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Symmetries of quantum graphs and the inverse scattering problem

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Abstract

The Schrödinger equation on a graph together with a set of self-adjoint boundary conditions at the vertices determine a quantum graph. If the graph has one or more infinite edges one can associate a scattering matrix to the quantum graph. It is proved that if such a graph has internal symmetries then the boundary conditions, and hence the self-adjoint operator describing the quantum system, in general cannot be reconstructed from the scattering matrix. In addition it is shown that if the Schrödinger operator possesses internal symmetry then there exists a different quantum graph associated with the same scattering matrix.

Keywords: Quantum graph; Schrödinger operator; Inverse scattering problem

1. Introduction

Mathematical theory of differential operators on graphs is a rapidly developing area of modern mathematical physics, whose importance is explained by possible applications to solid state physics and nanoelectronics in particular. A metric graph together with second order self-adjoint differential operators defined on the graph's edges is usually called a

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quantum graph. Such a collection of differential operators is a natural generalization of the one-dimensional Schrödinger operator and can be applied to describe the motion of a quantum particle along the graph. A self-adjoint operator on a given metric graph is determined by differential operators on the edges and certain boundary conditions at the vertices. The differential operators describe the movement of the quantum particle along the edges. The boundary conditions determine the transition probabilities across the vertices. From the mathematical point of view these operators are interesting, building a certain class of problems lying between ordinary and partial differential operators. To study spectral and scattering problems for quantum graphs methods developed originally for both ordinary and partial differential equations have to be applied.

Scattering problems for quantum graphs are of great importance for applications. In fact the scattering matrix is formed by transition coefficients between different not necessarily directly connected edges. To define the scattering problem one divides the edges into two classes: external and internal edges. The latter form the compact part of the quantum graph corresponding to a nanoelectronic device. The external edges can be seen as infinite wires attached to such a device. Then the scattering matrix associated with the external edges contains essentially all information that can be measured in an experiment and is the main characteristic of a quantum graph. In this context the inverse scattering problem is to reconstruct the quantum graph from the scattering matrix. It has been proven that this reconstruction in general is not unique [22]. Explicit examples of quantum graphs have been given showing that neither the potentials on the edges, the lengths of the edges, nor the topological type of the graph can be determined from the scattering matrix. All these examples presenting different operators having the same scattering matrix are based on symmetries of the underlying graph. On the other hand it was shown using the trace formula approach that the quantum graph is uniquely determined by the scattering matrix if the lengths of the edges are rationally independent [15]. The main goal of the present article is to show that for any quantum graph having internal symmetries (symmetries preserving the external edges) there is another quantum graph having the same scattering matrix. It is clear that any graph having non-trivial internal symmetries necessarily has edges of the same length and therefore our result narrows the gap between the results of [22] and [15].

Description of the recent developments in the theory of quantum graphs can be found in [20]. Differential operators on graphs were first considered in the 80s by N.I. Gerasimenko, B.S. Pavlov [13,14], and Y. Colin de Verdière [7,8]. Several physically relevant models were considered by P. Exner and P. Seba [11,12]. The corresponding problem for discrete operators has been studied recently by S.P. Novikov [23]. It was shown that the boundary conditions at the vertices can be described via Lagrangian subspaces for the symplectic boundary form corresponding to the maximal operator associated with the formal differential operator [16,23] (see, e.g., (3)). The idea to use hermitian-symplectic boundary forms to describe self-adjoint extensions of symmetric operators has been discussed earlier in a more general context [3,9,10,24]. These methods were developed first for ordinary differential operators [9,10] and for Hamiltonians with point interactions [2–4,21,24]. Numerous possible applications of quantum graphs to the theory of nanoelectronic devices [1] caused an explosion of publications in this area in the recent years. V. Kostrykin and R. Schrader [18] presented the most general boundary conditions leading to self-adjoint operators on graphs. The relations between the boundary conditions and the structure of the graph are discussed in detail in [22].

The inverse scattering and spectral problems were first addressed in [13,14], where the inverse scattering problem on a star-shaped graph was studied using the generalized Marchenko equation. Reconstruction of the boundary conditions from the scattering matrix was studied in [19]. Special cases of inverse problems have been discussed also in [5, 6,17,19]. In the current article we develop ideas from [22] and [15] as described above.

