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branching graphs**

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On the inverse scattering problem on branching graphs.

P.Kurasov and F.Stenberg

ABSTRACT. The inverse scattering problem on branching graphs is studied. The definition of the Schrödinger operator on such graph 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.

1. Introduction.

The scattering problem on branching graphs attracted attention of many scientists [1, 20, 21, 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, 34, 39, 44, ?]. 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. 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 the current paper is to study the inverse scattering problem on such graph. 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, 38]. Historically the first inverse problem for this Schrödinger operator was the inverse spectral problem solved by I.Gelfand and B.Levitan [26]. The inverse eigenvalue problem on compact graphs was recently studied by R.Carlson [15, 16]. It appears that this problem is much more complicated than the inverse spectral problem for Sturm-Liouville operator on an interval. Therefore one can expect that the inverse scattering problem on noncompact graphs has several new features compared with the inverse problem on the line. This problem has been studied first by N.I.Gerasimenko and B.S.Pavlov [27, 28] and later by V.Kostykin and R.Schrader [31, 32, 33]. It has been shown that the inverse scattering problem can be solved for graphs having special structure. In our paper we are going to consider mainly examples of graphs that do not have

such 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 graph.

The first mathematically rigorous definition of the Schrödinger operator on branching graph was given by N.I.Gerasimenko and B.S.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 symplectic boundary form makes all calculations explicit [40, 30]. The idea to use symplectic boundary forms to describe self-adjoint extensions has been discussed earlier in [41, 42, 6]. This method is especially effective when applied to ordinary differential operators, in particular to point interactions [4, 12, 35]. 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 did not attract enough attention in the literature. Therefore Section 2 is devoted to 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 to 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 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 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 what follow we show different counterexamples to all these inverse problems. It appears that to solve the inverse problems one has to either to restrict the set of admissible graphs or to enlarge the set of scattering data. These possibilities are discussed in the last section, where one conjecture is formulated as well.

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 tend to infinity. Such edges will be called external. The following geometrical definition of a graph will be used.

DEFINITION 1. The graph $\Gamma = (\mathbf{E}, \mathbf{V})$ consists of a finite set \mathbf{E} of edges and a finite set \mathbf{V} of N vertices. The edge-set \mathbf{E} consists of k arbitrary finite (not degenerated) intervals $l_j = [a_{2j-1}, a_{2j}] \subset \mathbf{R}$, $j = 1, 2, \dots, k$ and n arbitrary half-infinite intervals $d_j = [a_{2k+j}, \infty) \subset \mathbf{R}$ called **internal** and **external edges** respectively. The vertex-set \mathbf{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 a individual copy of \mathbf{R} . In what follows only the lengths of the intervals will play 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 the edges is equal to 2. The valency of the points will be denoted by $\text{val}(x)$.

DEFINITION 3. Two points on the graph are called **equivalent**, $x_1 \sim x_2$ if and only if either they are end points 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 end point 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

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

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 $[x_1, x_2]$

$$|x_2 - x_1| \geq \text{dist}(x_1, x_2).$$

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

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

Isomorphism between the two graphs does not preserve the vertex structure. Consider e.g. decoration defined in the following section. The following is true

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

The distance introduced above satisfy all axioms of the metrics and can be used to define topological structure on 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 valency of the points.*

PROOF. Consider 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 $\text{val}(x)$ and any real $r : 0 < r < \rho/2$ there exist exactly $\text{val}(x)$ distinct points $y_l \in \Gamma, l = 1, 2, \dots, \text{val}(x)$ with the property

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

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

$$\text{dist}(\mathbf{I}x, \mathbf{I}y_l) = r.$$

It follows that $\text{val}(\mathbf{I}x) \geq \text{val}(x)$. This implies the theorem, since the roles of the points x and $\mathbf{I}x$ can be exchanged. \square

The theorem implies that every vertex with valency ≥ 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 important role in constructing Schrödinger operators on graphs. Consider an arbitrary graph

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

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 disjointed 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 shores of the cut. Then **the edge-cut at the point O graph** is the new graph Γ' with the edges

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

and vertices

$$A_1, A_2, \dots, A_N, o_-, o_+,$$

where O_{\pm} denote the equivalence classes consisting of the points o_- and o_+ .

