On the inverse scattering problem on branching graphs

2002 J. Phys. A: Math. Gen. 35 101

(http://iopscience.iop.org/0305-4470/35/1/309)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **35** (2002) 101–121 PII: S0305-4470(02)23537-4

On the inverse scattering problem on branching graphs

P Kurasov[1] **and F Stenberg**

Department of Mathematics, Stockholm University, 106 91 Stockholm, Sweden

E-mail: pak@matematik.su.se and kurasov@maths.lth.se

Received 30 March 2001, in final form 29 October 2001
Published 21 December 2001
Online at stacks.iop.org/JPhysA/35/101

Abstract

The inverse scattering problem on branching graphs is studied. The definition of the Schrödinger operator on such graphs is discussed. The operator is defined with real potentials with finite first momentum and using special boundary conditions connecting values of the functions at the vertices. It is shown that in general the scattering matrix does not determine the topology of the graph, the potentials on the edges and the boundary conditions uniquely.

PACS numbers: 02.30.Zz, 02.10.Ab, 03.65.Sq, 05.45.Mt

1. Introduction

The scattering problem on branching graphs has attracted the attention of many scientists [1, 20–22, 27, 28]. Recent interest in these problems is explained by possible applications of the constructed models in nanoelectronics, quantum computing and studies of quantum chaos [9, 10, 19, 36, 41, 46–48]. The models which can be obtained investigating differential operators on graphs have both features of ordinary and partial differential operators. Many of the problems can be solved exactly. Such models have already been used by physicists, a good review of such publications can be found, for example, in [33, 34, 48]. To construct such models the method of point interactions can be used, since any graph can be understood as a collection of edges joined together at point vertices [5, 6]. The main goal of this paper is to study the inverse scattering problem on such graphs. This problem can be considered as a generalization of the classical inverse scattering problem for the Schrödinger operator on the line [2, 3, 17, 23, 24, 40]. Historically the first inverse problem for this Schrödinger operator was the inverse spectral problem solved by Gelfand and Levitan [26]. The inverse eigenvalue problem on compact graphs was recently studied by Carlson [15, 16]. It appears that this problem is much more complicated than the inverse spectral problem for the Sturm–Liouville operator on an interval. Therefore one can expect that the inverse scattering problem

[1] Current address: Department of Mathematics, Lund Institute of Technology, Box 118, 221 00 Lund, Sweden.

on noncompact graphs has several new features compared with the inverse problem on the line. This problem was studied first by Gerasimenko and Pavlov [27,28] and later by Kostrykin and Schrader [33–35]. It has been shown that the inverse scattering problem can be solved for graphs having special structure. In this paper we are going to mainly consider examples of graphs that do not have such a property. Several examples of graphs having the same scattering matrix are presented. All these examples are simple, but not trivial. In order to separate trivial examples we had to reconsider the definition of the Schrödinger operator on such graphs.

The first mathematically rigorous definition of the Schrödinger operator on a branching graph was given by Gerasimenko and Pavlov [27, 28]. Let Γ be an arbitrary graph, then the Schrödinger operator in $L_2(\Gamma)$ can be defined using second-order formally symmetric differential operators acting along the edges of the graph and special boundary conditions at the vertices. All self-adjoint operators appearing in this way can be described using the extension theory for symmetric operators. It appears that the language of Lagrangian planes of the corresponding Hermitian-symplectic boundary form makes all calculations explicit [30,42]. The idea to use Hermitian-symplectic boundary forms to describe self-adjoint extensions was discussed earlier in [6, 43, 44]. This method is especially effective when applied to ordinary differential operators, in particular to point interactions [4, 12, 37]. The only difficulty that appears in this way is how to relate the boundary conditions describing self-adjoint extensions with the structure of the graph. In some sense the Hilbert space $L_2(\Gamma)$ does not depend on how the edges of graph are connected. It is the boundary conditions for the Schrödinger operator that form the graph. This problem has not attracted enough attention in the literature. Therefore section 2 is devoted to a mathematically rigorous treatment of this problem. We start with the definition of the graph, which appears to be more suitable for our applications. The family of Schrödinger operators on the graph is defined considering the minimal and maximal operators determined by the differential expression. Considering all such self-adjoint operators we concentrate our attention on the question: what type of boundary conditions can be used to describe the Schrödinger operator on a certain graph; and what conditions are related to the Schrödinger operator on its cut. To give a rigorous treatment of this problem we had to define different transformations of graphs called edge cutting, vertex cutting and decoration.

The second part of the paper is devoted to the scattering problem on the graph. After defining the scattering matrix we discuss four different inverse scattering problems, namely:

(1) Provided that the structure of the graph and the boundary conditions are known, determine the potentials v_j.
(2) Determine the topological structure of the graph from the scattering data.
(3) Provided that the topological structure of the graph and the boundary conditions at the vertices are known, determine the graph from the scattering matrix for the Laplace operator.
(4) Provided that the graph and all potentials v_j are known, determine the boundary conditions for the Schrödinger operator from its scattering matrix.

In the following we show different counter-examples to all these inverse problems. It appears that to solve the inverse problems one has to either restrict the set of admissible graphs or to enlarge the set of scattering data. These possibilities are discussed in the final section, where a conjecture is also formulated.

2. Schrödinger operators on graphs

2.1. Graph. Elementary definitions

Consider arbitrary graph as a collection of edges (lines, channels) joined in vertices (nodes). Thus we admit such examples in which more than one line may connect a given pair of points, and the two endpoints of an edge may coincide. The graphs we are going to study have a finite number of edges. Some of the edges can be infinite and such edges will be called external. The following geometrical definition of a graph will be used.

Definition 1. *The graph* $\Gamma = (\boldsymbol{E}, \boldsymbol{V})$ *consists of a finite set* $\boldsymbol{E}$ *of edges and a finite set* $\boldsymbol{V}$ *of N vertices. The edge-set* $\boldsymbol{E}$ *consists of k arbitrary finite (not degenerated) intervals* $l_j = [a_{2j-1}, a_{2j}] \subset \boldsymbol{R},\ j = 1, 2, \dots, k$ *and n arbitrary half-infinite intervals* $d_j = [a_{2k+j}, \infty) \subset \boldsymbol{R}$ *called internal and external edges respectively. The vertex-set* $\boldsymbol{V}$ *is determined by an arbitrary partition of the set* $\{a_j\}_{j=1}^{2k+n}$ *of end-points into N equivalence classes* $A_i,\ i = 1, 2, \dots, N$ *called vertices.*

In the definition each edge is considered as a subset of an individual copy of $\boldsymbol{R}$. In what follows only the lengths of the intervals will play an important role.

This definition of the graph suitable for our consideration differs slightly from the standard definition used in discrete mathematics, since:

- with every edge we associate an interval on the real line with finite or infinite length;
- two different vertices can be joined by several edges;
- some edges are infinite and therefore do not connect two vertices.

The definition of the graph we are going to use is similar to the definition of the weighted graph. One can assume that with every edge of the graph we associate some weight—the length of the corresponding interval.

Definition 2. *The number of elements in the equivalence class* A_j *is called the valency of the vertex point* A_j. *The valency of any inner point of an edge is equal to* 2. *The valency of the points will be denoted by* $\mathrm{val}\,(x)$.

Definition 3. *Two points on the graph are called equivalent,* $x_1 \sim x_2$ *if and only if, either they are endpoints and belong to the same equivalence class, or they are internal points of a certain edge and coincide:*

$$x_1 \sim x_2 \Leftrightarrow \begin{cases} \exists A_m : x_1, x_2 \in A_m \\ x_1 = x_2. \end{cases}$$

In what follows the equivalent points will be identified.

On each interval $l_j(d_j)$ the length of the subinterval connecting any two points x_1 and x_2 will be denoted by $|x_1 - x_2|$. To define the distance between two arbitrary points x_1 and x_2 on the graph consider all paths S connecting the points. By pass we mean a sequence of intervals s_j such that the endpoint of each of the intervals in the sequence is equivalent to the starting point of the following interval. The length of the pass is then given by $|S| = \sum_j |s_j|$.

Definition 4. *The length of the shortest pass connecting any two points on the graph is called the distance between the points*

$$\mathrm{dist}(x_1, x_2) = \min_{S \supset \{x_1, x_2\}} |S|. \tag{1}$$

The distance between any two equivalent points is zero and *vice versa* if the distance between two points is zero then the points are equivalent. Suppose that two points x_1 and x_2 belong to the same edge, then the distance between them is always shorter than or equal to the length of the interval $[x_1, x_2]$

$$|x_2 - x_1| \geqslant \mathrm{dist}\,(x_1, x_2).$$

Definition 5. *Two graphs* Γ *and* Γ' *are called isomorphic (isometric) if, and only if, there exists a one-to-one map* $\boldsymbol{I}$ *between* Γ *and* Γ' *which preserves the distance*

$$x_1, x_2 \in \Gamma \Rightarrow \mathrm{dist}'(\boldsymbol{I}x_1, \boldsymbol{I}x_2) = \mathrm{dist}(x_1, x_2).$$

Isomorphism between the two graphs does not preserve the vertex structure. Consider, for example, the decoration defined in the following section. The following is true:

$$a_j \sim a_l \Leftrightarrow \boldsymbol{I}a_j \sim' \boldsymbol{I}a_l.$$

The distance introduced above satisfies all axioms of the metrics and can be used to define the topological structure on the graphs. Therefore in what follows we are going to speak about topologically equivalent graphs. Two isomorphic graphs are always topologically equivalent. The inverse is false in general.

