\mathsf{k}; \underline{a})]_{e,e'} = \sum_{\underline{n} \in \mathcal{N}_{e,e'}} [\widehat{\widetilde{S}}_{\underline{n},\underline{1}}(\mathsf{k})]_{e,e'}\, \mathrm{e}^{\mathrm{i}\mathsf{k}\langle \underline{n}, \underline{a}\rangle}$$

is absolutely convergent for all $\mathsf{k} > 0$. By Theorem 6.9 $\widehat{\widetilde{S}}_{\underline{n},\underline{1}}(\mathsf{k})_{e,e'}$ does not vanish identically if and only if there is a walk on the graph $\mathcal{G}$ from e' to e visiting every vertex of the graph at least once.

By Theorem 7.2 and Remark 7.3 the function $\mathsf{k} \mapsto [\widetilde{S}_\sharp(\mathsf{k}; \underline{a}_0)]_{e,e'}$ determines the lengths of all walks from e' to e on the graph $\mathcal{G}$ visiting every vertex of the graph at least once. Let w be the smallest number in this set. In particular, we have

$$w = \lim_{\mathrm{Im}\, \mathsf{k} \to \infty} \frac{1}{\mathrm{i}} \frac{\partial}{\partial \mathsf{k}} \log [\widetilde{S}_\sharp(\mathsf{k}; \underline{a}_0)]_{e,e'}.$$

By Assumption 2 there is a unique $\underline{n} \in (\mathbb{N}_0)^{|\mathcal{I}|}$ such that $w = \langle \underline{n}, \underline{a}_0 \rangle$. Obviously, $\underline{n}$ is the score of a walk from e' to e on the graph $\mathcal{G}$ solving TSP I. If HPP has a solution, then, by Theorem 9.3, the solution of TSP II is a walk with the score satisfying 9.5 and having the shortest metric length. TSP III has a solution if and only if $w \leq L$.

REFERENCES

[1] N. I. Akhiezer and I. M. Glazman, *Theory of Linear Operators in Hilbert Space*, Dover Publications, New York, 1993.

[2] J. C. Alexander, *The additive inverse eigenvalue problem and topological degree*, Proc. Amer. Math. Soc. **70** (1978), 5 – 7.

[3] D. Applegate, R. Bixby, V. Chvátal, and W. Cook, *On the solution of traveling salesman problems*, Documenta Mathematica, Extra Volume ICM 1998 - III, 645 – 656.