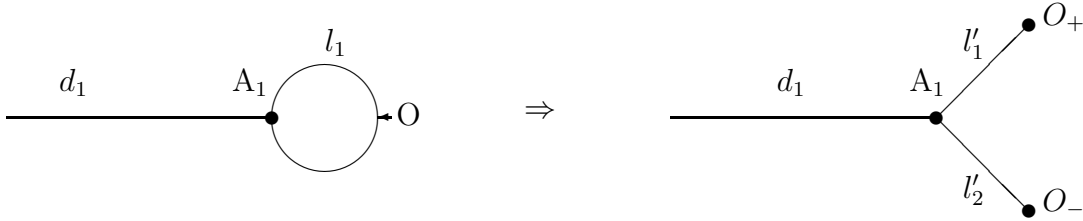


Fig.1 Edge cutting of graphs.

The edge cutting procedure is illustrated by Fig.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 disjoint subclasses B_1 and B_2

$$B_1 \cup B_2 = A_j, \quad B_1 \cap B_2 = \emptyset.$$

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

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

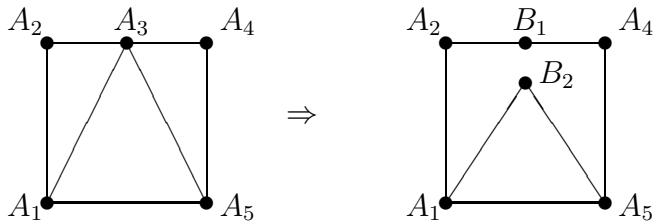


Fig.2 Vertex cutting of graphs.

The vertex cutting procedure is illustrated by Fig.2, where the graph with 5 vertices A_1, A_2, A_3, A_4, A_5 is chopped at the vertex A_3 . The new graph has 6 vertices $A_1, A_2, B_1, B_2, A_4, A_5$.

Another one transformation of a graph will be called **decoration**. 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 intervals

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

where O_{\pm} as before denote the two points on different shores of the cut. Then **the decorated at the point O graph** is the new graph Γ' with the edges

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

and vertices

$$A_1, A_2, \dots, A_N, O$$

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



Fig.3 Decoration of graphs.

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 its decoration 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 obviously is one-to-one and preserves the distance. \square

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

Let us define the transformation of graphs called cleaning. This transformation is 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

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

and the following vertices

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

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 one particle Hamiltonian on the graph consider the Hilbert space of square integrable functions defined on the graph's edges

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

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

$$\mathbf{F} = (f_1, f_2, \dots, f_k, f_{k+1}, \dots, f_{k+n}) \in \mathcal{H}; \\ f_j \in L_2[a_{2j-1}, a_{2j}], \quad j = 1, 2, \dots, k; \\ f_i \in L_2[a_{2k+i}, \infty), \quad i = k+1, k+2, \dots, k+n. \quad (3)$$

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 $\mathbf{I} : \Gamma \rightarrow \Gamma'$ between the graphs Γ and Γ' establishes a unitary transformation between the corresponding Hilbert spaces. In other words, the transformation*

$$\mathbf{U} : \mathcal{H}(\Gamma) \rightarrow \mathcal{H}(\Gamma') \\ f \mapsto (\mathbf{U}f)(x) = f(\mathbf{I}^{-1}x) \quad (4)$$

is unitary.

