On the Reconstruction of the Boundary Conditions for Star Graphs

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Abstract. The Laplace operator on a star graph is considered. The problem to recover the vertex matching boundary conditions from a part of the scattering matrix is investigated.

1. Introduction

Differential operator on geometric graphs have been studied from the beginning of 80-ies [**8, 11**], but recent interest in nano-structures has led to enormous interest in mathematical studies of the problem [**14, 16, 17, 19**]. In this article we discuss the possibility to reconstruct the matching (boundary) conditions at the unique vertex of a star graph from the corresponding scattering matrix. This problem can easily be solved if the total scattering matrix is known (see [**15**]), and it has been shown recently that the scattering matrix at a particular value of the energy can effectively be used to uniquely parameterize the matching conditions [**18**]. The problem we are interested in is the possibility to reconstruct the matching conditions if only a part of the scattering matrix is known, more precisely the principal $(v-1)\times(v-1)$ block $(S_v(k_0))_{v;v}$, where v is the valency of the vertex. This problem can be considered as the first step towards reconstruction of the vertex matching conditions for trees from the corresponding scattering matrix.

The problem of reconstructing the Schrödinger operator on a star graph was first discussed by N.I. Gerasimenko and B.S. Pavlov [**11, 12**] using the Gelfand-Levitan-Marchenko method. The inverse spectral and scattering problems for trees have intensively been studied in recent years by M. Belishev, M. Brown, R. Carlson, G. Freiling, A. Vakulenko, R. Weikard, V. Yurko, and the authors [**1, 2, 4, 5, 6, 7, 9, 10, 21**]. It has been proven that the knowledge of the Dirichlet-to-Neumann map, or Titchmarsh-Weyl matrix function allows one to calculate the potential for standard boundary conditions at the vertices. The case of more general boundary conditions has been discussed in [**10**], but the whole family of boundary conditions has not been investigated yet.

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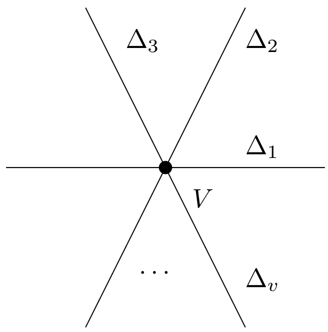

In the current article we consider the most general family of properly connecting self-adjoint boundary conditions. It is discovered that so-called *asymptotically properly connecting* conditions play a very important role. Such boundary conditions correspond to vertex scattering matrices $S_v(k)$ tending to the limit matrix S_v^∞ as $k \to \infty$, which cannot be written in the block-diagonal form (after a certain permutation of the coordinates). It appeared that for such boundary conditions the principal $(v-1) \times (v-1)$ block of the scattering matrix known for one particular value of the energy essentially determines the boundary conditions (up to one real parameter, which in principle cannot be recovered and provided one additional easily checked condition is satisfied). Explicit interpretation of this free parameter is given using unitary equivalent operators. In the second part of the paper it is shown that knowing in addition the diagonal elements of the principal block for a finite number of energies one may reconstruct the boundary conditions even in the case of just *properly connecting* boundary conditions.

All results are proven so far for the Laplace operator on the star graph with most general self-adjoint matching conditions at the vertex, but it is not hard to generalize these conditions to include potentials with compact support using Boundary Control method [**3**] following ideas already developed in [**1**]. It is our future aim to apply these results to solve the most general inverse problem for trees consisting of recovering the geometric tree, potential on it and boundary conditions at the vertices.

The paper is organized as follows. In the following section main notations and definitions are given. The cases of asymptotically properly connecting and just properly connecting matching conditions are considered in sections 3 and 4.