[4] V. I. Arnold and A. B. Givental, *Symplectic Geometry*, in V. I. Arnold and S. P. Novikov (Eds.) “Dynamical Systems, Vol. IV”, Springer, Berlin, 1990. pp. 1 – 138.
[5] V. I. Arnold, *The complex Lagrangian Grassmannian*, Funct. Anal. Appl. **34** (2000), 208 – 210.
[6] M. I. Belishev, *Boundary spectral inverse problem on a class of graphs (trees) by the BC method*, Inverse Problems **20** (2004), 647 – 672.
[7] J. von Below, *Can one hear the shape of a network?*, in F. Ali Mehmeti, J. von Below, and S. Nicaise (Eds.) “Partial Differential Equations on Multistructures”, (Proceedings of the Int. Conference, Luminy, April 19-24, 1999), Lecture Notes in Pure and Appl. Math., Vol. 219, Dekker, New York, 2001. pp. 19 – 36.
[8] J. Boman and P. Kurasov, *Symmetries of quantum graphs and the inverse scattering problem*, Adv. in Appl. Math. **35** (2005), 58 – 70.
[9] R. Brooks and P. A. Perry, *Isophasal scattering manifolds in two dimensions*, Comm. Math. Phys. **223** (2001), 465 – 474.
[10] J. Brüning and V. A. Geyler, *Scattering on compact manifolds with infinitely thin horns*, J. Math. Phys. **44** (2003), 371 – 405.
[11] R. Carlson, *Inverse eigenvalue problems on directed graphs*, Trans. Amer. Math. Soc. **351** (1999), 4069 – 4088.
[12] Y. Colin de Verdière, *Spectres de graphes*, Cours Spécialisés, Vol. 4. Société Mathématique de France, Paris, 1998.
[13] B. Dekoninck and S. Nicaise, *The eigenvalue problem for networks of beams*, Linear Algebra Appl. **314** (2000), 165 – 189.
[14] R. Diestel, *Graph Theory*, Springer, New York, 2000.
[15] R. J. Eden, P. V. Landshoff, D. I. Olive, and J. C. Polkinghorne, *The Analytic S-matrix*, Cambridge University Press, Cambridge, 1966.
[16] W. N. Everitt and L. Markus, *Elliptic Partial Differential Operators and Symplectic Algebra*, Mem. Amer. Math. Soc. Vol. 162 (2003), no. 770.
[17] P. Exner and O. Post, *Convergence of spectra of graph-like thin manifolds*, J. Geom. Phys. **54** (2005), 77 – 115.
[18] S. Friedland, *Matrices with prescribed off-diagonal elements*, Israel J. Math. **11** (1972), 184 – 189.
[19] S. Friedland, *Inverse eigenvalue problems*, Linear Algebra and Appl. **17** (1977), 15 – 51.
[20] M. R. Garey and D. S. Johnson, *Computers and Intractability. A Guide to the Theory of NP-Completeness*, W. H. Freeman and Co., San Francisco, 1979.
[21] B. Gaveau, M. Okada, and T. Okada, *Explicit heat kernels on graphs and spectral analysis*, in J. E. Fornaess (Ed.) “Several Complex Variables”, (Proceedings of the Mittag-Leffler Institute, Stockholm, 1987-88), Princeton Math. Notes Vol. 38, Princeton University Press, 1993. pp. 364 – 388.
[22] B. Gaveau and M. Okada, *Differential forms and heat diffusion on one-dimensional singular varieties*, Bull. Sci. Math., II. Sér., **115** (1991), 61 – 80.
[23] N. I. Gerasimenko and B. S. Pavlov, *Scattering problems on non-compact graphs*, Theor. Math. Phys. **74** (1988), 230 – 240.
[24] N. I. Gerasimenko, *Inverse scattering problems on noncompact graphs*, Theor. Math. Phys. **75** (1988), 460 – 470.
[25] F. M. Goodman, P. de la Harpe, and V. F. R. Jones, *Coxeter Graphs and Towers of Algebras*, Springer, New York, 1989.
[26] C. Gordon, D. Webb, and S. Wolpert, *One cannot hear the shape of a drum*, Bull. Amer. Math. Soc. **27** (1992), 134 – 138.
[27] C. Gordon, *Survey of isospectral manifolds*, in F. J. E. Dillen and L. C. A. Verstraelen (Eds.) “Handbook of Differential Geometry, Vol. I”. North-Holland, Amsterdam, 2000. pp. 747 - 778.
[28] B. Gutkin and U. Smilansky, *Can one hear the shape of a graph?*, J. Phys. A: Math. Gen. **34** (2001), 6061 – 6068.
[29] M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics*, Interdiscipinary Applied Mathematics, Vol. 1, Springer, New York, 1990.
[30] M. Harmer, *Hermitian symplectic geometry and extension theory*, J. Phys. A: Math. Gen. **33** (2000), 9193 – 9203.
[31] M. Harmer, *Hermitian symplectic geometry and the factorizatuion of the scattering matrix on graphs*, J. Phys. A: Math. Gen. **33** (2000), 9015 – 9032.
[32] M. Harmer, *Inverse scattering for the matrix Schrödinger operator and Schrödinger operator on graphs with general self-adjoint boundary conditions*, ANZIAM J. **44** (2002), 161 – 168.
[33] M. Harmer, *Inverse scattering on matrices with boundary conditions*, J. Phys. A: Math. Gen. **38** (2005), 4875 – 4885.
[34] A. Hassell and S. Zelditch, *Determinants of Laplacians in exterior domains*, Int. Math. Res. Notes **18** (1999), 971 – 1004.
[35] L. Hörmander, *An Introduction to Complex Analysis in Several Variables*, North-Holland, Amsterdam, 1973.
[36] R. A. Horn and C. R. Johnson, *Topics in Matrix Analysis*, Cambridge University Press, Cambridge, 1991.