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

$$|x_1 - x_2| = |\mathbf{I}x_1 - \mathbf{I}x_2|',$$

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

2.4. The Hamiltonian. Consider real potentials $v_j(x)$ defined on each edge such that

$$\begin{aligned} v_j &\in L_1[a_{2j-1}, 2j], \quad j = 1, 2, \dots, k; \\ \int_{a_{2k+i}}^{\infty} (1 + |x|)|v_j(x)|dx &< \infty, \quad j = k + 1, k + 2, \dots, k + n. \end{aligned} \quad (5)$$

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

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

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

$$(\mathbf{H}\mathbf{F})_j = -\frac{d^2}{dx^2}f_j + v_j f_j. \quad (6)$$

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

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

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

$$\text{Dom}(\mathbf{H}_{\max}) = \left(\bigoplus_{j=1}^k W_2^2[a_{2j-1}, a_{2j}] \right) \oplus \left(\bigoplus_{i=1}^n W_2^2[a_{2k+i}, \infty) \right).$$

The functions from this domain are continuous and have 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

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

where $\frac{d}{dn}$ denotes the normal derivative at the end point of the interval.¹ Then the self-adjoint operators are defined by Lagrangian planes with respect to the symplectic structure 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 plane coincides with the restriction of the operator \mathbf{H}_{\max} to the set of functions satisfying the boundary conditions.² The set of boundary conditions leading to self-adjoint operators and the relations between the symplectic structure and von Neumann formulas have been described in details in [31, 30] following the main ideas of [27, 28]. The same connection have been discussed in [40, 41, 42, 6].

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 end points. Namely the boundary conditions cannot connect the boundary values of the function at the end points 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. vertex joining together m edges (see Fig.4).

¹The normal derivatives at the vertices are defined as follows

$$\begin{aligned} \frac{df}{dn}(a_{2j-1}) &= \frac{df}{dx}(a_{2j-1}), \quad j = 1, 2, \dots, k; & \frac{df}{dn}(a_{2j}) &= -\frac{df}{dx}(a_{2j}), \quad j = 1, 2, \dots, k; \\ \frac{df}{dn}(a_j) &= \frac{df}{dx}(a_j), \quad j = 2k+1, 2k+2, \dots, 2k+n. \end{aligned}$$

²Another 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 formulas [11, 43].

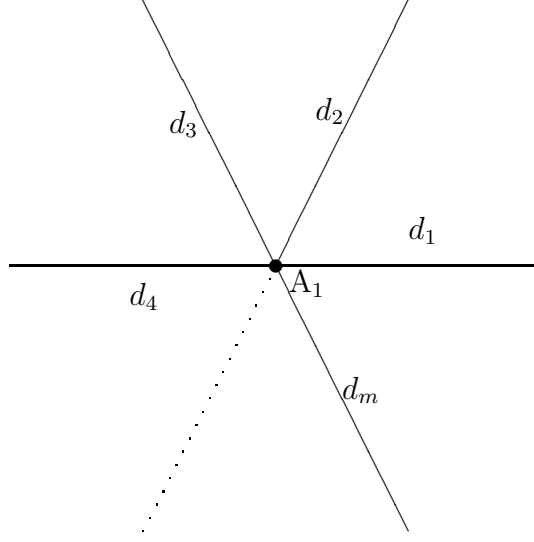


Fig.4 Star-like graph.

The boundary form of the maximal operator in this case is

$$\langle \mathbf{F}, \mathbf{H}_{\max}^m \mathbf{G} \rangle - \langle \mathbf{H}_{\max}^m \mathbf{F}, \mathbf{G} \rangle = \sum_{j=1}^m \left(\bar{f}(a_j) \frac{dg}{dn}(a_j) - \frac{d\bar{f}}{dn}(a_j) g(a_j) \right),$$

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

LEMMA 9. (Lemmas 2.2 and 2.3 from [31]) All self-adjoint extensions of the minimal operator \mathbf{H}_{\min}^m are described by the boundary conditions