2. Scattering on a star graph

Let us denote by Γ_{star} the star graph formed by v edges $\Delta_j = [x_{2j-1}, \infty)$ joined together at one vertex $V = \{x_{2j-1}\}_{j=1}^v$. Consider the Laplace operator $L = -\frac{d^2}{dx^2}$ in $L_2(\Gamma_{\text{star}})$ defined on the set of functions from $W_2^2(\Gamma_{\text{star}} \setminus V)$ satisfying the following matching conditions at the vertex

$$i(S-I)\boldsymbol{\psi}(V) = (S+I)\partial_n \boldsymbol{\psi}(V), \tag{2.1}$$

where S is a $v \times v$ unitary matrix and $\boldsymbol{\psi}(V)$ and $\partial_n \boldsymbol{\psi}(V)$ are v-dimensional vectors of the values of ψ and its normal derivative at the vertex V. The unitary matrix appearing in (2.1) is just the vertex scattering matrix $S_v(k), k^2 = E$ for $k = 1$. The vertex scattering matrix may be defined by considering scattering waves on Γ_{star}. Every solution to the equation $-\psi''(k,x) = k^2 \psi(k,x)$ can be written as a combination of the incoming $e^{-ik|x-x_{2j-1}|}$ and outgoing $e^{ik|x-x_{2j-1}|}$ waves:

$$\psi(k,x) = b_j e^{-ik|x-x_{2j-1}|} + a_j e^{ik|x-x_{2j-1}|}, \ x \in \Delta_j.$$

Substitution into the matching conditions (2.1) determines connection between the amplitudes of incoming and outgoing waves

$$\boldsymbol{a} = S_v(k)\boldsymbol{b}, \tag{2.2}$$

where $S_v(k)$ is the vertex scattering matrix

$$S_v(k) = \frac{(k+1)S + k - 1}{(k-1)S + k + 1}, \ k \neq 0. \tag{2.3}$$

This formula allows one to establish explicit connection between vertex scattering matrices for different values of the energy parameter (see [**15**])

$$S_v(k) = \frac{(k+k_0)S_v(k_0) + k - k_0}{(k-k_0)S_v(k_0) + k + k_0}, \ k, k_0 \neq 0. \tag{2.4}$$

The unitary matrix S parameterizes the boundary conditions in the unique way and therefore encodes all information concerning these conditions. In particular, one may understand whether the boundary conditions connect all edges properly or not. In what follows we shall need the notion of asymptotically properly connecting boundary conditions. It is possible to prove that for $k \to \infty$ the vertex scattering matrix $S_v(k)$ tends to a certain limit. If the boundary conditions are properly connecting there is no guarantee, that the limit scattering matrix corresponds to properly connecting conditions. In other words it may happen that the connection between certain channels becomes weak and therefore for large energies the corresponding vertex is seen as two (or more) independent vertices. Let us therefore use the following

Definition 1. Vertex boundary conditions are called **properly connecting** if the vertex cannot be divided into two (or more) vertices so that the boundary conditions connect together only boundary values belonging to each of the new vertices. Vertex boundary conditions are called **asymptotically properly connecting** if the limit scattering matrix S_v^∞ corresponds to certain properly connecting boundary conditions.

It is clear that every asymptotically properly connecting boundary condition is properly connecting. In the rest of this article we consider first asymptotically properly connecting and then just properly connections matching conditions.

Criteria for S to be properly connecting is rather simple: the matching conditions are properly connecting if and only if the matrix S cannot be transformed into a block-diagonal form by a permutation of the indices. To understand whether S is asymptotically properly connecting or not one has to use its spectral representation as a unitary matrix. Let us denote by $N_{e^{i\theta_j}}$ the eigensubspace corresponding to the eigenvalue $e^{i\theta_j}$. Then it is possible to prove that the limit scattering matrix $S_v^\infty = \lim_{k\to\infty} S_v(k)$ has eigenvalues ± 1 with the following eigensubspaces [**13, 18**]

$$N_{-1}^\infty = N_{-1} \ \text{ and } \ N_1^\infty = \mathbb{C}^v \ominus N_{-1} = N_{-1}^\perp. \tag{2.5}$$