2. Geometry of quantum graphs

In this section we will give a definition of graph which is very close to the notion of metric, or weighted graph.

Definition 1. A graph $\Gamma = \Gamma(\mathbf{E}, \sigma)$ consists of a finite set $\mathbf{E}$ of finite or semi-infinite closed intervals E_j, called edges, and a partition σ of the set $\mathbf{A}$ of endpoints of edges, $\mathbf{A} = \bigcup A_i$. The equivalence classes A_i will be called vertices, and the number of elements of A_i will be called the valence of A_i. The finite and semi-infinite intervals will be called internal and external edges, respectively.

Specifically, if there are n external and k internal edges, the set $\mathbf{A}$ of endpoints has $n + 2k$ elements. The number of equivalence classes (vertices) A_i will be denoted by N.

Definition 2. A permutation J of the set $\mathbf{A}$ of endpoints will be called an *automorphism* of Γ if

(1) J is consistent with the vertex structure in the sense that the equivalence relation induced by the partition σ of $\mathbf{A}$ is preserved by J, and
(2) the pair of endpoints of any edge are mapped to the pair of endpoints of an edge with the same length.

The automorphism is called non-trivial if the permutation J (as a permutation on $\mathbf{A}$) is different from the identity.

Definition 3. A graph Γ is called *symmetric* if and only if there exists a non-trivial automorphism of Γ in the sense of Definition 2. If the automorphism preserves all external edges then we say that the graph has *internal symmetry*.

Example 1. Γ consists of one external edge E_0 with endpoint a and one internal edge $E_1 = [b, c]$, and there is just one vertex $\{a, b, c\}$. See Fig. 1. Let J be the permutation $b \leftrightarrow c$ which leaves a invariant and permutes b and c. Clearly J satisfies (1) and (2) and J is non-trivial. Intuitively J leaves E_0 invariant and changes the orientation of E_1.

Example 2. Γ consists of one external edge E_0 with endpoint a and three internal edges $E_j = [b_j, c_j]$, $j = 1, 2, 3$, where $|E_1| = |E_3|$. The vertices are the three equivalence classes

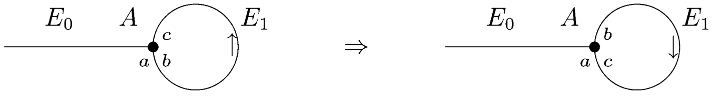

Fig. 1. Non-trivial internal symmetry.

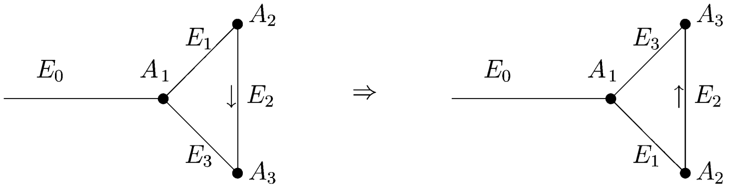

Fig. 2. Non-trivial internal symmetry.

$\{a, b_1, c_3\}$, $\{c_1, b_2\}$, $\{c_2, b_3\}$. See Fig. 2. Let J be the permutation $b_1 \leftrightarrow c_3$, $c_1 \leftrightarrow b_3$, $b_2 \leftrightarrow c_2$. Then J is non-trivial, and can be viewed as the automorphism which permutes the edges E_1 and E_3 and reverses the orientation of E_2.

A *weighted* graph is a (combinatorial) graph with a positive number associated to each edge. To any graph in the sense of Definition 1 one can associate a weighted graph by associating to each edge its length. The automorphism considered in Example 1 becomes trivial if the graph is considered as a weighted graph. Our motivation behind Definition 1 was that we wanted any graph containing a loop to have internal symmetry in order to make our theorems applicable to such graphs.

When considering functions on the graph Γ we shall identify Γ with the disjoint union $\widetilde{\Gamma}$ of all edges in Γ with endpoints belonging to the same vertex identified. An automorphism J of Γ induces in an obvious way a mapping of $\widetilde{\Gamma}$ into itself whose restriction to each edge E_j is isometric. Since functions on $\widetilde{\Gamma}$ may have different values at endpoints belonging to the same vertex, we shall usually consider our functions on $\widetilde{\Gamma}$ to be undefined on the vertices. From now on we shall use the same notation, Γ, for the graph as defined above and the graph as a set of points, and we hope that there will be no risk for misunderstanding. Thus, denoting the union of all vertices (considered as a set of points) by V we shall consider functions defined on $\Gamma \setminus V$.