Theorem 6. *Isomorphism between the graphs preserves the valency of the points.*

Proof. Consider the strictly positive real number

$$\rho = \min_j \{|a_{2j} - a_{2j-1}|, |a'_{2j} - a'_{2j-1}|\} > 0.$$

Then for each point $x \in \Gamma$ with valency $\mathrm{val}(x)$ and any real $r : 0 < r < \rho/2$ there exist exactly $\mathrm{val}(x)$ distinct points $y_l \in \Gamma, l = 1, 2, \ldots, \mathrm{val}(x)$ with the property

$$\mathrm{dist}(x, y_l) = r.$$

Any isomorphism $\boldsymbol{I}$ maps the points y_l into $\mathrm{val}(x)$ different points on the graph Γ' with the similar property

$$\mathrm{dist}(\boldsymbol{I}x, \boldsymbol{I}y_l) = r.$$

It follows that $\mathrm{val}(\boldsymbol{I}x) \geqslant \mathrm{val}(x)$. This implies the theorem, since the roles of the points x and $\boldsymbol{I}x$ can be exchanged. □

The theorem implies that every vertex with valency $\geqslant 3$ is mapped by any isomorphism to a certain vertex with the same valency. Every vertex with valency 2 or any inner point of any edge is mapped to a vertex with valency 2 or to an inner point of a certain edge.

2.2. Surgery of graphs

One can obtain new graphs by cutting the graphs into certain subgraphs. Let us define two procedures called *edge cutting* and *vertex cutting*. These procedures play an important role in constructing Schrödinger operators on graphs. Consider an arbitrary graph

$$\Gamma = (\boldsymbol{E}, \boldsymbol{V}) = (\{l_j\}_{j=1}^k \cup \{d_i\}_{i=1}^n, \{A_j\}_{j=1}^N).$$

Let O be arbitrary internal point belonging to one of the edges, $O \in l_j$ or $O \in d_i$. Consider the case where the point O divides the edge l_j into two disjoined intervals

$$l_j = [a_{2j-1}, a_{2j}] = [a_{2j-1}, O_-] \cup [O_+, a_{2j}]$$

where $O_\pm$ denote the two points on different sides of the cut. Then *the edge-cut at the point* O *graph* is the new graph Γ' with the edges

$$[a_1, a_2], \ldots, [a_{2j-1}, O_-], [O_+, a_{2j}], \ldots, [a_{2k-1}, a_{2k}]; \{d_i\}_{i=1}^n$$

and vertices

$$A_1, A_2, \ldots, A_N, O_-, O_+$$

Figure 1. Edge cutting of graphs.

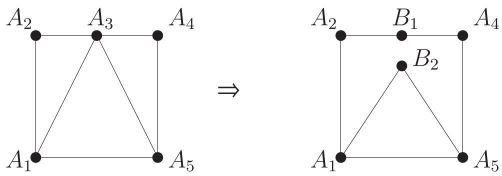

Figure 2. Vertex cutting of graphs.

where $O_\pm$ denotes the equivalence classes consisting of the points O_- and O_+.

The edge cutting procedure is illustrated by figure 1. The edge l_1 of the left graph is cut into two intervals l'_1 and l'_2.

To define vertex cutting of the graph Γ consider arbitrary decomposition of any equivalence class A_j into two disjoined subclasses B_1 and B_2

$$B_1 \cup B_2 = A_j \qquad B_1 \cap B_2 = \emptyset.$$

Then *the vertex cut graph* (at the vertex A_j) is the graph Γ' having the same edges $\{l_j\}_{j=1}^k$, $\{d_i\}_{i=1}^n$ and the following vertices:

$$A_1, A_2, \ldots, A_{j-1}, B_1, B_2, A_{j+1}, \ldots, A_N.$$

The vertex cutting procedure is illustrated by figure 2, where the graph with five vertices A_1, A_2, A_3, A_4, A_5 is chopped at the vertex A_3. The new graph has six vertices $A_1, A_2, B_1, B_2, A_4, A_5$.

Another transformation of a graph will be called *decoration* (see figure 3). Let O be an arbitrary internal point belonging to one of the edges $O \in l_j$ or $O \in d_i$. Consider the case where the point O divides the edge l_j into two intervals

$$l_j = [a_{2j-1}, a_{2j}] = [a_{2j-1}, O_-] \cup [O_+, a_{2j}]$$

where $O_\pm$ as before denotes the two points on different sides of the cut. Then *the graph decorated at the point* O is the new graph Γ' with the edges

$$[a_1, a_2], \ldots, [a_{2j-1}, O_-], [O_+, a_{2j}], \ldots, [a_{2k-1}, a_{2k}]; \{d_i\}_{i=1}^n$$

and vertices

$$A_1, A_2, \ldots, A_N, O$$

where $O = \{O_-, O_+\}$ denotes the equivalence class consisting of two points on the different sides of the cut.

It is obvious that the edge cutting can be considered as a combination of the decoration and vertex cutting.

Lemma 7. *The graph and any of its decorations are isomorphic.*

Proof. The isomorphism between these two graphs can be defined by the identical transformation mapping, in particular, the decorated edge $l_j = [a_{2j-1}, a_{2j}]$ onto the intervals $[a_{2j-1}, O_-]$ and $[O_+, a_{2j}]$ so that the point $O \in l_j$ is mapped to the equivalent points O_-, O_+. This transformation is obviously one to one and preserves the distance. □

The lemma shows that the two isomorphic graphs can have a different number of edges and vertices. In what follows two isomorphic graphs will be identified[2].

Let us define the transformation of graphs called cleaning. This transformation is the inverse one to decoration. Let Γ be any graph defined as above with the vertex A_l having valency 2. Suppose that the bivalent vertex A_l joins together the end points a_{2j} and a_{2m-1}. Then the *cleaned* graph Γ' is the graph having the following edges:

$$\{l_1, \ldots, l_{j-1}, [a_{2j-1}, a_{2j} + a_{2m} - a_{2m-1}], l_{j+1}, \ldots, l_{m-1}, l_{m+1}, \ldots, l_k\} \qquad \{d_1, \ldots, d_k\}$$

and the following vertices:

$$A_1, A_2, \ldots, A_{j-1}, A_{j+1}, \ldots, A_N.$$

The new graph has exactly one vertex and one edge less.

It is easy to see now that the cleaning of the graph and decoration are inverse transformations. Therefore any graph is isomorphic to the cleaned graph.

2.3. Hilbert space

To define the self-adjoint operator describing a one-particle Hamiltonian on the graph consider the Hilbert space of square integrable functions defined on the graph's edges:

$$\mathcal{H} = \left(\oplus \sum_{j=1}^{k} L_2[a_{2j-1}, a_{2j}] \right) \oplus \left(\oplus \sum_{i=1}^{n} L_2[a_{2k+i}, \infty) \right). \qquad (2)$$

The elements from the Hilbert space will be denoted by bold letters and the following vector notations will be used:

$$\begin{aligned} &\boldsymbol{F} = (f_1, f_2, \ldots, f_k, f_{k+1}, \ldots f_{k+n}) \in \mathcal{H} \\ &f_j \in L_2[a_{2j-1}, a_{2j}] \qquad j = 1, 2, \ldots, k \\ &f_i \in L_2[a_{2k+i}, \infty) \qquad i = k+1, k+2, \ldots, k+n. \end{aligned} \qquad (3)$$

The Hilbert space $\mathcal{H}$ is defined without taking into account the vertex structure of the graph. The same Hilbert space corresponds to graphs having the same edges, but different vertices. Even two topologically different graphs can have the same Hilbert space. The vertex structure of the graph will be used in the definition of the self-adjoint operator only. In what follows we are going to identify the Hilbert spaces corresponding to a graph and its decoration, as well as to a graph and its cutting.

Lemma 8. *The isomorphism $\boldsymbol{I} : \Gamma \to \Gamma'$ between the graphs Γ and Γ' establishes a unitary transformation between the corresponding Hilbert spaces. In other words, the transformation*

$$\begin{aligned} &\boldsymbol{U} : \mathcal{H}(\Gamma) \to \mathcal{H}(\Gamma') \\ &f \mapsto (\boldsymbol{U} f)(x) = f(\boldsymbol{I}^{-1} x) \end{aligned} \qquad (4)$$

is unitary.

[2] Using this identification we automatically consider every vertex with valency 2 as the inner point of the corresponding edge. This does not restrict the set of models as far as standard boundary conditions are concerned (see below). Boundary conditions at points with valency 2 can be considered as additional point interactions on the graph edges.