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

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 [31]. \square

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

Consider now the case of 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 end points. In other words with each vertex A_j we associate two matrices C_j and D_j having the dimension equal to the valency $\text{val}(A_j)$ of the vertex A_j and satisfying the conditions of Lemma 9

$$C_j \begin{pmatrix} f(a_{i_1}) \\ f(a_{i_2}) \\ \dots \\ f(a_{j_{\text{val}(A_j)}}) \end{pmatrix} = D_j \begin{pmatrix} \frac{d}{dn} f(a_{i_1}) \\ \frac{d}{dn} f(a_{i_2}) \\ \dots \\ \frac{d}{dn} f(a_{j_{\text{val}(A_j)}}) \end{pmatrix}, \quad \{a_{i_1}, a_{i_2}, \dots, a_{j_{\text{val}(A_j)}}\} = A_j,$$

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

(9)

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 back to the discussion of the operator \mathbf{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 corresponds 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 end points belonging to two different subsets of the equivalence class describing the vertex. Such boundary conditions corresponds to the graph with the vertex chopped into 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 exist equivalent boundary conditions which connect only the boundary values at equivalent end points 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 [36, 6]. The following boundary conditions are nonseparable and will be called **standard** ³

$$\left\{ \begin{array}{l} f(a_{i_1}) = f(a_{i_2}) = \dots = f(a_{i_{\text{val}(A_j)}}) \\ \sum_{l=1}^{\text{val}(A_j)} f'(a_{i_l}) = 0, \\ \{a_{i_1}, a_{i_2}, \dots, a_{i_{\text{val}(A_j)}}\} = A_j, \quad j = 1, 2, \dots, N. \end{array} \right. \quad (10)$$

The functions satisfying these conditions have remarkable property: they are continuous at each vertex.⁴ 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 graph's isomorphism.

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

$$f(a_1) = f(a_2), \quad \frac{d}{dn}f(a_1) = -\frac{d}{dn}f(a_2),$$

and one 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 $\frac{d^2}{dx^2} + q$ on the line with the potential $q = Uv$. The functions from the domain of the operator are continuous and have continuous first derivative at the origin. It follows that the domain of the transformed operator is $W_2^2(\mathbf{R})$. 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

³These boundary conditions are described in canonical way by the matrices

$$C = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -1 & \dots & 0 & 0 \\ 0 & 0 & 1 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 1 & -1 \\ 0 & 0 & 0 & \dots & 0 & 0 \end{pmatrix}; D = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & 0 & 0 & \dots & 0 & 0 \\ 1 & 1 & 1 & \dots & 1 & 1 \end{pmatrix}$$

⁴This property is always appreciated by physicists, even if it is not necessary for physical applications.

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 its decoration are unitary 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 \mathbf{I} are unitary equivalent if the potentials are invariant under the isomorphism*

$$v(\mathbf{I}x) = v(x). \quad (11)$$

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 $\frac{d^l}{dx^l}(\mathbf{U}f)(\mathbf{I}x) = \frac{d^l}{dx^l}f(x)$ for any sufficiently smooth function f . Using (11) one can see that the minimal operators are unitary equivalent. Moreover the standard boundary conditions are mapped to standard boundary conditions. It follows that the Schrödinger operators on the isomorphic graphs are unitary equivalent. \square

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 , $1 \leq l \leq n$ of the Schrödinger equation

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

satisfying the boundary conditions and having the following asymptotics

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

It is straightforward to show that solutions to the Schrödinger equation (12) always have asymptotics (13) (see e.g. [38]). Thus the scattering matrix is well defined. It is convenient to write the coefficients s_{jl} as unitary $n \times n$ matrix $\mathbf{S}(E)$.

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 $[a_j, \infty)$, $j = 1, 2, \dots, n$ and $[a'_j, \infty)$, $j = 1, 2, \dots, n$ respectively. The the scattering matrices for the corresponding Schrödinger operators are

related by

$$\mathbf{S}'(E) = \text{diag}\{\exp(ik(a_l - a'_l))\} \mathbf{S}(E) \text{diag}\{\exp(ik(a_l - a'_l))\}, \quad (14)$$

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 Introduction can be discussed. One of the main goals of the present paper is to provide some counterexamples to the above mentioned inverse problems.