3. Hilbert space and differential operators

The functions on the graph which are square integrable with respect to the Lebesque measure on the edges form the Hilbert space $L^2(\Gamma)$. This Hilbert space can be decomposed into the orthogonal sum of L^2-spaces on the edges

$$L^2(\Gamma) = \bigoplus \sum L^2(E_j).$$

The inner product in each $L^2(E_j)$ is defined as $\langle f, g\rangle = \int_{E_j} f\,\bar{g}\,\mathrm{d}x$. The definition of $L^2(\Gamma)$ is obviously independent of the vertex structure of the graph.

Consider the linear operator L, which is defined as the orthogonal sum of the operators of the second differentiation, $-\mathrm{d}^2/\mathrm{d}x^2$, along the edges. This operator will be called the Laplace operator on the graph. It is defined on the natural domain, the Sobolev space $W_2^2(\Gamma \setminus V)$ of all functions on Γ whose restriction to each E_j belongs to $W_2^2(E_j)$. To make this operator self-adjoint one needs to restrict it to the set of functions satisfying certain boundary conditions at the vertices. The following boundary conditions are called standard, or natural:

$$u(a_j) = u(a_k), \quad a_j, a_k \in A_i,\ i = 1, 2, \ldots, N, \tag{1}$$

$$\sum_{a_j \in A_i} \partial_n u(a_j) = 0, \quad i = 1, 2, \ldots, N; \tag{2}$$

here $\partial_n u(a)$ denotes the "normal derivative" of the function u at the endpoint a, that is, the first derivative oriented outward from the interval in question. Condition (1) implies that u can be considered as a continuous function on the entire graph Γ, including vertices.

In the case of a vertex of valence 2 the standard conditions imply that the function and its first derivative are continuous across the vertex, and thus the vertex can be removed without changing the domain of the operator.

In addition to the Laplace operator L we are going to consider the Schrödinger operator $H = L + Q$, where Q is a real-valued potential function. About the potential $Q = \{q_j\}$ we shall assume that

$$\int_\Gamma \bigl(1 + |x|\bigr)\bigl|Q(x)\bigr|\,\mathrm{d}x < \infty,$$

which is the same as saying that $q_j \in L^1(E_j)$ for each edge E_j, and in addition, q_j satisfies the Faddeev condition $\int_{E_j} (1 + |x|)|q_j(x)|\,\mathrm{d}x < \infty$ on all external edges.

The following two operators in the Hilbert space $L^2(\Gamma)$ are naturally associated with the formal differential operator H:

- the maximal operator $H_{\max}$ defined on the domain

$$\mathrm{Dom}(H_{\max}) = \bigl\{u \in L^2(\Gamma);\ Hu \in L^2(\Gamma)\bigr\} \equiv W_2^2(\Gamma \setminus V);$$

- the minimal operator $H_{\min}$ being the closure of the operator $H|_{C_0^\infty(\Gamma\setminus V)}$ and having the domain

$$\mathrm{Dom}(H_{\min}) = \bigl\{u \in W_2^2(\Gamma \setminus V);\ u(a_j) = 0 = \partial_n u(a_j),\ j = 1, 2, \ldots, n + 2k\bigr\}.$$

Here $C_0^\infty(\Gamma \setminus V)$ denotes the set of functions that are infinitely differentiable and compactly supported in the open set $\Gamma \setminus V$. Then every self-adjoint operator H associated with the formal differential operator is an extension of $H_{\min}$ and a restriction of $H_{\max}$ at the same time

$$H_{\min} \prec H \prec H_{\max}.$$

To determine all such operators H the von Neumann extension theory can be applied to the symmetric operator $H_{\min}$. Another possibility is to describe H by imposing boundary conditions on the functions from the domain of $H_{\max}$. In this approach one uses instead of unitary operators acting between the deficiency subspaces for $H_{\min}$ (like in von Neumann theory) the Lagrangian subspaces for the boundary form of $H_{\max}$.