Proof. The proof follows immediately from the fact that the isomorphism preserves the distance between the points and therefore for sufficiently small $|x_1 - x_2|$ the following holds:

$$|x_1 - x_2| = |\boldsymbol{I}x_1 - \boldsymbol{I}x_2|'$$

where x_1 and x_2 are two points on the same edge. Hence the Jacobian of this transformation is trivial. □

2.4. The Hamiltonian

Consider real potentials $v_j(x)$ defined on each edge such that

$$\begin{aligned} &v_j \in L_1[a_{2j-1}, a_{2j}] \qquad j = 1, 2, \ldots, k \\ &\int_{a_{2k+i}}^{\infty} (1 + |x|)|v_j(x)|\,\mathrm{d}x < \infty \qquad j = k+1, k+2, \ldots, k+n. \end{aligned} \tag{5}$$

It will be convenient to introduce the function $\boldsymbol{V} \in L_1(\Gamma)$ defined on the graph as follows:

$$\begin{aligned} &x \in l_j \to \boldsymbol{V}(x) = v_j(x) \\ &x \in d_j \to \boldsymbol{V}(x) = v_{k+j}(x). \end{aligned}$$

The function $\boldsymbol{V}$ can be defined arbitrarily at the vertex points, since the vertices have Lebesque measure zero. Then the differential Hamilton operator is given by

$$(H\boldsymbol{F})_j = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} f_j + v_j f_j. \tag{6}$$

In the case where all potentials v_j are equal to zero, the operator H will be denoted by L and we call it the *Laplace* operator on the graph. Different self-adjoint operators can be associated with the last differential expression. The minimal operator $\boldsymbol{H}_{\min}$ determined by the last differential expression is symmetric and has the following domain:

$$\mathrm{Dom}\,(\boldsymbol{H}_{\min}) = \left(\oplus \sum_{j=1}^{k} C_0^\infty[a_{2j-1}, a_{2j}] \right) \oplus \left(\oplus \sum_{i=1}^{n} C_0^\infty[a_{2k+i}, \infty) \right).$$

Every self-adjoint extension of the minimal operator is a certain restriction of the adjoint (maximal) operator $\boldsymbol{H}_{\max}$ defined by the same differential expression on the domain

$$\mathrm{Dom}\,(\boldsymbol{H}_{\min}) = \left(\oplus \sum_{j=1}^{k} W_2^2[a_{2j-1}, a_{2j}] \right) \oplus \left(\oplus \sum_{i=1}^{n} W_2^2[a_{2k+i}, \infty) \right).$$

The functions from this domain are continuous and have a continuous first derivative on each edge. The values of the functions at the vertices are not well defined, since the functions on the edges can have different limits as x approaches the same vertex along different edges. Therefore the functions from this domain are not necessarily continuous on the whole graph. In order to define self-adjoint operators corresponding to (6) it is natural to calculate the boundary form of the maximal operator

$$\langle \boldsymbol{F}, \boldsymbol{H}_{\max}\boldsymbol{G}\rangle - \langle \boldsymbol{H}_{\max}\boldsymbol{F}, \boldsymbol{G}\rangle = \sum_{j=1}^{2k+n} \left(\bar{f}(a_j)\frac{\mathrm{d}g}{\mathrm{d}n}(a_j) - \frac{\mathrm{d}\bar{f}}{\mathrm{d}n}(a_j)g(a_j) \right) \tag{7}$$

where $\frac{\mathrm{d}}{\mathrm{d}n}$ denotes the normal derivative at the end point of the interval[3]. Then the self-adjoint operators are defined by Lagrangian planes with respect to the Hermitian-symplectic structure

[3] The normal derivatives at the vertices are defined as follows:

$$\frac{\mathrm{d}f}{\mathrm{d}n}(a_{2j-1}) = \frac{\mathrm{d}f}{\mathrm{d}x}(a_{2j-1}) \qquad j = 1, 2, \ldots, k \qquad \frac{\mathrm{d}f}{\mathrm{d}n}(a_{2j}) = -\frac{\mathrm{d}f}{\mathrm{d}x}(a_{2j}) \qquad j = 1, 2, \ldots, k$$

$$\frac{\mathrm{d}f}{\mathrm{d}n}(a_j) = \frac{\mathrm{d}f}{\mathrm{d}x}(a_j) \qquad j = 2k+1, 2k+2, \ldots, 2k+n.$$

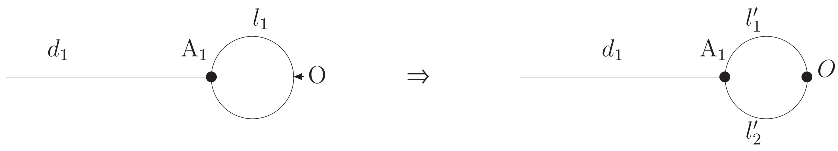

Figure 3. Decoration of graphs.

determined by the boundary form. These Lagrangian planes can be described by different boundary conditions involving the values of the functions and their normal derivatives at the vertices. Then the self-adjoint operator determined by such Lagrangian planes coincide with the restriction of the operator $\boldsymbol{H}_{\max}$ to the set of functions satisfying the boundary conditions[4]. The set of boundary conditions leading to self-adjoint operators and the relations between the Hermitian-symplectic structure and von Neumann formulae have been described in detail in [30–33] following the main ideas of [27, 28]. The same connections have been discussed in [6, 42–44].

2.5. Boundary conditions and vertex structure

Provided that the vertex structure of the graph Γ is fixed, not all symmetric boundary conditions should be allowed. The boundary conditions for the graph should respect the equivalence classes (vertices) of the endpoints. Namely the boundary conditions cannot connect the boundary values of the function at the endpoints which are not equivalent. Since the number of vertices is finite, each boundary condition respecting the vertex structure can be decomposed into the set of N independent boundary conditions at each vertex.

Let us study the set of self-adjoint boundary conditions at a vertex of degree m, i.e. a vertex joining together m edges (see figure 4).

The boundary form of the maximal operator in this case is

$$\langle \boldsymbol{F}, \boldsymbol{H}^m_{\max}\boldsymbol{G}\rangle - \langle \boldsymbol{H}^m_{\max}\boldsymbol{F}, \boldsymbol{G}\rangle = \sum_{j=1}^{m}\left(\bar{f}(a_j)\frac{\mathrm{d}g}{\mathrm{d}n}(a_j) - \frac{\mathrm{d}\bar{f}}{\mathrm{d}n}(a_j)g(a_j)\right)$$

where $\boldsymbol{H}^m_{\max} = \oplus\sum_{j=1}^{m}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + v_j\right)|_{W_2^2[a_j,\infty)}$.

Lemma 9 (lemmas 2.2 and 2.3 from [33]). *All self-adjoint extensions of the minimal operator* $\boldsymbol{H}^m_{\min}$ *are described by the boundary conditions*

$$C\begin{pmatrix} f(a_1)\\ f(a_2)\\ \dots\\ f(a_m)\end{pmatrix} = D\begin{pmatrix} f'(a_1)\\ f'(a_2)\\ \dots\\ f'(a_m)\end{pmatrix} \tag{8}$$

where C, D *are* $m \times m$ *matrices having the following properties:*

(1) The matrix (C, D) *has rank* m.
(2) The matrix CD^* *is Hermitian.*

Proof. The proof of this lemma can be deduced from lemmas 2.2 and 2.3 of [33]. □

It is clear that different matrices can define the same Lagrangian planes, since the boundary conditions can be multiplied by any invertible matrix.

[4] Another more traditional way to define the self-adjoint operator is to study the restriction of the differential operator to C_0^∞ functions and consider its self-adjoint extensions described by von Neumann formulae [11, 45].

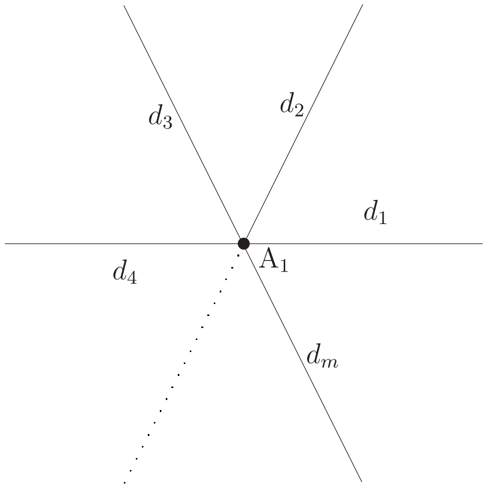

Figure 4. Star-like graph.

Consider now the case of an arbitrary finite graph. The self-adjoint boundary conditions *respecting the vertex structure* are defined by the set of N boundary conditions connecting the boundary values of the functions from the domain of the operator at equivalent endpoints. In other words with each vertex A_j we associate two matrices, C_j and D_j, having the dimension equal to the valency val (A_j) of the vertex A_j and satisfying the conditions of lemma 9:

$$C_j \begin{pmatrix} f(a_{i_1}) \\ f(a_{i_2}) \\ \dots \\ f(a_{j_{\mathrm{val}(A_j)}}) \end{pmatrix} = D_j \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}n} f(a_{i_1}) \\ \frac{\mathrm{d}}{\mathrm{d}n} f(a_{i_2}) \\ \dots \\ \frac{\mathrm{d}}{\mathrm{d}n} f(a_{j_{\mathrm{val}(A_j)}}) \end{pmatrix} \qquad \{a_{i_1}, a_{i_2}, \dots, a_{j_{\mathrm{val}(A_j)}}\} = A_j \tag{9}$$

$$j = 1, 2, \dots, N.$$

Again different boundary conditions (matrices C_j, D_j) can determine the same self-adjoint operator. All boundary conditions leading to the same self-adjoint operator will be called *equivalent*.