Then it is not hard to prove the following

Proposition 1 (Theorem 6.5 from [**18**]). *The boundary conditions are asymptotically properly connecting if and only if N_{-1} is not perpendicular to any coordinate subspace.*

By coordinate subspace we mean any subspace in $\mathbb{C}^n$ spanned by one or several vectors from the standard basis, which does not coincide with $\mathbb{C}^n$

3. Recovering of the asymptotically properly connecting matching conditions

In this section we discuss the possibility to reconstruct the matching conditions from the principal $(v-1)\times(v-1)$ block $(S_v(k))_{v;v}$ of the vertex scattering matrix. This part of the matrix is obtained when we send plane waves along the first $v-1$ edges and measure the reflected waves coming along the same edges. Let us discuss first whether this reconstruction is unique or not. Consider the following unitary transformation in $L_2(\Gamma_{\rm star})$

$$(T_\theta f)(x) = \begin{cases} f(x), & x\in\Delta_j, j=1,2,...,v-1; \\ e^{i\theta}f(x), & x\in\Delta_v. \end{cases} \tag{3.1}$$

This transformation does not change the differential operator but do change the matching conditions at the vertex, i. e. the operator $L^\theta = T_\theta^{-1}LT_\theta$ is given by the same differential expression $-\mathrm{d}^2/\mathrm{d}x^2$, but the matrix S in boundary conditions (2.1) has to be substituted with

$$S^\theta = R_\theta S^0 R_{-\theta}, \quad S^0 = S, \tag{3.2}$$

where R_θ is the following $v\times v$ matrix:

$$R_\theta = \mathrm{diag}\,\{1,1,...,1,e^{i\theta}\} = \begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \\ 0 & 0 & \dots & 0 & e^{i\theta} \end{pmatrix}. \tag{3.3}$$

It is clear that this transformation does not change the block $(S_v(k))_{v;v}$ of the matrix S. The same holds for the vertex scattering matrix, since (2.3) implies that

$$S_v^\theta(k) = R_\theta S_v^0(k) R_{-\theta}, \tag{3.4}$$

where $S_v^\theta(k)$ is the vertex scattering matrix corresponding to the new conditions.

The following theorem implies that the knowledge of the principal $(v-1)\times(v-1)$ block of the vertex scattering matrix allows one to reconstruct the whole matrix up to one real parameter corresponding to the transformation T_θ, provided the boundary conditions at the vertex are asymptotically properly connecting.

THEOREM 1. *Consider the set of $v\times v$ vertex scattering matrices S_v determined by certain asymptotically properly connecting vertex boundary conditions and having the same principal $(v-1)\times(v-1)$ block $(S_v(k_0))_{v;v}$ with $\det((S_v(k_0))_{v;v}+1)\neq 0$. This family of matrices can be described by one real phase parameter so that*

$$S_v^\theta(k) = R_\theta S_v^0(k) R_{-\theta}, \tag{3.5}$$

where R_θ is given by (3.3) *and $S_v^0(k)$ is a certain particular member of the family.*

PROOF. Reconstruction of an unitary matrix from its principal $(v-1)\times(v-1)$ block in general contains two arbitrary phase parameters and can be carried out using the fact that the entries of an unitary matrix satisfy the normalization and orthogonality conditions:

$$\begin{array}{cc} \sum_{j=1}^{v} |s_{ij}|^2 = 1, & \sum_{i=1}^{v} |s_{ij}|^2 = 1; \\ \sum_{j=1}^{v} s_{ij}\overline{s_{lj}} = 0, & \sum_{i=1}^{v} s_{ij}\overline{s_{il}} = 0. \end{array}$$