4. Boundary conditions and vertex structure

If $\mathbf{A}$ is the set of $n+2k$ endpoints of edges of the graph, then we have the following identity for $f, g \in W_2^2(\Gamma \setminus V)$

$$\langle f, Hg\rangle - \langle Hf, g\rangle = \sum_{a\in\mathbf{A}} \bigl(\partial_n f(a)\overline{g(a)} - f(a)\overline{\partial_n g(a)}\bigr). \tag{3}$$

This form vanishes if at least one of the functions f, g belongs to $\mathrm{Dom}(H_{\min})$. Let $\mathbf{B} \simeq \mathbf{C}^{n+2k}$ be the $(n+2k)$-dimensional vector space of all boundary values $\{(u(a), \partial_n u(a));\ a \in \mathbf{A}\}$. Writing $F = (f(a), \partial_n f(a))_{a\in\mathbf{A}}$ and letting G have the analogous meaning we introduce the symplectic form $\mathcal{B}$ on $\mathbf{B}$ by defining $\mathcal{B}[F, G]$ as the expression in the right hand side of (3). The form $\mathcal{B}$ defines a symplectic structure on $\mathbf{B}$. The self-adjoint restrictions of L are in 1–1-correspondence with the Lagrangian subspaces of $\mathbf{B}$.

We are only going to allow boundary conditions which relate boundary values at the same vertex to each other. This requirement can be expressed as follows. The partition σ of the set of boundary points into equivalence classes corresponding to vertices determines a decomposition of the space $\mathbf{B}$ into an orthogonal sum of symplectic spaces $\mathbf{B}_1 \oplus \cdots \oplus \mathbf{B}_N$, where $\mathbf{B}_i = \{u(a), \partial_n u(a);\ a \in A_i\}$. We shall say that a set of boundary conditions is *compatible with the vertex structure of the graph* $\Gamma(\mathbf{E}, \sigma)$ if the corresponding Lagrangian subspace of $\mathbf{B}$ can be written as the orthogonal sum of Lagrangian subspaces of the $\mathbf{B}_i$. The set of partitions σ of the set $\mathbf{A}$ of endpoints of edges is partially ordered in an obvious way: let us write $\sigma' \succcurlyeq \sigma$ if σ' is a refinement of σ. We shall say that a set of boundary conditions on the graph $\Gamma(\mathbf{E}, \sigma)$ is *non-separable*, if the partition σ is a maximal element in the set of partitions for which the corresponding vertex structure is compatible with this set of boundary conditions. This means that if we form a new graph with the same set of edges and with one or more new vertices by choosing a strictly finer partition of the set of endpoints, then our boundary conditions will not be compatible with the new vertex structure.

As an example we consider the case when Γ consists of precisely m external edges with endpoints $a_1, \dots, a_m$, joined at one vertex. Setting $\vec{f} = (f(a_1), \dots, f(a_m))$, $\partial_n \vec{f} = (\partial_n f(a_1), \dots, \partial_n f(a_m))$, we can describe a subspace of $\mathbf{B}$ by $C\vec{f} = D\partial_n \vec{f}$, where (C, D) is an $m \times 2m$ matrix. It is rather easy to prove that the boundary conditions $C\vec{f} = D\partial_n \vec{f}$ define a Lagrangian subspace of $\mathbf{B}$ if and only if (C, D) has rank m and CD^* is Hermitean. In the case of a general graph we get a similar condition on each vertex [18]. The matrices (C, D) and (C', D') define the same Lagrangian subspace and hence the same operator if and only if there exists an invertible matrix A such that $C' = AC$, $D' = AD$. The boundary conditions are separable if and only if they can be written $C\vec{f} = D\partial_n \vec{f}$, where

$$C = \begin{pmatrix} C_1 & 0 \\ 0 & C_2 \end{pmatrix}, \qquad D = \begin{pmatrix} D_1 & 0 \\ 0 & D_2 \end{pmatrix},$$

with respect to a suitable ordering of the endpoints in the vertex, the matrices C_j and D_j having the same size.