Let us return to the discussion of the operator $\boldsymbol{H}^m$ defined on the star-like graph. Suppose that one of the equivalent boundary conditions (8) can be written in the form

$$\begin{pmatrix} C^1 & 0 \\ 0 & C^2 \end{pmatrix} P \begin{pmatrix} f(a_1) \\ f(a_2) \\ \dots \\ f(a_m) \end{pmatrix} = \begin{pmatrix} D^1 & 0 \\ 0 & D^2 \end{pmatrix} P \begin{pmatrix} f'(a_1) \\ f'(a_2) \\ \dots \\ f'(a_m) \end{pmatrix}$$

where C^1, D^1 and C^2, D^2 are square matrices of the same rank, and P is a certain $m \times m$ permutation matrix. It is obvious that these boundary conditions correspond to the graph cut at the vertex. Really the boundary conditions can be written as (at least) two independent sets of linear equations connecting the boundary values of the functions at the endpoints belonging to two different subsets of the equivalence class describing the vertex. Such boundary conditions correspond to the graph with the vertex chopped in two.

Definition 10. *The boundary conditions (9) for the Schrödinger operator on the graph* Γ *are called nonseparable if, and only if, the graph cannot be cut to another graph* Γ' *in such a way that there exists equivalent boundary conditions which connect only the boundary values at equivalent endpoints of* Γ'.

In what follows we are going to study nonseparable boundary conditions only, since separable boundary conditions obviously correspond to a different (cut) graph. Here we follow terminology suggested in [6, 38]. The following boundary conditions are nonseparable and will be called *standard* [5]

$$\begin{aligned} & f(a_{i_1}) = f(a_{i_2}) = \cdots = f(a_{i_{\mathrm{val}(A_j)}}) \\ & \sum_{l=1}^{\mathrm{val}\,(A_j)} f'(a_{i_l}) = 0 \\ & \{a_{i_1}, a_{i_2}, \ldots, a_{i_{\mathrm{val}\,(A_j)}}\} = A_j \qquad j = 1, 2, \ldots, N. \end{aligned} \tag{10}$$

The functions satisfying these conditions have a remarkable property: they are continuous at each vertex[6]. Thus the functions from the domain described by these boundary conditions are well defined on the graph (even at the vertex points). Another important property is related to the graph's isomorphism.

Consider the star-like graph with the valency of the unique vertex equal to 2 (see figure 4, for $m = 2$). Then the corresponding standard boundary conditions at the points $a_1 \sim a_2$ are

$$f(a_1) = f(a_2) \qquad \frac{\mathrm{d}}{\mathrm{d}n} f(a_1) = -\frac{\mathrm{d}}{\mathrm{d}n} f(a_2)$$

and one can easily see that the Hilbert space

$$\mathcal{H} = L_2[a_1, \infty) \oplus L_2[a_2, \infty)$$

can be unitarily mapped to the Hilbert space $L_2(-\infty, \infty)$

$$U : f \mapsto (Uf)(x) = \begin{cases} f_1(a_1 + x) & x > 0 \\ f_2(a_2 - x) & x < 0. \end{cases}$$

The Schrödinger operator on the graph is mapped to the Schrödinger operator $\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q$ on the line with the potential $q = Uv$. The functions from the domain of the operator are continuous and have a continuous first derivative at the origin. It follows that the domain of the transformed operator is $W_2^2(\boldsymbol{R})$. This domain coincides with the domain of the unperturbed operator on the line. All other boundary conditions describe operators with certain point interactions at the origin. One can say that the vertex can be removed by this transformation provided that the functions from the domain of the operator satisfy natural boundary conditions. Any other boundary condition at the vertex lead to the Schrödinger operator with a certain point interaction at the origin [5, 6]. The above example shows that the Schrödinger operator on the graph and any of its decorations are unitarily equivalent as far as natural boundary conditions are concerned.

Theorem 11. *Two Schrödinger operators defined by standard boundary conditions on two isomorphic graphs with the isomorphism* $\boldsymbol{I}$ *are unitarily equivalent if the potentials are invariant under the isomorphism*

$$v(\boldsymbol{I}x) = v(x). \tag{11}$$

[5] These boundary conditions are described in a canonical way by the matrices

$$C = \begin{pmatrix} 1 & -1 & 0 & \ldots & 0 & 0 \\ 0 & 1 & -1 & \ldots & 0 & 0 \\ 0 & 0 & 1 & \ldots & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & 1 & -1 \\ 0 & 0 & 0 & \ldots & 0 & 0 \end{pmatrix} \qquad D = \begin{pmatrix} 0 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & 0 & \ldots & 0 & 0 \\ 0 & 0 & 0 & \ldots & 0 & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & 0 & \ldots & 0 & 0 \\ 1 & 1 & 1 & \ldots & 1 & 1 \end{pmatrix}.$$

[6] This property is always appreciated by physicists, even if it is not necessary for physical applications [48].

Proof. We have already seen that the isomorphism of two graphs establishes the unitary map between the corresponding Hilbert spaces (see lemma 8). Similar reasoning shows that $\frac{d^l}{dx^l}(\boldsymbol{U}f)(\boldsymbol{I}x) = \frac{d^l}{dx^l}f(x)$ for any sufficiently smooth function f. Using (11) one can see that the minimal operators are unitarily equivalent. Moreover the standard boundary conditions are mapped to standard boundary conditions. It follows that Schrödinger operators on isomorphic graphs are unitary equivalent. □

3. Scattering problem on graphs

3.1. Definition of the scattering matrix

The $n \times n$ scattering matrix $S(k)$, $k^2 = E$ can be defined for all energies $E > 0$ by looking at the solutions ψ^l, $1 \leqslant l \leqslant n$ of the Schrödinger equation

$$(H\Psi)_j = -\frac{d^2}{dx^2}\psi_j + v_j\psi_j = E\psi_j \tag{12}$$

satisfying the boundary conditions and having the following asymptotics:

$$\psi_j^l(x, E) = \begin{cases} s_{jl}(k)\exp(ikx) & \text{for} \quad j \neq l \\ \exp(-ikx) + s_{ll}(k)\exp(ikx) & \text{for} \quad j = l. \end{cases} \tag{13}$$

It is straightforward to show that solutions to the Schrödinger equation (12) always have asymptotics (13) (see e.g. [40]). Thus the scattering matrix is well defined. It is convenient to write the coefficients s_{jl} as the unitary $n \times n$ matrix $\boldsymbol{S}(E)$.

The scattering matrix so defined depends on the parametrization of the external edges. Really consider two isomorphic graphs Γ and Γ' with the external edges $[a_j, \infty)$, $j = 1, 2, \ldots, n$ and $[a'_j, \infty)$, $j = 1, 2, \ldots, n$ respectively. The scattering matrices for the corresponding Schrödinger operators are related by

$$\boldsymbol{S}'(E) = \mathrm{diag}\{\exp(ik(a_l - a'_l))\}\boldsymbol{S}(E)\mathrm{diag}\{\exp(ik(a_l - a'_l))\} \tag{14}$$

where S and S' are the scattering matrices corresponding to the two Schrödinger operators. Therefore in what follows two such scattering matrices will be called *similar*. The corresponding Schrödinger operators are unitary equivalent and therefore similar scattering matrices should be identified.

The size of the scattering matrix is determined by the number of external channels in the graph. The scattering matrix depends on the structure of the graph, on the boundary conditions and on the potentials appearing in the Schrödinger equation. It is clear that all this information about the graph and Schrödinger operator can be reconstructed from the scattering data only in very special situations.

Therefore the four inverse scattering problems stated in the introduction can be discussed. One of the main goals of this paper is to provide some counter-examples to the above-mentioned inverse problems.

3.2. Determining potentials

The following theorem was proven by Bargmann back in 1948 [7, 8]:

Theorem 12 (Bargmann). *The knowledge of the graph, the self-adjoint boundary conditions at the vertices and the scattering matrix* $\boldsymbol{S}$ *for the Schrödinger operator* $\boldsymbol{H}$ *is generally not enough to determine the real-valued potentials satisfying (5).*

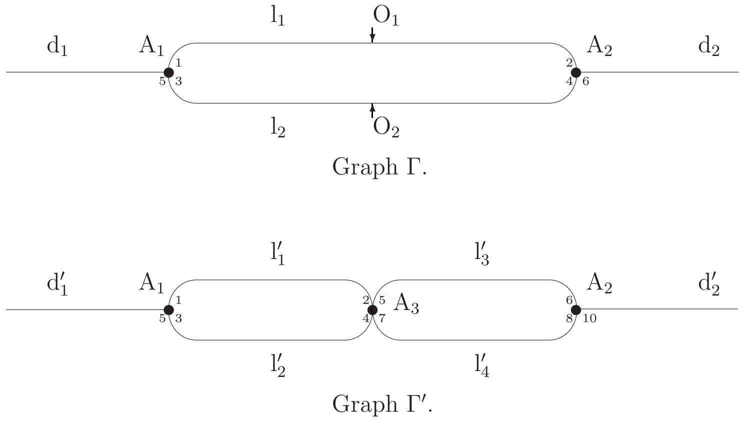

Figure 5. Two topologically different graphs having the same scattering matrix (arabic numbers indicate positions of the points a_j and a'_j).