[37] V. C. L. Hutson and J. S. Pym, *Application of Functional Analysis and Operator Theory*, Academic Press, New York, 1980.
[38] D. Jungnickel, *Graphs, Networks and Algorithms*, Algorithms and Computation in Mathematics, Vol. 5. Springer, Berlin, 2005.
[39] M. Kac, *Can one hear the shape of a drum?*, Amer. Math. Monthly **73** (1966), 1 – 27.
[40] T. Kato, *Perturbation Theory for Linear Operators*, Springer, Berlin, 1966.
[41] A. N. Kočubeĭ, *Extensions of symmetric operators and of symmetric binary relations*, Math. Notes **17** (1975), 25 – 28.
[42] V. Kostrykin and R. Schrader, *Kirchhoff's rule for quantum wires*, J. Phys. A: Math. Gen. **32** (1999), 595 – 630.
[43] V. Kostrykin and R. Schrader, *Kirchhoff's rule for quantum wires II: The inverse problem with possible applications to quantum computers*, Fortschr. Phys. **48** (2000), 703 – 716.
[44] V. Kostrykin and R. Schrader, *The generalized star product and the factorization of scattering matrices on graphs*, J. Math. Phys. **42** (2001), 1563 – 1598.
[45] V. Kostrykin and R. Schrader, *Quantum wires with magnetic fluxes*, Comm. Math. Phys. **237** (2003), 161 – 179.
[46] V. Kostrykin and R. Schrader, *Generating functions of random walks on graphs*, preprint `arXiv:math.CO/0404467` (2004).
[47] V. Kostrykin and R. Schrader, *Laplacians on metric graphs: Eigenvalues, resolvents and semigroups*, Contemp. Math. (to appear). Preprint `arXiv:math-ph/0601041`.
[48] T. Kottos and U. Smilansky, *Periodic orbit theory and spectral statistics for quantum graphs*, Ann. Phys. (N.Y.) **274** (1999), 76 – 124.
[49] T. Kottos and U. Smilansky, *Chaotic scattering on graphs*, Phys. Rev. Lett. **85** (2000), 968 – 971.
[50] T. Kottos and U. Smilansky, *Quantum graphs: A simple model for chaotic scattering*, J. Phys. A: Math. Gen. **36** (2003), 3501 – 3524.
[51] S. G. Krantz and H. R. Parks, *A Primer of Real-Analytic Functions*, Birkhauser, Basel, 1992.
[52] P. Kuchment, *Graph models for waves in thin structures*, Waves Random Media **12** (2002), R1 – R24.
[53] P. Kuchment, *Quantum graphs: I. Some basic structures*, Waves Random Media **14** (2004), S107 – S128.
[54] P. Kuchment, *Quantum graphs: II. Some spectral properties of quantum and combinatorial graphs*, J. Phys. A: Math. Gen. **38** (2005), 4887 – 4900.
[55] P. Kuchment and H. Zeng, *Convergence of spectra of mesoscopic systems collapsing onto a graph*, J. Math. Anal. Appl. **258** (2001), 671 – 700.
[56] P. Kuchment and H. Zeng, *Asymptotics of spectra of Neumann Laplacians in thin domains*, in Yu. Karpeshina, G. Stolz, R. Weikard, and Y. Zeng (Eds.) "Advances in Differential Equations and Mathematical Physics", Contemp. Math. **327**, Amer. Math. Soc., Providence, RI, 2003. pp. 199 – 213.
[57] P. Kurasov and F. Stenberg, *On the inverse scattering problem on branching graphs*, J. Phys. A: Math. Gen. **35** (2002), 101 – 121.
[58] P. Kurasov and M. Novaszek, *Inverse spectral problem for quantum graphs*, J. Phys. A: Math. Gen. **38** (2005), 4901 – 4915.
[59] E. L. Lawler, J. K. Lenstra, A. H. G. Rinnooy Kan, and D. B. Shmoys, *The Traveling Salesman Problem : A Guided Tour of Combinatorial Optimization*, Wiley, New York, 1985.
[60] D. McDuff and D. Salamon, *Introduction to Symplectic Topology*, Claredon Press, Oxford, 1995.
[61] H. P. McKean, *Selberg's trace formula as applied to a compact Riemann surface*, Comm. Pure Appl. Math. **25** (1972), 225 – 246; *Correction to: "Selberg's trace formula as applied to a compact Riemann surface"*, Comm. Pure Appl. Math. **27** (1974), 134.
[62] K. Naimark and M. Solomyak, *Eigenvalue estimates for the weighted Laplacian on metric trees*, Proc. London Math. Soc. **80** (2000), 690 – 724.
[63] S. Nicaise, *Spectre des réseaux topologiques finis*, Bull. Sci. Math., II. Sér., **111** (1987), 401 – 413.
[64] S. Nicaise, *Le laplacien sur les résaux deux-dimensionnels polygonaux topologiques*, J. Math. Pures Appl., IX. Sér., **67** (1988), 93 – 113.
[65] S. P. Novikov, *Schrödinger operators on graphs and symplectic geometry*, in E. Bierstone, B. Khesin, A. Khovanskii, and J. Marsden (Eds.) "The Arnoldfest" (Proceedings of a Conference in Honour V. I. Arnold for His Sixtieth Birthday), Fields Institute Communications Series, Vol. 24, American Mathematical Society, Providence, R.I., 1999. pp. 397 – 413.
[66] D. I. Olive, *Unitarity and the evaluation of discontinuities*, Nuovo Cimento **26** (1962), 73 – 102.
[67] B. Osgood, R. Phillips, and P. Sarnak, *Compact isospectral sets of surfaces*, J. Funct. Anal. **80** (1988), 212 – 234.
[68] C. M. Papadimitriou, *Computational Complexity*, Addison-Wesley, Reading, Massachusetts, 1994.
[69] B. S. Pavlov, *The theory of extensions and explicitly solvable models*, Russian. Math. Surveys **42**:6 (1987), 127 – 168.
[70] V. Pivovarchik, *Inverse problem for the Sturm-Liouville equation on a simple graph*, SIAM J. Math. Anal. **32** (2001), 801 – 819.