3.2. Determining potentials. The following theorem was proven by V.Bargmann back in 1948 [7, 8]:

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

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 V.A.Marchenko and L.D.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, 38]. The use of their results by J.Green, C.Gardner, M.Kruskal and R.Miura [25] allows to show that extra parameters in the solution of the inverse scattering problem are related to soliton solutions of KdV equation. The inverse scattering problem for the star-like graph with standard boundary conditions at the vertex was studied by N.Gerasimenko and B.Pavlov [27, 28]. 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 matrix Schrödinger equation on the line (see [18, 29] for comprehensive study of the problem). It was shown that as in scalar case the Schrödinger operator is determined uniquely by the Weyl-Titchmarsh function extending results of G.Borg and V.A.Marchenko [13, 14, 37]. 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 \mathbf{S} for the Laplace operator \mathbf{L} described by standard boundary conditions at the vertices generally is 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 by Fig.5. Suppose that the following conditions on the lengths of the edges hold

$$\begin{aligned} |l_1| &= |l_2| = |l'_1| + |l'_3| = |l'_2| + |l'_4|, \\ |l'_1| &= |l'_2|. \end{aligned} \tag{15}$$

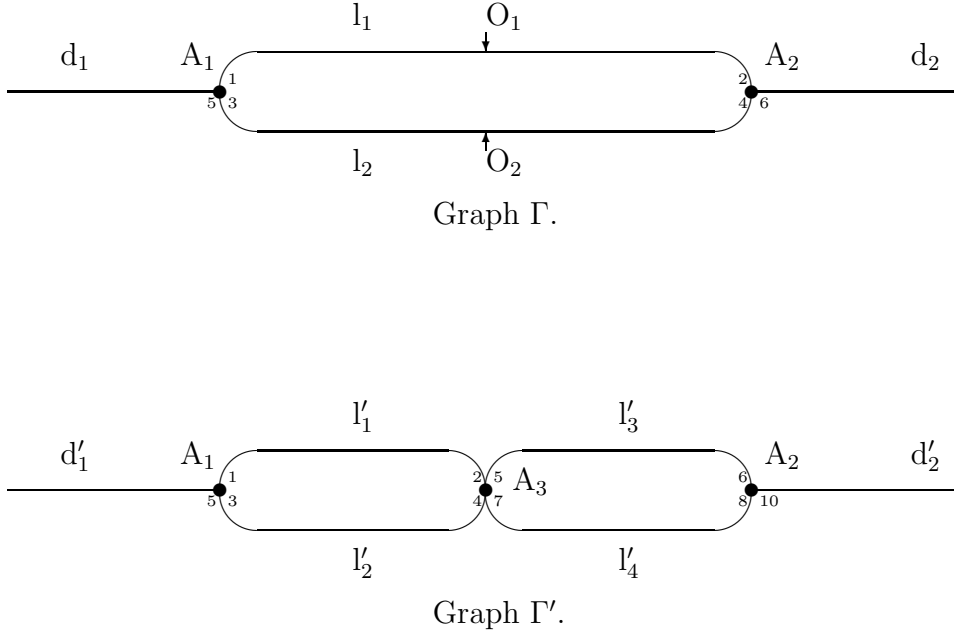


Fig.5 Two topologically different graphs having the same scattering matrix.

(Arabic numbers indicate positions of the points a_j and a'_j .)

Consider the automorphism \mathbf{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 automorphism exists, 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 $\tilde{\Psi}(x) = \Psi(\mathbf{J}x)$ is a solution to the same differential equation and boundary conditions. Consider then the symmetrized function

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

which has just the same as the function Ψ asymptotics at infinity (since the components $\psi_{3,4}$ of the functions Ψ and Ψ' are equal) and satisfies the symmetry relation⁵

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

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 $|O_1 - a_1| = |O_2 - a_3| = |l'_1|$ ($= |l'_2|$).