Bargmann considered the simplest graph formed by one half-infinite edge. It was shown that the potential cannot be reconstructed uniquely from the scattering matrix only in the presence of bound states. It was shown later by Marchenko and Faddeev that in order to ensure the unique solution of the inverse problem the set of scattering data has to be enlarged in order to include the energies of the bound states and corresponding normalizing constants [2,3,23]. The corresponding problem on the whole real line was studied by the same authors [24,40]. The use of their results by Gardner *et al* [25] allows one to show that extra parameters in the solution of the inverse scattering problem are related to soliton solutions of the KdV equation. The inverse scattering problem for the star-like graph with standard boundary conditions at the vertex was studied by Gerasimenko *et al* [27, 28, 31]. The results obtained were similar to those for the inverse problem on the half-line. This inverse problem is similar to the inverse problem for the matrix Schrödinger equation on the line (see [18,29] for a comprehensive study of the problem). It was shown that as in the scalar case the Schrödinger operator is determined uniquely by the Weyl–Titchmarsh function extending results of Borg and Marchenko [13, 14, 39]. Therefore the main obstacle in solving the inverse scattering problem is the reconstruction of the Weyl–Titchmarsh function from the scattering data. The scattering matrix does not always determine the Weyl–Titchmarsh function uniquely. Nonuniqueness in the solution of this scattering problem leads to interesting connections with nonlinear partial differential equations. Similar connection can be found studying Schrödinger operators on graphs.

3.3. Topological structure

Theorem 13. *The knowledge of the scattering matrix* $\boldsymbol{S}$ *for the Laplace operator* $\boldsymbol{L}$ *described by standard boundary conditions at the vertices is generally not enough to determine the topological structure of the graph uniquely.*

Proof. Let us remind that the Laplace operator is uniquely defined by the graph if one assumes standard boundary conditions at the vertices. Consider the two graphs presented in figure 5. Suppose that the following conditions on the lengths of the edges hold:

$$\begin{aligned} |l_1| = |l_2| = |l'_1| + |l'_3| = |l'_2| + |l'_4| \\ |l'_1| = |l'_2|. \end{aligned} \qquad (15)$$

Consider the automorphism $\boldsymbol{J}$ of the graph Γ, which preserves the external edges d_1 and d_2 and exchanges the two internal edges l_1 and l_2. Such automorphisms exist, since the edges l_1 and l_2 connect the same vertices and have equal lengths. Suppose that Ψ is a scattering solution to the equation $L\Psi = E\Psi$ on the graph Γ satisfying standard boundary conditions at the vertices. Then the function $\tilde{\Psi}(x) = \Psi(\boldsymbol{J}x)$ is a solution to the same differential equation and boundary conditions. Then consider the symmetrized function

$$\Phi = \frac{1}{2}(\Psi + \tilde{\Psi})$$

which has just the same asymptotics as the function Ψ at infinity (since the components $\psi_{3,4}$ of the functions Ψ and Ψ' are equal) and satisfies the symmetry relation[7]

$$\Phi(x) = \Phi(\boldsymbol{J}x).$$

One can obtain the graph Γ' from Γ by identifying two points O_1 and O_2 from l_1 and l_2 respectively. We suppose that $|O_1 - a_1| = |O_2 - a_3| = |l_1'| \ \ (= |l_2'|)$. Let us denote by $\boldsymbol{T}$ the natural map from Γ onto Γ' which:

- maps the points $O_{1,2}$ to the vertex A_3;
- maps the external edges $d_{1,2}$ onto $d'_{1,2}$, respectively;
- maps the intervals $(a_1, O_1), (O_1, a_2), (a_3, O_2)$, and (O_2, a_4) onto the intervals $(a_1', a_2'), (a_5', a_6'), (a_3', a_4)$, and (a_7', a_8') respectively;
- preserves the distance between any two internal points of the intervals d_1, d_2, (a_1, O_1), (O_1, a_2), (a_3, O_2) and (O_2, a_4).

The symmetrized function Φ attains equal values at the points O_1 and O_2

$$\Phi(O_1) = \Phi(O_2). \tag{16}$$

Therefore one can define the function Ψ' on Γ' by the following equality:

$$\Psi'(x) = \Psi(\boldsymbol{T}^{-1}x).$$

The function Ψ' so defined satisfies the differential equation $L'\Psi' = E\Psi$ on each edge of the graph Γ'. Moreover it satisfies the standard boundary conditions at all vertices of Γ', since:

- the function Ψ satisfies standard boundary conditions at the vertices $A_{1,2}$,
- the function Ψ is continuous at the points $O_{1,2}$ and has continuous first derivative, and (16) holds.

Obviously the functions Ψ and Ψ' have exactly the same asymptotics on the external edges and therefore define equivalent scattering matrices. □

Figure 6 presents two graphs with the same scattering matrix, provided the lengths of the edges are chosen properly.

These examples are interesting, since one of the graphs (graph Γ_1) cannot be realized in $\boldsymbol{R}^2$ whereas the graph Γ_2 is planar. To see that the scattering matrices are equal one can consider the following graph of Γ presented in figure 7.

The graphs Γ_1 and Γ_2 can be obtained from the graph Γ_3 by cutting it at the vertex A_7.

[7] Considering the antisymmetrized function $F = \frac{1}{2}(\Psi - \tilde{\Psi})$ we get either a zero function, or an eigenfunction for the eigenvalue E.

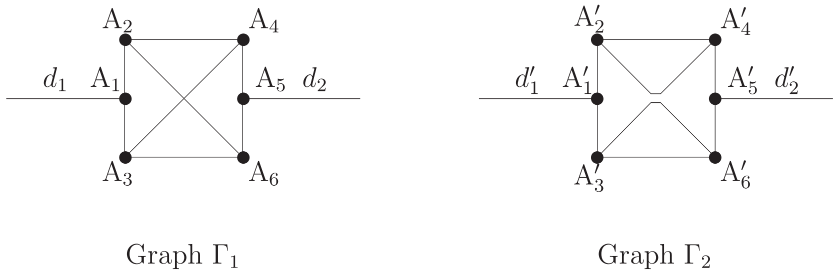

Figure 6. Planar and nonplanar graphs having equal scattering matrices.

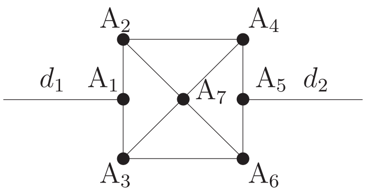

Figure 7. Graph Γ_3.

3.4. Geometrical structure

Theorem 14. *The knowledge of the topological structure of the graph and of the scattering matrix* $\boldsymbol{S}$ *for the Laplace operator* $\mathbf{L}$ *described by standard boundary conditions at the vertices is generally not enough to determine the graph uniquely (up to isomorphism).*

Proof. Consider the graph Γ' plotted in figure 5 and used in the proof of theorem 13. Since the (equal) lengths of the internal edges l'_1 and l'_2 can be chosen arbitrarily subject to the inequality $|l'_j| < |l_j|$, the same example shows that one cannot reconstruct the lengths of all edges uniquely from the scattering matrix, even if the topological structure of the graph is known. □

3.5. Boundary conditions

Sometimes it is possible to determine the boundary conditions at the vertices from the scattering matrix. Kostrykin and Shrader considered such an inverse scattering problem for the star-like graph [34] (see figure 4). It has been shown that the knowledge of the scattering matrix for one value of the energy is enough to determine the matrix in the boundary conditions (up to the equivalence described in section 2.5).

Consider the arbitrary graph Γ and the function Θ which is constant on each edge of the graph and is equal to a certain complex number having an absolute value 1 on every internal edge and is equal to 1 on the external edges:

$$\Theta|_{l_j} = \mathrm{e}^{\mathrm{i}\theta_j} \qquad \Theta|_{d_j} = 1.$$

Suppose that some of the parameters θ_j are different, then the operator of multiplication by this function maps any Schrödinger operator $\boldsymbol{H}$ on the graph to the Schrödinger operator $\Theta^{-1}\boldsymbol{H}\Theta$ defined by the same differential expression and some other boundary conditions at the vertices (since the function Θ is not continuous at the vertices). The new Schrödinger operator has just the same scattering matrix. This shows that in general the scattering matrix does not determine the boundary conditions at the vertices for the Schrödinger operator on the graph. However, the two Schrödinger operators just considered are unitarily equivalent and therefore should be identified as far as physical applications are concerned.