Assume that the principal $(v-1)\times(v-1)$ block $(S_v(k_0))_{v;v}$ of the matrix $S_v(k_0)$ is known. Consider the last row in $S_v(k_0)$. The absolute values of $s_{vj}(k_0), j = 1, 2, ..., v-1$ can be calculated from the normalization conditions. At least one of these numbers is different from zero, otherwise the matrix $S_v(k_0)$ is block-diagonal and does not correspond to asymptotically properly connecting boundary conditions. Consider any such different from zero element, say with the index $v1$. All possible values of this element can be described by one real phase parameter α as follows $s_{v1} = |s_{v1}|e^{i\alpha}$. Then all other elements $s_{vj}, j = 2, ..., v-1$ can be reconstructed using orthogonality conditions. In the same way one may consider the last column and introduce a parameter $\beta \in \mathbb{R}$ such that $s_{1v} = |s_{1v}|e^{i\beta}$. Then the element s_{vv} is uniquely determined.[7]

Let us summarize our calculations by stating the following result: the family of vertex scattering matrices having the same principal $(v-1)\times(v-1)$ block can be described by two real parameters so that

$$S_v^{\alpha,\beta}(k_0) = R_\alpha S_v^0(k_0) R_\beta, \tag{3.6}$$

where $S_v^0(k_0)$ is a certain particular member of the family. It remains to prove that the subfamily corresponding to asymptotically properly connecting matching conditions is described by just one parameter using (3.5). Assume that $S_v^0(k_0)$ is a particular member of the subfamily. Every vertex scattering matrix corresponding to asymptotically properly connecting boundary conditions has eigenvalue -1, which implies that

$$\det(S_v^{\alpha,\beta}(k_0) + I) = 0 \Rightarrow \det(S_v^0(k_0) + R_{-(\alpha+\beta)}) = 0.$$

In the last equality we may use that the determinant is linear with respect to the entry with the index vv to get

$$0 = \det(S_v^0(k_0) + I) + (e^{-i(\alpha+\beta)} - 1)\det(S_v(k_0))_{v;v} = (e^{-i(\alpha+\beta)} - 1)\det(S_v(k_0))_{v;v},$$

where we have taken into account that $\det(S_v^0(k_0) + I) = 0$. It follows that $\alpha = -\beta$, since $\det(S_v(k_0))_{v;v} \neq 0$. We have proven that all possible $S_v(k)$ satisfy (3.5) for $k = k_0$. Then formula (2.4) implies that (3.5) holds for any real k. □

It follows that in the case of asymptotically properly connecting matching conditions the vertex scattering matrix for all values of the energy can be recovered from its principal $(v-1)\times(v-1)$ block given for a certain value of the energy parameter k up to one real parameter connected with the unitary transformation given by (3.4) (provided $\det((S_v(k_0))_{v;v} + I) \neq 0$). The corresponding Laplace operators are all unitary equivalent to each other.

We would like to mention that the result just proven is an extension of Theorem 1 from [**15**], where it is shown that the knowledge of the (whole) scattering matrix for a certain energy allows one to reconstruct the boundary conditions at the vertex and therefore determine the vertex scattering matrix for all other values of the energy.

[7] Only if the matrix $S_v(k_0)$ is block-diagonal, the element s_{vv} has to be chosen with unit absolute value but otherwise arbitrarily, but this case cannot occur under our assumptions.

4. Recovering of the properly connecting matching conditions

In the rest of this article we discuss the possibility to recover the matching conditions from the principal $(v-1)\times(v-1)$ block of the scattering matrix given for different energies, but without assuming that the boundary conditions are asymptotically properly connecting. It is assumed that the boundary conditions are just properly connecting. This restriction is not essential, since in the case of not properly connecting conditions one may solve the inverse problem for each block separately. The only case that has to be excluded is where the last edge is not connected to the rest of the star graph. It is clear that in this case no information concerning the boundary condition for edge number v is contained in the principal $(v-1)\times(v-1)$ block of the scattering matrix.