⁵Considering the antisymmetrized function $F = \frac{1}{2} (\Psi - \tilde{\Psi})$ we get either a zero function, or an eigenfunction for the eigenvalue E .

Let us denote by \mathbf{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

$$\Phi(O_1) = \Phi(O_2). \quad (16)$$

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

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

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. \square

The following figure presents two graphs with the same scattering matrix, provided the lengths of the edges are chosen properly.

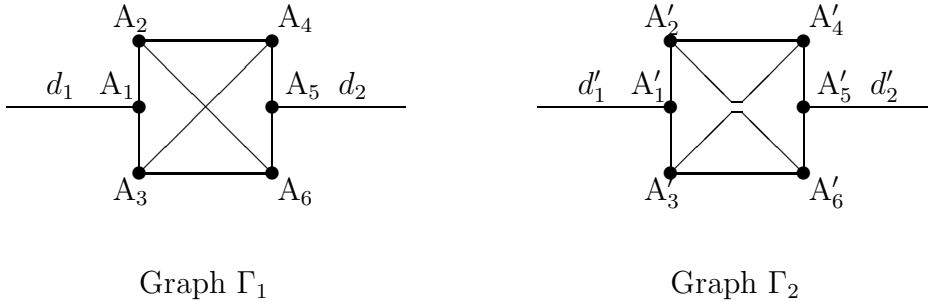
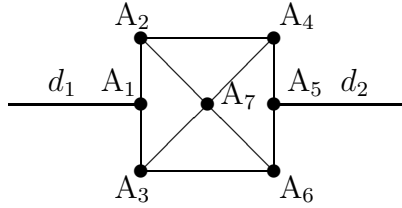


Fig.6 Planar and nonplanar graphs
 having equal scattering matrices.

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


 Fig.7 Graph Γ_3 .

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

3.4. Geometrical structure.

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

PROOF. Consider the graph Γ' plotted in Fig.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 arbitrary 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. \square

3.5. Boundary conditions. Sometimes it is possible to determine the boundary conditions at the vertices from the scattering matrix. V.Kostykin and R.Shrader considered such inverse scattering problem for the star-like graph [32] (see Fig.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 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 absolute value 1 on every internal edge and is equal to 1 on the external edges:

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

Suppose that some of the parameters θ_j are different, then the operator of multiplication by this function maps any Schrödinger operator \mathbf{H} on the graph

to the Schrödinger operator $\Theta^{-1}\mathbf{H}\Theta$ 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. But the two Schrödinger operators just considered are unitary equivalent and therefore should be identified as far as physical applications are concerned.

THEOREM 15. *The knowledge of the graph, real valued potentials satisfying (5) and scattering matrix \mathbf{S} for the Schrödinger operator \mathbf{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 Fig.8.

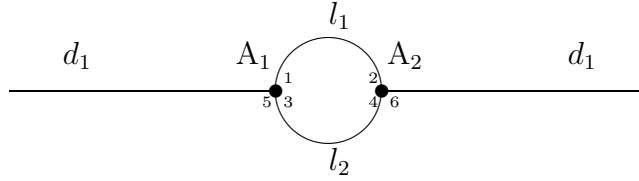


Fig.8 Graph Γ .

(Arabic numbers indicate positions of the points a_j .)

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

$$\begin{cases} f_4(a_6) = \frac{1}{2} (f_1(a_2) + f_2(a_4)) \\ \frac{d}{dn} f_4(a_6) = - \left(\frac{d}{dn} f_1(a_2) + \frac{d}{dn} f_2(a_4) \right) \\ \frac{d}{dn} f_1(a_2) - \frac{d}{dn} f_2(a_4) = h (f_1(a_2) - f_2(a_4)) \end{cases} \quad (17)$$

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

We denote by \mathbf{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 \mathbf{L}_h can be divided onto two classes: symmetric and antisymmetric with respect to the automorphism \mathbf{J} . The antisymmetric functions are obviously equal to zero on the external edges and do not contribute to the scattering matrix et 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 \mathbf{L}_h have different discrete spectra and therefore are not unitary equivalent. \square