5. The scattering matrix

Let Γ be a graph with n external edges, let $H = L + V$ be a Schrödinger operator with potential q_j on the jth edge, and assume that a set of self-adjoint boundary conditions is given. The scattering matrix for this problem is an $n \times n$ unitary matrix $S(k) = (s_{jl}(k))$, $k \in \mathbf{R}$, which is defined as follows. Let us number the edges so that $E_1, \dots, E_n$ are external and $E_{n+1}, \dots, E_{n+k}$ are internal edges. For any positive energy $\lambda = k^2$ and any l, $1 \leqslant l \leqslant n$, let ψ_j^l, $1 \leqslant j \leqslant k + n$, be a solution of the system

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi_j^l + q_j \psi_j^l = \lambda \psi_j^l \quad \text{on } E_j,\ 1 \leqslant j \leqslant n + k, \tag{4}$$

satisfying the given boundary conditions at all vertices and the following asymptotic conditions on all external edges

$$\begin{aligned} &\psi_j^l(x,\lambda) = s_{jl}(k)e^{ikx} + o(1), \quad \text{as } x \to \infty \text{ on } E_j,\ 1 \leqslant j, l \leqslant n,\ j \neq l, \\ &\psi_l^l(x,\lambda) = e^{-ikx} + s_{ll}(k)e^{ikx} + o(1), \quad \text{as } x \to \infty \text{ on } E_l,\ 1 \leqslant l \leqslant n, \end{aligned} \tag{5}$$

for some constants $s_{jl}(k)$. In the last formula we have assumed, without loss of generality, that all external edges are of the form $[0, \infty)$.

It is straightforward to show that such solutions always exist. If λ is not an eigenvalue of the operator, the solution $\psi^l = (\psi_1^l, \dots, \psi_{n+k}^l)$ is unique. If λ is an eigenvalue, then the solution ψ^l is not always unique on internal edges, but the coefficients $s_{jl}(k)$ of the scattering matrix are still uniquely determined. If the potentials q_j are zero, then the remainder terms $o(1)$ can be omitted.

6. The inverse scattering problem for symmetric graphs

We can now formulate our first theorem. As usual we shall say that a graph is *connected* if any pair of vertices can be joined by a finite sequence of edges, each attached to the next one by an endpoint belonging to the same vertex. It is obvious that the scattering matrix carries no information whatsoever about a compact part of the graph which is not connected with any of the external edges. Moreover, if the graph has more than one non-compact connected component it is clearly enough to consider one of those components.

Theorem 1. *Let Γ be a graph with at least one external edge, and assume that there exists a non-trivial automorphism of Γ in the sense of Definition 2, which preserves all external edges and preserves the potential $Q(x)$ in the sense that $Q(Jx) = Q(x)$. Then the self-adjoint boundary conditions at the vertices defining the operator $H = L + Q$ in general cannot be determined from the scattering matrix. More precisely, there exists an infinite family of self-adjoint boundary conditions for H such that the scattering matrix for H with any of those boundary conditions is the same.*

For the proof we shall need a couple of lemmas.

Lemma 1. *Let Γ be a connected graph with at least one external edge, and assume that there exists a non-trivial automorphism J of Γ which preserves all external edges. Then there exists a vertex A, preserved by J, and a set of distinct endpoints $a_0, a_1, \dots, a_m$, $m \geqslant 2$, in A such that $Ja_0 = a_0$ and J operates cyclically on $a_1, \dots, a_m$ in the sense that $Ja_k = a_{k+1}$ for $1 \leqslant k \leqslant m-1$ and $Ja_m = a_1$.*

Proof. Let A_1 be a vertex containing the endpoint a_0 of one of the external edges of Γ. Assume first that there exists an endpoint $a_1 \in A_1$ such that $Ja_1 \neq a_1$. Set $J^k a_1 = a_{k+1}$ for $k = 2, 3, \dots$. Since J is a permutation of the endpoints in A_1, there must exist a smallest $m \geqslant 2$ such that $Ja_m = a_1$. This proves the lemma in this case. Assume next that J fixes all endpoints in A_1. Since Γ is connected and J is non-trivial we can choose a vertex $A_2 \neq A_1$ containing the other endpoint a_0 of one of the (internal) edges attached to A_1. If J does not fix all endpoints in A_2 we can choose $a_1, \dots, a_m$ as before and the lemma is proved. If J fixes all endpoints in A_2 we can choose $A_3 \neq A_2$ containing the other endpoint a_0 of one of the edges attached to A_2. Continuing in this way, since Γ is connected and J is a non-trivial automorphism, we must eventually find a vertex A_p on which J does not fix all endpoints. This completes the proof of the lemma. □

If J is an automophism of Γ we introduce the isometric map on $L^2(\Gamma)$, also denoted J, which takes $f \in L^2(\Gamma)$ into $Jf(x) = f(J^{-1}x)$.