In the following theorem we are proving that the knowledge of the principal block $(S_v(k))_{v;v}$ for several energies allows one to reconstruct the boundary conditions at the vertex up to the unitary transformation given by (3.2) and (3.3).

THEOREM 2. *Consider the set of $v\times v$ vertex scattering matrices S_v determined by certain properly connecting vertex boundary conditions and having the same principal $(v-1)\times(v-1)$ block $(S_v(k_0))_{v;v}$, $k_0>0$. Assume in addition that these matrices have the same diagonal elements $s_{jj}(k_n)$, $j=1,2,...,v-1$ for certain different $k_n>0, k_n\neq k_0$, $n=1,2,...,2v-3$. Then this family of matrices can be described by one real phase parameter so that*

$$S_v^\theta(k)=R_\theta S_v^0(k)R_{-\theta}, \tag{4.1}$$

where R_θ is given by (3.3) and $S_v^0(k)$ is a certain particular member of the family.

PROOF. Assume that one particular unitary matrix $S_v^0(k_0)$ has been calculated from the value of its principal $(v-1)\times(v-1)$ block. Then any other unitary matrix with the same principal block is given by (3.6). This formula includes two arbitrary parameters and it remains to show, that the knowledge of $v-1$ diagonal elements allows one to eliminate one of these parameters.

Consider one of the matrices $S_v^{\alpha,\beta}(k_0)$ from the two-parameter family described by (3.6). Then the scattering matrix for all values of the energy parameter k can be calculated using (2.4)

$$S_v^{\alpha,\beta}(k)=\frac{(k+k_0)S_v^{\alpha,\beta}(k_0)+k-k_0}{(k-k_0)S_v^{\alpha,\beta}(k_0)+k+k_0}. \tag{4.2}$$

In particular, its element with the index 11 is

$$\begin{aligned}\left(S_v^{\alpha,\beta}(k)\right)_{11} &= \frac{k+k_0}{k-k_0}-\frac{4kk_0}{k^2-k_0^2}\left(S_v^{\alpha,\beta}(k_0)+\frac{k+k_0}{k-k_0}\right)^{-1}_{11}\\ &= \frac{k+k_0}{k-k_0}-\frac{4kk_0}{k^2-k_0^2}\left(S_v^{0}(k_0)+\frac{k+k_0}{k-k_0}R_{-\alpha-\beta}\right)^{-1}_{11},\end{aligned} \tag{4.3}$$

where we used the fact that the matrices R_θ do not change the principle $(v-1)\times(v-1)$ block and, in particular, the element with the index 11. In what follows we are going to use the notion of rejected minor. Let A be any quadratic $n\times n$ matrix, then the rejected minor $A_{i;j}$ is the quadratic matrix of dimension $(n-1)\times(n-1)$ obtained from A by rejecting the row i and the column j. Similarly the rejected minor $A_{i_1,i_2;j_1,j_2}$ is obtained from the matrix A by rejecting the rows i_1,i_2 and the columns j_1, j_2 [**20**]. With these notations the diagonal element of the scattering matrix can be calculated

(4.4)

$$\left(S_v^{\alpha,\beta}(k)\right)_{11} = \sigma - \left(\sigma - \frac{1}{\sigma}\right) \frac{\det(S_v^0(k_0)+\sigma)_{1;1} + \sigma(e^{-i\gamma}-1)\det(S_v^0(k_0)+\sigma)_{1,v;1,v}}{\det(S_v^0(k_0)+\sigma) + \sigma(e^{-i\gamma}-1)\det(S_v^0(k_0)+\sigma)_{v;v}},$$

where $\sigma = \frac{k+k_0}{k-k_0}$, $\gamma = \alpha+\beta$ and $k \neq k_0$. All determinants appearing in this formula are different from zero, since the matrix $S_v^0(k_0)$ is unitary and $\sigma > 1$ (remember that $k > 0$). This formula shows that in general situation the knowledge of $\left(S_v^{\alpha,\beta}(k)\right)_{11}$ for a certain $k \neq k_0$ allows one to calculate γ (up to unessential factor 2π). This is impossible if and only if $\left(S_v^{\alpha,\beta}(k)\right)_{11}$ does not depend on γ, *i.e.* the equality