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 details. In fact all examples presented in current article have one common feature: There exists a nontrivial automorphism \mathbf{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 $\mathbf{J}^2 = \mathbf{I}$, where \mathbf{I} is the trivial isomorphism. This allows one to decompose the Hilbert space \mathcal{H} into the orthogonal sum of two Hilbert spaces

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

if functions symmetric and antisymmetric with respect to the automorphism

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

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

$$\mathbf{H} = \mathbf{H}_+ \oplus \mathbf{H}_-,$$

where \mathbf{H}_\pm are self-adjoint operators in \mathcal{H}_\pm . Only one of the two operators had 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 finish the article by formulating the following

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

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

In [36] 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.

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Appendix A. 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. We consider here a little bit more sophisticated example. The following graph is a generalization of the graph plotted in Fig.8

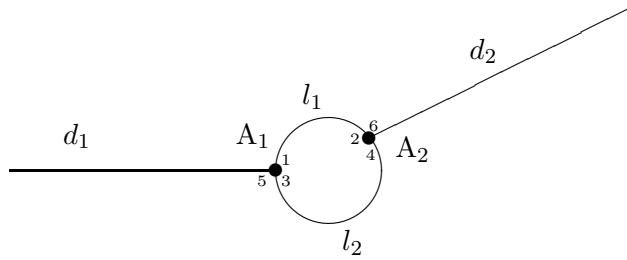


Fig.9 Non-symmetric graph.

(Arabic numbers indicate positions of the points a_j .)

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. Consider the isomorphism \mathbf{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

$$C \begin{pmatrix} f_1(a_1) \\ f_2(a_3) \\ f_3(a_5) \end{pmatrix} = \begin{pmatrix} \frac{d}{dn} f_1(a_1) \\ \frac{d}{dn} f_2(a_3) \\ \frac{d}{dn} f_3(a_5) \end{pmatrix}, \quad C \begin{pmatrix} f_1(a_2) \\ f_2(a_4) \\ f_3(a_6) \end{pmatrix} = \begin{pmatrix} \frac{d}{dn} f_1(a_2) \\ \frac{d}{dn} f_2(a_4) \\ \frac{d}{dn} f_3(a_6) \end{pmatrix}$$

where C is a certain 3×3 Hermitian matrix to be determined. It is obvious that one cannot calculate this matrix (having 9 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

$$\begin{aligned} a_1 + a_2 &= 0, \\ a_3 + a_4 &= 0, \\ a_5 = a_6 &= 0. \end{aligned}$$

Consider scattering solutions which are symmetric with respect to the isomorphism \mathbf{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 this asymptotics is

$$\begin{cases} f_1 = \alpha \cos kx \\ f_2 = \beta \cos kx \\ f_3 = f_4 = \exp(-ikx) + R(k) \exp(ikx) \end{cases},$$

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

$$C \begin{pmatrix} \alpha \cos k|l_1|/2 \\ \beta \cos k|l_2|/2 \\ 1 + R(k) \end{pmatrix} = \begin{pmatrix} k\alpha \sin k|l_1|/2 \\ k\beta \sin k|l_2|/2 \\ -ik(1 - R(k)) \end{pmatrix}. \quad (18)$$

To prove that (18) determines the matrix C uniquely consider first the following values of k : $k_n|l_1|/2 = \pi/2 + \pi n$. The system (18) reduces to

$$\begin{aligned} c_{22}\beta \cos k_n|l_2|/2 + c_{23}(1 + R(k_n)) &= k_n\beta \sin k_n|l_2|/2 \\ c_{32}\beta \cos k_n|l_2|/2 + c_{33}(1 + R(k_n)) &= -ik_n(1 - R(k_n)) \end{aligned}$$

and implies that

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

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 rationally dependent. 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 (18). We know that the system of equations

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

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

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