Lemma 2. *Let Γ be a connected graph with at least one external edge, assume that there exists a non-trivial automorphism J of Γ which preserves all external edges, and let m have the same meaning as in Lemma 1. Then there exists an infinite family $L(h)$, $h \in \mathbf{R}^{m-1}$, of self-adjoint restrictions of the operator L such that*

$$\mathrm{Dom}\big(L(h)\big) \cap \big\{ f \in L^2(\Gamma);\ Jf = f \big\} \text{ is independent of } h \qquad \text{for } h \in \mathbf{R}^{m-1}, \tag{6}$$

but

$$\mathrm{Dom}\big(L(h)\big) \neq \mathrm{Dom}\big(L\big(h'\big)\big) \quad \text{if } h \neq h',\ h \in \mathbf{R}^{m-1}. \tag{7}$$

Proof. Let A, $a_0, a_1, \dots, a_m$ be a vertex and endpoints as in Lemma 1. Let $M > m$ be the valence of A, set $a_{m+1} = a_0$, and if $M > m+1$ let $a_{m+2}, \dots, a_M$ be the remaining endpoints in A.

Let us now introduce a set of boundary conditions for the operator $L = -\mathrm{d}^2/\mathrm{d}x^2$ on Γ. At the vertex A we first take the $M - m + 1$ conditions

$$f(a_{m+1}) = f(a_2) = \cdots = f(a_M) = \frac{1}{\sqrt{m}} \sum_{k=1}^{m} f(a_k), \tag{8}$$

$$\sum_{k=m+1}^{M} \partial_n f(a_k) = -\sum_{k=1}^{m} \partial_n f(a_k). \tag{9}$$

Note that the last condition can be written $\sum_{k=1}^{M} \partial_n f = 0$. For arbitrary real constants $h_1, \ldots, h_{m-1}$ we further introduce the $m - 1$ conditions

$$\sum_{k=1}^{m} e^{i2\pi kp/m} \partial_n f(a_k) = h_p \sum_{k=1}^{m} e^{i2\pi kp/m} f(a_k), \quad p = 1, 2, \ldots, m - 1. \tag{10}$$

Thus we have given M conditions at the vertex A. At all other vertices we introduce natural boundary conditions. Since the linear forms $\mathbf{C}^m \ni x \mapsto \sum_{k=1}^{m} e^{i2\pi kp/m} x_k,\ p = 1, 2, \ldots, m - 1$, are linearly independent, it is clear that (7) is true.

We will now show that these conditions determine a self-adjoint operator. Since we have the correct number of conditions and those conditions are obviously linearly independent, it is sufficient to show that the operator is symmetric.

We start from formula (3), which is valid for all functions $f, g \in W_2^2(\Gamma \setminus V)$. We need to show that this expression is zero if f and g satisfy our boundary conditions. Since we have natural boundary conditions at all vertices except A, the sum over all those vertices must vanish. So it remains only to consider the sum in (3) restricted to the vertex A, that is

$$\sum_{k=1}^{M} \big(\partial_n f(a_k) \overline{g(a_k)} - f(a_k) \overline{\partial_n g(a_k)}\big). \tag{11}$$

Denote the mth root of unity $e^{i2\pi/m}$ by α. If we introduce the notation

$$f_p = \frac{1}{\sqrt{m}} \sum_{k=1}^{m} \alpha^{pk} f(a_k), \qquad \partial_n f_p = \frac{1}{\sqrt{m}} \sum_{k=1}^{m} \alpha^{pk} \partial_n f(a_k), \tag{12}$$

for $p = 0, 1, 2, \ldots, m - 1$, we can write the conditions (10) as

$$\partial_n f_p = h_p f_p, \quad p = 1, 2, \ldots, m - 1. \tag{13}$$

We now claim that the following identity holds

$$\sum_{k=1}^{m} \big(\partial_n f(a_k) \overline{g(a_k)} - f(a_k) \overline{\partial_n g(a_k)}\big) = \sum_{p=0}^{m-1} \big(\partial_n f_p \overline{g_p} - f_p \overline{\partial_n g_p}\big). \tag{14}$$

Let S be the $m \times m$ van der Monde matrix whose kth row is

$$m^{-1/2}\bigl(1, \alpha^k, \dots, \alpha^{(m-1)k}\bigr), \quad k = 0, 1, \dots, m-1.$$