(4.5)

$$\det(S_v^0(k_0)+\sigma)\det(S_v^0(k_0)+\sigma)_{1,v;1,v} - \det(S_v^0(k_0)+\sigma)_{1;1}\det(S_v^0(k_0)+\sigma)_{v;v} = 0$$

holds. It might happen that γ cannot be recovered even if the element 11 of $S_v^{\alpha,\beta}(k)$ is known for all $k > 0$. This occurs if (4.5) holds for all $\sigma > 0$ (remember that $\sigma = \frac{k+k_0}{k-k_0}$). Using Jacobi identity (Section 3.6.1 from [**20**])

(4.6)

$$\begin{aligned} &\det(S_v^0(k_0)+\sigma)\det(S_v^0(k_0)+\sigma)_{1,v;1,v} \\ &= \det(S_v^0(k_0)+\sigma)_{1;1}\det(S_v^0(k_0)+\sigma)_{v;v} - \det(S_v^0(k_0)+\sigma)_{1;v}\det(S_v^0(k_0)+\sigma)_{v;1} \end{aligned}$$

condition (4.5) can be written as

$$\det(S_v^0(k_0)+\sigma)_{1;v}\det(S_v^0(k_0)+\sigma)_{v;1} = 0, \tag{4.7}$$

and it holds for $\sigma = \frac{k_n+k_0}{k_n-k_0}$, $n = 1,2,...,2v-3$. This implies that at least one of the determinants, say $\det(S_v^0(k_0)+\sigma)_{v;1}$ is equal to zero for $v-1$ different values of σ. But this determinant is a polynomial in σ of order $v-2$ with the zero and leading coefficients equal to $\det(S_v^0(k_0))_{v;1}$ and $(S_v^0(k_0))_{1v}$ respectively. It follows that $\det(S_v^0(k_0))_{v;1} = 0 = (S_v^0(k_0))_{1v}$, but taking into account that $S_v^0(k_0)$ is unitary $\det(S_v^0(k_0))_{v;1} = 0$ implies that $(S_v^0(k_0))_{v1} = 0$. Summing up we see that the parameter γ cannot be recovered from $(S_v(k))_{11}$ only if $(S_v^0(k_0))_{1v} = (S_v^0(k_0))_{v1} = 0$.

Consider now any element $(S_v(k))_{mm}$, $m = 2,...,v-1$. Similar analysis implies that the parameter γ can be recovered from $(S_v(k_n))_{mm}$, $n = 1,2,...,2v-3$ unless the entries $(S_v^0(k_0))_{1m}$ and $(S_v^0(k_0))_{m1}$ are equal to zero. In other words the parameter γ can be calculated from one of the diagonal elements $(S_v(k))_{mm}$, $m = 1,...,v-1$, unless all entries $(S_v^0(k_0))_{1m}$ and $(S_v^0(k_0))_{m1}$ $m = 1,...,v-1$ are equal to zero. But this means that $S_v^0(k_0)$ has a block diagonal form and hence the corresponding boundary conditions are not properly connecting. □

This theorem can be improved, which we would like to illustrate by the following example. Let $v = 3$. Then the parameter γ cannot be recovered from $(S_v(k_n))_{11}, n = 1,2,3$ only if $(S_v^0(k_0))_{13} = 0$ and $\det(S_v^0(k_0))_{3;1} = 0$, which implies that at least one of the entries $(S_v^0(k_0))_{12}$ and $(S_v^0(k_0))_{23}$ is equal to zero. Hence $S_v(k_0)$ is block-diagonal and the boundary conditions are not properly connecting.

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