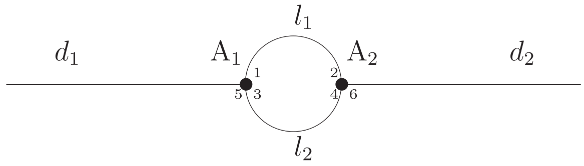

Figure 8. Graph Γ (arabic numbers indicate positions of the points a_j).

Theorem 15. *The knowledge of the graph, the real-valued potentials satisfying (5) and the scattering matrix $\boldsymbol{S}$ for the Schrödinger operator $\boldsymbol{H}$ generally is not enough to determine the Schrödinger operator uniquely (up to unitary equivalence).*

Proof. To prove the theorem consider the graph Γ plotted in figure 8.

Suppose that $|l_1| = |l_2|$. Consider the family of Laplace operators $\boldsymbol{L}_h$ on this graph determined by standard boundary conditions at the vertex A_1 and the following boundary conditions at A_2

$$\begin{aligned} & f_4(a_6) = \tfrac{1}{2}\left(f_1(a_2) + f_2(a_4)\right) \\ & \frac{\mathrm{d}}{\mathrm{d}n} f_4(a_6) = -\left(\frac{\mathrm{d}}{\mathrm{d}n} f_1(a_2) + \frac{\mathrm{d}}{\mathrm{d}n} f_2(a_4)\right) \\ & f_1(a_2) - f_2(a_4) = \frac{h}{2}\left(\frac{\mathrm{d}}{\mathrm{d}n} f_1(a_2) - \frac{\mathrm{d}}{\mathrm{d}n} f_2(a_4)\right) \end{aligned} \tag{17}$$

where $h \in \boldsymbol{R}$ is arbitrary real parameter. It is easy to see that conditions (17) determine the self-adjoint operator.

We denote by $\boldsymbol{J}$ the automorphism of the graph which preserves the external edges and maps l_1 onto l_2. The boundary conditions (17) as well as the standard boundary conditions at A_1 are invariant under this automorphism. Therefore the eigenfunctions of the operator $\boldsymbol{L}_h$ can be divided into two classes: symmetric and antisymmetric with respect to the automorphism $\boldsymbol{J}$. The antisymmetric functions are obviously equal to zero on the external edges and do not contribute to the scattering matrix at all. The symmetric eigenfunctions determine the scattering matrix for the graph Γ. The third boundary condition (17) is automatically satisfied for symmetric functions. It follows that the scattering matrix does not depend on the real parameter h. This parameter determines the discrete spectrum of antisymmetric eigenfunctions, which cannot be calculated from the scattering matrix. It is clear that the operators $\boldsymbol{L}_h$ have different discrete spectra and therefore are not unitarily equivalent. □

4. Discussion and generalizations

We have shown that the inverse scattering problem on branching graphs, in general, cannot be solved uniquely in contrast to the inverse scattering problem on the real line. It is clear that examples of different graphs having the same scattering matrices are not rare. Therefore this phenomenon has to be studied in detail. In fact all examples presented in this paper have one common feature: there exists a nontrivial automorphism $\boldsymbol{J}$ which preserves the external edges. The boundary conditions at the vertices are invariant with respect to the isomorphism. In all considered examples the isomorphism was equal to its inverse $\boldsymbol{J}^2 = \boldsymbol{I}$, where $\boldsymbol{I}$ is the trivial isomorphism. This allows one to decompose the Hilbert space $\mathcal{H}$ into the orthogonal sum of two Hilbert spaces

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$$

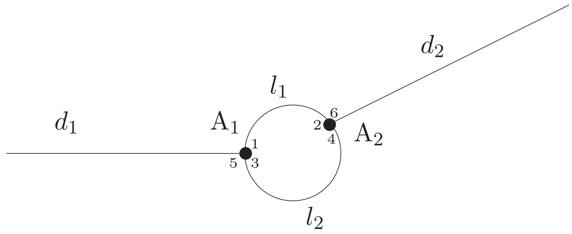

Figure 9. Non-symmetric graph (arabic numbers indicate positions of the points a_j).

if functions symmetric and antisymmetric with respect to the automorphism

$$\psi \in \mathcal{H}_\pm \Rightarrow (\boldsymbol{J}\psi) = \pm\psi.$$

In all examples the self-adjoint operator on the graph was reduced by these subspaces

$$\boldsymbol{H} = \boldsymbol{H}_+ \oplus \boldsymbol{H}_-$$

where $\boldsymbol{H}_\pm$ are self-adjoint operators in $\mathcal{H}_\pm$. Only one of the two operators had a nontrivial continuous spectrum and therefore determined the scattering matrix. It is not surprising that no information concerning the other operator could be obtained from the scattering matrix.

We would like to conclude this paper by formulating the following conjecture:

Conjecture. *Let the graph Γ be known and have no nontrivial automorphisms preserving the external edges. Then the potentials and the scattering matrix $\boldsymbol{S}$ determine the Schrödinger operator uniquely (up to unitary equivalence).*

See the appendix where one of such graphs is considered. Similar conjectures can be formulated for the other inverse scattering problems on graphs.

In [38] it was shown that the Laplace operator in an extended space can have the same scattering matrix as the Schrödinger operator. It shows that probably Schrödinger operators on graphs with complicated internal structure can have just the same scattering matrices as Schrödinger operators on simple graphs.

Acknowledgments

The first author would like to thank The Swedish Royal Academy of Sciences for financial support. The authors are grateful to J Boman for many fruitful discussions and for E von Schwerin for providing the example presented in figure 6. The authors would like to thank the referee for careful reading of the manuscript and making several suggestions leading to improvements, in particular for pointing out reference [48].

Appendix. The scattering matrix can determine the boundary conditions

We have discussed that the boundary conditions for the star-like graph can be determined by the scattering matrix. This fact is not surprising, since the size of the scattering matrix just coincides with the size of the matrix appearing in the boundary conditions. Here we consider a slightly more sophisticated example. The following graph is a generalization of the graph plotted in figure 8.

Suppose that $|l_1| \neq |l_2|$, then there is no (nontrivial) isomorphism which preserves the external edges. We are going to show that the boundary conditions at the vertices can be calculated from the scattering matrix[8]. In order to illustrate this proposition we are going to consider two examples.

Example 1. Consider the operator L_h being a generalization of the operator considered in section 3.5. It is the second derivative operator on the nonsymmetric graph Γ described by the standard boundary conditions at the point A_1 and conditions (17) at the point A_2. We are going to show that the real parameter h can be calculated from the scattering matrix.

Proposition 1. *Let L_h be the self-adjoint second derivative operator defined in $L_2(\Gamma)$ by standard boundary conditions at A_1 and h-dependent boundary conditions (17) at A_2. Then the scattering matrix determines the boundary conditions uniquely.*

Proof. To proof this proposition we are going to work with the transfer matrix instead of the scattering matrix. To define the transfer matrix consider arbitrary solution $f(k)$ to the second-order differential equation $-\frac{d^2}{dx^2} f = k^2 f$ on the edges and satisfying the boundary conditions at the vertices. Let us consider the case when k^2 does not belong to the discrete spectrum of the operator L_h. Then every solution described is just a combination of the scattering solutions and is uniquely determined by Cauchy data (function and its first derivative) at any point on the external edges. In particular, Cauchy data at point a_5, i.e. $f(k, a_5)$, $\frac{d}{dn} f(k, a_5)$ determine the solution. Then the Cauchy data at point a_6 can be calculated. The transfer matrix $T(k)$ transforms Cauchy data at point a_5 into Cauchy data at point a_6:

$$\begin{pmatrix} f_4(a_6) \\ \frac{d}{dn} f_4(a_6) \end{pmatrix} = T(k) \begin{pmatrix} f_3(a_5) \\ \frac{d}{dn} f_3(a_5) \end{pmatrix}. \tag{18}$$

The matrix $T(k)$ is uniquely determined by the scattering matrix. In fact there is a one-to-one correspondence between the sets of transfer and scattering matrices. Therefore we are going to prove that the transfer matrix for L_h determines the boundary conditions in unique way.

Let us reconstruct the solution to the second-order differential equation from its Cauchy data at point a_5. Without loss of generality let us use the following parametrization of the internal edges: $a_1 = 0, a_2 = |l_1|$ and $a_3 = 0, a_4 = |l_2|$. Then the general solution to the second order equation on the internal edges is given by

$$\begin{aligned} f_1 &= \alpha \cos kx + \beta \sin kx \\ f_2 &= \gamma \cos kx + \delta \sin kx \end{aligned}$$

where α, β, γ, and δ are constants to be determined by the boundary conditions. The parameters α and γ can be calculated from the boundary conditions at A_1

$$\begin{aligned} \alpha &= f_3(a_5) \\ \gamma &= f_3(a_5) \\ \beta k + \delta k &= -\frac{d}{dn} u_3(a_5). \end{aligned} \tag{19}$$

Then the boundary conditions at A_2 take the form

$$\begin{pmatrix} f_4(a_6) \\ \frac{d}{dn} f_4(a_6) \\ f_3(a_5)(\cos k|l_1| - \cos k|l_2|) + \beta \sin k|l_1| - \delta \sin k|l_2| \end{pmatrix}$$
$$= \begin{pmatrix} \frac{1}{2}\left(f_3(a_5)(\cos k|l_1| + \cos k|l_2|) + \beta \sin k|l_1| + \delta \sin k|l_2|\right) \\ k\left(f_3(a_5)(\sin k|l_1| + \sin k|l_2|) - \beta \cos k|l_1| - \delta \cos k|l_2|\right) \\ hk\left(-f_3(a_5)(\sin k|l_1| - \sin k|l_2|) + \beta \cos k|l_1| - \delta \cos k|l_2|\right) \end{pmatrix}.$$

[8] We would like to thank one of the referees for pointing out [48], where the transfer problem for graph Γ is investigated.