[71] V. P. Potapov, *The multiplicative structure of J-contractive matrix functions*, Amer. Math. Soc. Transl., Ser. 2, **15** (1960), 131 – 243.
[72] J.-P. Roth, *Spectre du laplacien sur un graphe*, C. R. Acad. Sci. Paris, Sér. I Math. **296** (1983), 793 – 795.
[73] J.-P. Roth, *Le spectre du laplacien sur un graphe*, in G. Mokobodzki and D. Pinchon (Eds.), "Théorie du potentiel", (Proceedings of the Colloque Jacques Deny, Orsay, June 20-23, 1983), Lecture Notes in Math., Vol. 1096, Springer, Berlin, 1984. pp. 521 – 539.
[74] J. Rubinstein and M. Schatzman, *Variational problems on multiply connected thin strips. I. Basic estimates and convergence of the Laplacian spectrum*, Arch. Ration. Mech. Anal. **160** (2001), 271 – 308.
[75] Y. Saito, *The limiting equation for Neumann Laplacians on shrinking domains*, Electron. J. Differ. Equ. (2000), Paper No. 31, 25 p. `http://ejde.math.unt.edu/`
[76] Y. Saito, *Convergence of the Neumann Laplacian on shrinking domains*, Analysis **21** (2001), 171 – 204.
[77] H. Schanz and U. Smilansky, *Combinatorial identities from the spectral theory of quantum graphs*, Electron. J. Combin. **8** (2001), no. 2, Research Paper 16, 16 pp.
[78] A. Selberg, *Harmonic analysis and discontinuous groups in weakly symmetric spaces with applications to Dirichlet series*, J. Indian Math. Soc. **20** (1956), 47 – 87.
[79] M. Solomyak, *On the spectrum of the Laplacian on regular metric trees*, Waves Random Media **14** (2004), S155 – S171.
[80] B. Sz.-Nagy and C. Foias, *Harmonic Analysis of Operators on Hilbert Space*, North-Holland, Amsterdam, 1970.
[81] Traveling Salesman Problem, `http://www.tsp.gatech.edu/`.
[82] V. S. Varadarajan, *An Introduction to Harmonic Analysis on Semisimple Lie Groups*, Cambridge Studies in Advanced Mathematics, Vol. 16. Cambridge University Press, Cambridge, 1989.
[83] D. R. Yafaev, *Mathematical Scattering Theory. General Theory*, Amer. Math. Soc. Transl. of Math. Monographs Vol. 105, Providence, RI, 1992.
[84] V. Yurko, *Inverse spectral problems for Sturm-Liouville operators on graphs*, Inverse Problems **21** (2005), 1075 – 1086.
[85] S. Zelditch, *The inverse spectral problem*, in A. Grigor'yan and S.-T. Yau (Eds.) "Surveys in Differential Geometry, Vol. IX: Eigenvalues of Laplacians and Other Geometric Operators", International Press, Somerville, 2004. pp. 401 – 467.

VADIM KOSTRYKIN, INSTITUT FÜR MATHEMATIK, TECHNISCHE UNIVERSITÄT CLAUSTHAL, ERZSTRASSE 1, D-38678 CLAUSTHAL-ZELLERFELD, GERMANY
E-mail address: `kostrykin@math.tu-clausthal.de, kostrykin@t-online.de`

ROBERT SCHRADER, INSTITUT FÜR THEORETISCHE PHYSIK, FREIE UNIVERSITÄT BERLIN, ARNIMALLEE 14, D-14195 BERLIN, GERMANY
E-mail address: `schrader@physik.fu-berlin.de`