Denote elements of $\mathbf{C}^{2m}$ by $X = (x, x')$, $Y = (y, y')$, and let $T : \mathbf{C}^{2m} \to \mathbf{C}^{2m}$ be the transformation given by $(x, x') \mapsto (Sx, Sx')$. Then T is symplectic (with respect to the form $\mathcal{B}[X, Y] = \langle x', y\rangle - \langle x, y'\rangle$ introduced above), for

$$\mathcal{B}(TX, TY) = \bigl\langle Sx', Sy\bigr\rangle - \bigl\langle Sx, Sy'\bigr\rangle = \bigl\langle x', y\bigr\rangle - \bigl\langle x, y'\bigr\rangle = \mathcal{B}(X, Y),$$

because S is unitary. Applying this identity with

$$x = \bigl(f(a_1), \dots, f(a_m)\bigr), \qquad x' = \bigl(\partial_n f(a_1), \dots, \partial_n f(a_m)\bigr),$$

etc., we obtain (14).

Let us now go back to the expression (11). If we rewrite the sum of the first m terms by means of (14), this expression becomes

$$\begin{aligned} &\sum_{p=1}^{m-1}\bigl(\partial_n f_p \overline{g_p} - f_p \overline{\partial_n g_p}\bigr) + \bigl(\partial_n f_0 \overline{g_0} - f_0 \overline{\partial_n g_0}\bigr) \\ &\quad + \sum_{k=m+1}^{M}\bigl(\partial_n f(a_k)\overline{g(a_k)} - f(a_k)\overline{\partial_n g(a_k)}\bigr). \end{aligned} \tag{15}$$

Each term in the first sum must vanish according to the conditions (13). Applying first (8) and then (9) we can rewrite the last sum in (15) as follows

$$\begin{aligned} \sum_{k=m+1}^{M}(\dots) &= \frac{\overline{g_0}}{\sqrt{m}}\sum_{k=m+1}^{M}\partial_n f(a_k) - \frac{f_0}{\sqrt{m}}\sum_{k=m+1}^{M}\overline{\partial_n g(a_k)} \\ &= -\frac{\overline{g_0}}{\sqrt{m}}\sum_{1}^{m}\partial_n f(a_k) + \frac{f_0}{\sqrt{m}}\sum_{1}^{m}\overline{\partial_n g(a_k)} \\ &= -\overline{g_0}\partial_n f_0 + f_0\overline{\partial_n g_0}. \end{aligned}$$

Hence the last two terms in (15) cancel each other. The proof is complete. □

Proof of Theorem 1. As was already explained it is enough to consider the case when Γ is connected. Let J be a non-trivial automorphism of Γ, let m have the same meaning as in Lemma 1, and let $L(h)$ be the operators constructed in Lemma 2. We have seen that $L(h') \neq L(h)$ if $h' \neq h$. We must show that the scattering matrix is the same for all $L(h)$.

Let G be the cyclic group of automorphisms generated by J and let q be the order of G. Then q must be a multiple of m. We claim that the Hilbert space $\mathcal{H} = W_2^2(\Gamma \setminus V)$ can be decomposed into an orthogonal sum

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \cdots \oplus \mathcal{H}_{q-1}$$

of subspaces $\mathcal{H}_k$ such that

$$J^k f(x) = f\big(J^{-k}x\big) = e^{ik2\pi/q} f(x) \quad \text{for } f \in \mathcal{H}_k,\ k = 0, 1, \ldots, q-1. \tag{16}$$

This follows immediately from the fact that the map which takes $J^k \in G$ into the linear transformation $f \mapsto J^k f$ of $\mathcal{H}$ into itself is a representation of the finite cyclic group G, and the irreducible representations of that group are 1-dimensional with characters $e^{ik2\pi/q}$, $k = 0, 1, \ldots, q-1$. Let $P_k : \mathcal{H} \to \mathcal{H}_k$ be the orthogonal projection onto $\mathcal{H}_k$. Let $\psi_h = \{\psi_{h,j}^l\}$ be the solution of the system (4) satisfying the boundary conditions (13), and the asymptotic conditions (5). We shall show that ψ_h is independent of h on all external edges; this implies of course that the scattering matrix is independent of h. First we claim that

$$P_k \psi_h = 0 \quad \text{for } 1 \leqslant k \leqslant q-1 \text{ on all external edges.} \tag{17}$$