This linear system together with the last equation in (19) form the following 4×4 linear system:

$$\begin{pmatrix} \sin k|l_1|\beta + \sin k|l_2|\delta - 2f_4(a_6) \\ k\cos k|l_1|\beta + k\cos k|l_2|\delta + \frac{\mathrm{d}}{\mathrm{d}n} f_4(a_6) \\ (\sin k|l_1| - hk\cos k|l_1|)\beta + (-\sin k|l_2| + kh\cos k|l_2|)\delta \\ k\beta + k\delta \end{pmatrix}$$

$$= \begin{pmatrix} -f_3(a_5)(\cos k|l_1| + \cos k|l_2|) \\ kf_3(a_5)(\sin k|l_1| + \sin k|l_2|) \\ -f_3(a_5)(\cos k|l_1| - \cos k|l_2|) - hf_3(a_5)k(\sin k|l_1| - \sin k|l_2|) \\ -\frac{\mathrm{d}}{\mathrm{d}n} f_3(a_5) \end{pmatrix} \tag{20}$$

where $\beta, \delta, f_4(a_6)$ and $\frac{\mathrm{d}}{\mathrm{d}n} f_4(a_6)$ are unknown variables. The parameters α and δ can be determined from the last two equations, provided the determinant

$$2k\cos k\frac{|l_1| - |l_2|}{2}\left(-\sin k\frac{|l_1| + |l_2|}{2} + hk\cos k\frac{|l_1| + |l_2|}{2}\right)$$

is different from zero (which is true for almost all values of k). Only the nonspecial case will be considered in what follows. Then the two parameters are given by

$$\beta = \tan k\frac{|l_1| - |l_2|}{2} f_3(a_5) + \frac{\sin k|l_2| - hk\cos k|l_2|}{2k\cos k\frac{|l_1|+|l_2|}{2}\left(-\sin k\frac{|l_1|+|l_2|}{2} + hk\cos k\frac{|l_1|+|l_2|}{2}\right)}\frac{\mathrm{d}}{\mathrm{d}n} f_3(a_5)$$

$$\delta = -\tan k\frac{|l_1| - |l_2|}{2} f_3(a_5) + \frac{\sin k|l_1| - hk\cos k|l_1|}{2k\cos k\frac{|l_1|+|l_2|}{2}\left(-\sin k\frac{|l_1|+|l_2|}{2} + hk\cos k\frac{|l_1|+|l_2|}{2}\right)}\frac{\mathrm{d}}{\mathrm{d}n} f_3(a_5).$$

Finally $f_4(a_6)$ and $\frac{\mathrm{d}}{\mathrm{d}n} f_4(a_6)$ can be calculated from the first two equations and the transfer matrix can be determined (for all nonspecial k such that $\cos k\frac{|l_1|-|l_2|}{2} \neq 0$)

$$T(k) = \begin{pmatrix} \frac{\cos k\frac{|l_1|+|l_2|}{2}}{\cos k\frac{|l_1|-|l_2|}{2}} & \frac{\sin k|l_1|\sin k|l_2| - \frac{hk}{2}\sin k(|l_1|+|l_2|)}{2k\cos k\frac{|l_1|+|l_2|}{2}\left(-\sin k\frac{|l_1|+|l_2|}{2} + hk\cos k\frac{|l_1|+|l_2|}{2}\right)} \\ 2k\frac{\sin k\frac{|l_1|+|l_2|}{2}}{\cos k\frac{|l_1|-|l_2|}{2}} & \frac{k(-\sin k(|l_1|+|l_2|) + 2hk\cos k|l_1|\cos k|l_2|)}{2k\cos k\frac{|l_1|+|l_2|}{2}\left(-\sin k\frac{|l_1|+|l_2|}{2} + hk\cos k\frac{|l_1|+|l_2|}{2}\right)} \end{pmatrix}. \tag{21}$$

One can easily see that such two matrices corresponding to different values of the real parameter h are equal only if $\sin^2 k\frac{|l_1|-|l_2|}{2} = 0$, which holds for almost all k only if $|l_1| = |l_2|$. The last formula proves the proposition. One can see that the reason that the parameter h cannot be determined for symmetric graphs is just that the parameters β and δ determined by (20) do not depend on h and therefore the transfer matrix is independent of h as well. □

Example 2. Consider the isomorphism $\boldsymbol{P}$, which maps d_1 onto d_2 and *vice versa* and inverts the internal edges. Suppose that the boundary conditions at the vertices are invariant with respect to the chosen isomorphism. Almost all such boundary conditions can be written in the form

$$C\begin{pmatrix} f_1(a_1) \\ f_2(a_3) \\ f_3(a_5) \end{pmatrix} = \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}n} f_1(a_1) \\ \frac{\mathrm{d}}{\mathrm{d}n} f_2(a_3) \\ \frac{\mathrm{d}}{\mathrm{d}n} f_3(a_5) \end{pmatrix} \qquad C\begin{pmatrix} f_1(a_2) \\ f_2(a_4) \\ f_3(a_6) \end{pmatrix} = \begin{pmatrix} \frac{\mathrm{d}}{\mathrm{d}n} f_1(a_2) \\ \frac{\mathrm{d}}{\mathrm{d}n} f_2(a_4) \\ \frac{\mathrm{d}}{\mathrm{d}n} f_3(a_6) \end{pmatrix}$$

where C is a certain 3×3 Hermitian matrix. Let us denote the corresponding operator by L_C.

Proposition 2. *Let L_C be the second derivative operator in $L_2(\Gamma)$ determined by equal boundary conditions at the vertices. Then the operator can be reconstructed up to a unitary equivalence from its scattering matrix if $|l_1| \neq |l_2|$.*

Proof. It is obvious that one cannot calculate this matrix (having nine real parameters) from the value of the scattering matrix (which is 2×2 unitary matrix) for certain energy. Therefore we are going to use the knowledge of the scattering matrix for different values of the energy. Let us choose the parametrization on each edge so that

$$a_1 + a_2 = 0$$
$$a_3 + a_4 = 0$$
$$a_5 = a_6 = 0.$$

Consider scattering solutions which are invariant with respect to the isomorphism $\boldsymbol{P}$. Then the asymptotics of such function on the external edges is determined by the reflection coefficient

$$R(k) = s_{11}(k) + s_{21}(k).$$

The most general solution to the differential equation having these asymptotics is

$$f_1 = \alpha \cos kx$$
$$f_2 = \beta \cos kx$$
$$f_3 = f_4 = \exp(-\mathrm{i}kx) + R(k)\exp(\mathrm{i}kx)$$

where α, β are certain constants. We took into account that the function is invariant under the automorphism $\boldsymbol{P}$. Substitution into the boundary conditions gives the following equation:

$$C \begin{pmatrix} \alpha \cos k|l_1|/2 \\ \beta \cos k|l_2|/2 \\ 1 + R(k) \end{pmatrix} = \begin{pmatrix} k\alpha \sin k|l_1|/2 \\ k\beta \sin k|l_2|/2 \\ -\mathrm{i}k(1 - R(k)) \end{pmatrix}. \tag{22}$$

To prove that (22) determines the matrix C uniquely consider first the following values of k: $k_n|l_1|/2 = \pi/2 + \pi n$. The system (22) reduces to

$$c_{22}\beta \cos k_n|l_2|/2 + c_{23}(1 + R(k_n)) = k_n\beta \sin k_n|l_2|/2$$
$$c_{32}\beta \cos k_n|l_2|/2 + c_{33}(1 + R(k_n)) = -\mathrm{i}k_n(1 - R(k_n))$$

and implies that

$$-\mathrm{i}k_n \frac{1 - R(k_n)}{1 + R(k_n)} = c_{33} + \frac{|c_{23}|^2 \cos k_n|l_2|/2}{k_n \sin k_n|l_2|/2 - c_{22}\cos k_n|l_2|/2}.$$

Then the constants c_{22}, c_{33} and $|c_{23}|$ can be calculated from the last formula if $|l_1|$ and $|l_2|$ are not equal. The coefficients c_{11} and $|c_{13}|$ can be calculated similarly considering $k : k_m|l_2|/2 = \pi/2 + \pi m$. The phases of the coefficients c_{13} and c_{23} do not play any role as far as unitary equivalent Schrödinger operators are not distinguished. Therefore we can suppose that the coefficients $c_{11}, c_{13}, c_{22}, c_{23}, c_{33}$ of the Hermitian matrix C are known. The last coefficient c_{12} can be calculated substituting all known parameters into (22). We know that the system of equations

$$\begin{pmatrix} c_{11}\cos k|l_1|/2 - k\sin k|l_1|/2 & c_{12}\cos k|l_2|/2 & c_{13}(1 + R(k)) \\ \bar{c}_{12}\cos k|l_1|/2 & c_{22}\cos k|l_2|/2 - k\sin k|l_2|/2 & c_{23}(1 + R(k)) \\ c_{31}\cos k|l_1|/2 & c_{32}\cos k|l_2| & c_{33}(1 + R(k)) + \mathrm{i}k(1 - R(k)) \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ 1 \end{pmatrix} = 0$$

has a nontrivial solution. Therefore the determinant of the matrix is zero and gives an equation to calculate c_{12}. □

The proof presented here fails if $|l_1| = |l_2|$. The example considered in section 3.5 can be easily generalized to show, that in case of equal lengths the scattering matrix does not always determine the operator (up to unitary equivalence).