In fact, since J is an automorphism of Γ leaving all external edges invariant, it is clear that $J\psi_h = \psi_h$, hence $JP_k\psi_h = P_kJ\psi_h$, on each external edge. On the other hand $JP_k\psi_h = e^{ik2\pi/q}\psi_h$ by (16). Combination of these equations proves (17). Moreover, it follows from (6) that $P_0\psi_h$ is independent of h (in fact on all edges). Thus $P_k\psi_h$ is independent of h on external edges for all k, in other words, ψ_h is independent of h on external edges as claimed. This completes the proof of the theorem. □

7. The same scattering matrix for two different symmetric graphs

Theorem 2. *Let Γ be a graph with at least one external edge, and assume that there exists a non-trivial automorphism of Γ in the sense of Definition 2, which preserves all external edges and preserves the potential $Q(x)$ in the sense that $Q(Jx) = Q(x)$. Assume in addition that the Schrödinger operator H on Γ possesses the same symmetry as Γ, i.e., that not only the potential Q but also the boundary conditions are invariant under the automorphism preserving the external edges of the graph. Then there exists a different graph Γ' and a Schrödinger operator H' on Γ' such that the scattering matrices for H and H' coincide.*

Proof. Let J be an automorphism preserving the external edges. Lemma 1 implies that the automorphism J operates cyclically on certain endpoints $a_1, a_2, \ldots, a_m$ joined at a vertex A. Consider the corresponding edges $[a_1, b_1], [a_2, b_2], \ldots, [a_m, b_m]$, having the same length d, and an arbitrary positive real number $\delta < d$. Let us denote by c_l the point on the interval $[a_l, b_l]$ having distance δ from the left end a_l. Consider then the graph Γ' obtained from Γ by joining together the points $c_1, c_2, \ldots, c_m$ into a new vertex denoted by C in

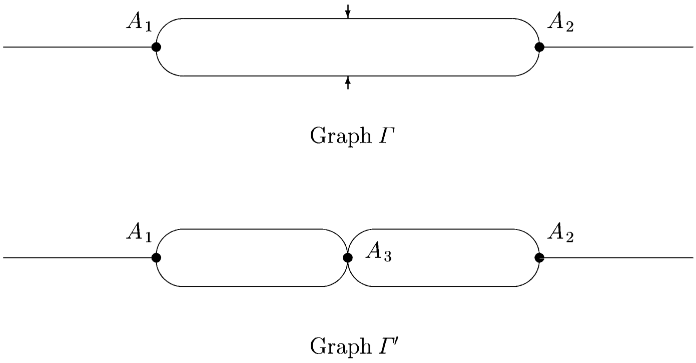

Fig. 3. Two different graphs with the same scattering matrix.

what follows. See Fig. 3. The automorphism J induces a unique automorphism J' of Γ'. Let us denote by τ the natural unitary map between the Hilbert spaces

$$\tau : L^2(\Gamma) \to L^2(\Gamma'),$$

which is determined by the pointwise map between Γ and Γ'. This map intertwines the two automorphisms

$$\tau J = J' \tau$$

and is the identity transformation when restricted to the external edges. Similarly the potential Q induces a unique potential $Q' = \tau Q$ on Γ'. Define then the Schrödinger operator H' in $L^2(\Gamma')$ by imposing natural boundary conditions at the vertex C and the same boundary conditions as for the operator H at all other vertices. The operator H' so defined is invariant under J'. It follows from the proof of Theorem 1, that all scattered waves can be chosen invariant under the automorphism. (If λ is not an eigenvalue, then the scattered waves are always invariant under J.) Consider such scattered waves ψ_j^l for the operator H. Then the functions $\tau \psi_j^l$ are scattered waves for the operator H' (satisfy the differential equation on all edges and the boundary conditions at all vertices including the vertex C, and having required asymptotics at all external edges). Since the map τ is trivial on external edges, the corresponding scattering matrices coincide. The theorem is proven. $\square$

Comment. The theorem states that if the graph has internal symmetry, then the knowledge of the scattering matrix is not enough to determine the graph. Explicit examples show that this statement does not hold in general for non-symmetric graphs, i.e., that some graphs are determined uniquely by the corresponding scattering matrices [15,22]. The operators H and H' have different spectra, but their parts restricted to functions invariant under the automorphism are unitarily equivalent.

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