These examples shows that the boundary conditions at the vertices can be determined by the scattering matrix, even if the dimension of the matrix is not very high.

References

[1] Adamyan V 1992 Scattering matrices for microschemes *Operator Theory: Adv. Appl.* **59** 1–10

[2] Agranovich Z S and Marchenko V A 1957 Reconstruction of the potential energy from the scattering matrix *Usp. Mat. Nauk* **12** 143–5 (in Russian)

[3] Agranovich Z S and Marchenko V A 1963 *The Inverse Problem of Scattering Theory* (New York: Gordon and Breach) pp xiii+291

[4] Albeverio S, Dabrowski L and Kurasov P 1998 Symmetries of Schrödinger operators with point interactions *Lett. Math. Phys.* **45** 33–47

[5] Albeverio S, Gesztesy F, Høegh-Krohn R and Holden H 1988 *Solvable Models in Quantum Mechanics* (Berlin: Springer)

[6] Albeverio S and Kurasov P 2000 *Singular Perturbations of Differential Operators (London Mathematical Society Lecture Notes N271)* (Cambridge: Cambridge University Press)

[7] Bargmann V 1949 Remarks on the determination of a central field of force from the elastic scattering phase shifts *Phys. Rev.* **75** 301–3

[8] Bargmann V 1949 On the connection between phase shifts and scattering potential *Rev. Mod. Phys.* **21** 488–93

[9] Berkolaiko G and Keating J P 1999 Two-point spectral correlations for star graphs *J. Phys. A: Math. Gen.* **32** 7827–41

[10] Berkolaiko G, Bogomolny E B and Keating J P 2001 Star graphs and Seba billiards *J. Phys. A: Math. Gen.* **34** 335–50

[11] Birman M and Solomjak M 1987 *Spectral Theory of Selfadjoint Operators in Hilbert Space* (Dordrecht: Reidel)

[12] Boman J and Kurasov P 1998 Finite rank singular perturbations and distributions with discontinuous test functions *Proc. Am. Math. Soc.* **126** 1673–83

[13] Borg G 1946 Inverse problems in the theory of characteristic values of differential systems *C. R. Dixième Congrès Math. Scand.* 172–80

[14] Borg G 1952 Uniqueness theorems in the spectral theory of $y'' + (\lambda - q(x))y = 0$ *Den 11te Skandinaviske Matematikerkongress (Trondheim 1949)* 276–87 (Oslo: Johan Grundt Tanums Forlag)

[15] Carlson R 1998 Adjoint and self-adjoint differential operators on graphs *Electronic J. Diff. Eqns* **1998** 1–10 webpage http://ejde.math.swt.edu/Volumes/1998/06/abstr.html

[16] Carlson R 1999 Inverse eigenvalue problems on directed graphs *Trans. Am. Math. Soc.* **351** 4069–88

[17] Chadan K and Sabatier P C 1989 *Inverse Problems in Quantum Scattering Theory* 2nd edn (New York: Springer)

[18] Clark S, Gesztesy F, Holden H and Levitan B 2000 Borg-type theorems for matrix-valued Schrödinger operators *J. Diff. Eqns* **167** 181–210

[19] Desbois J 2000 Spectral determinant of Schrödinger operators on graphs *J. Phys. A: Math. Gen.* **33** L63–7

[20] Exner P 1996 Contact interactions on graph superlattices *J. Phys. A: Math. Gen.* **29** 87–102

[21] Exner P 1996 Weakly coupled states on branching graphs *Lett. Math. Phys.* **38** 313–20

[22] Exner P and Šeba P 1989 Free quantum motion on a branching graph *Rep. Math. Phys.* **28** 7–26

[23] Faddeev L D 1959 The inverse problem in the quantum theory of scattering *Usp. Mat. Nauk* **14** 57–119

[24] Faddeev L D 1967 Properties of the S-matrix of the one-dimensional Schrödinger equation *Am. Math. Soc. Transl.* **65** 139–66

[25] Gardner C, Green J, Kruskal M and Miura R 1967 A method for solving the Korteweg–de-Vries equation *Phys. Rev. Lett.* **19** 1095–8

[26] Gelfand I M and Levitan B M 1951 On the determination of a differential equation from its spectral function *Izv. Akad. Nauk SSSR* **15** 309–60 (in Russian) (Engl. transl. 1955 *Am. Math. Soc. Transl. Ser. 2* **1** 253–304)

[27] Gerasimenko N I and Pavlov B S 1988 Scattering problems on noncompact graphs *Teor. Mat. Fiz.* **74** 345–59 (Engl. transl. 1988 *Teor. Math. Phys.* **74** 230–40)

[28] Gerasimenko N I 1988 Inverse scattering problem on a noncompact graph *Theor. Mat. Fiz.* **75** 187–200 (Engl. transl. 1988 *Theor. Math. Phys.* **75** 460–70)

[29] Gesztesy F and Simon B 2000 On local Borg–Marchenko uniqueness results *Commun. Math. Phys.* **211** 273–87

[30] Harmer M 2000 Hermitian symplectic geometry and extension theory *J. Phys. A: Math. Gen.* **33** 9193–203

[31] Harmer M Inverse scattering for the matrix Schrödinger operator and Schrödinger operator on graphs with general self-adjoint boundary conditions *J. Aust. Math. Soc.* at press

[32] Harmer M 2000 A relation between the spectrum of the laplacean and the geometry of a compact graph *Report* 446, Department of Mathematics, The University of Auckland

[33] Kostrykin V and Schrader R 1999 Kirchoff's rule for quantum wires *J. Phys. A: Math. Gen.* **32** 595–630

[34] Kostrykin V and Schrader R 2000 Kirchoff's rule for quantum wires II: The inverse problem with possible applications to quantum computers *Fortschr. Phys.* **48** 703–16

[35] Kostrykin V and Schrader R 2001 The generalized star product and the factorization of scattering matrices on graphs *J. Math. Phys.* **42** 1563–98

[36] Kottos T and Smilansky U 1997 Quantum chaos on graphs *Phys. Rev. Lett.* **79** 4794–7
[37] Kurasov P 1996 Distribution theory for discontinuous test functions and differential operators with generalized coefficients *J. Math. Anal. Appl.* **201** 297–323
[38] Kurasov P 1992 Zero-range potentials with internal structures and the inverse scattering problem *Lett. Math. Phys.* **25** 287–97
[39] Marchenko V A 1952 Some questions of the theory of one-dimensional linear differential operators of the second order *Trudy Moscov. Mat. Obsch.* **1** 327–420 (Engl. transl. 1973 *Am. Math. Soc. Transl. Ser. 2* **101** 1–104)
[40] Marchenko V A 1986 *Sturm-Liouville Operators and Applications* (Basel: Birkhäuser) pp xii+367
[41] Melnikov Yu B and Pavlov B S 1995 Two-body scattering on a graph and application to simple nanoelectronic devices *J. Math. Phys.* **36** 2813–25
[42] Novikov S 1998 Discrete Schrödinger operators and topology *Asian J. Math.* **2** 921–34
[43] Pavlov B S 1988 Boundary conditions on thin manifolds and the semiboundedness of the three-body Schrödinger operator with point potential *Mat. Sb.* **136(178)** 163–77 (in Russian)
[44] Pavlov B S 1987 The theory of extensions, and explicitly solvable models *Usp. Mat. Nauk* **42** 99–131 247 (in Russian)
[45] Reed M and Simon B 1975 *Methods of Modern Mathematical Physics* vol 2 (New York: Academic)
[46] Schanz H and Smilansky U 1999 Spectral statistics for quantum graphs: periodic orbits and combinatorics *Preprint* chao-dyn/9904007
[47] Schenker J H and Aizenman M 2000 The creation of spectral gaps by graph decoration *Lett. Math. Phys.* **53** 253–62
[48] Xia J-B 1992 Quantum waveguide theory for mesoscopic structures *Phys. Rev.* B **45** 3593–9