Inverse Problems for Graph Laplacians

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Preface

This thesis is devoted to inverse spectral problems for Laplace operators on metric graphs, and it is based on the following papers:

Paper I P. Kurasov and M. Nowaczyk 2005 Inverse spectral problem for quantum graphs *J. Phys. A: Math. Gen* **38** 4901–15

Paper II M. Nowaczyk 2007 Inverse spectral problem for quantum graphs with rationally dependent edges *Operator Theory, Analysis and Mathematical Physics* Operator Theory: Advances and Applications **147** 105–16

Paper III P. Kurasov and M. Nowaczyk 2007 Geometric properties of quantum graphs and vertex scattering matrices, Preprint 2007:21 Centre for Mathematical Sciences, Lund University.

Paper IV S. Avdonin, P. Kurasov and M. Nowaczyk 2007 On the Reconstruction of the Boundary Conditions for Star Graphs, Preprint 2007:29 Centre for Mathematical Sciences, Lund University.

In the first paper, we prove the trace formula and show that it can be used to reconstruct the metric graph in the case of rationally independent lengths of the edges and the Laplace operator with standard boundary conditions at the vertices.

The second paper generalises this result by showing that the condition of rational independence of lengths of the edges can be weakened.

In the third paper the possibility to parameterise vertex boundary conditions via the scattering matrix is investigated. The trace formula is generalised to include even arbitrary vertex boundary conditions leading to energy independent vertex scattering matrices, so-called non-resonant boundary conditions.

In the last paper, we turn to the problem of recovering boundary conditions and solve it for the special case of the star graph.

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Last but not least, my thanks go to my beloved husband Slawek, who has shown great understanding and help towards this work as well as everything else I do.

Contents

Introduction

1. Historical background

Although the spectral problems for quantum graphs have only recently become a rapidly developing field of mathematics and mathematical physics, the first problems of this kind have already been studied in the fifties by K. Ruedenberg and others [66]. In 1988, B. S. Pavlov and N. I. Gerasimenko gave the first mathematically rigorous definition for a Schrödinger operator on a metric graph [31]. They considered the Schrödinger equation with real potentials $q_i(x)$ (where index i goes over all edges) and with standard boundary conditions at the vertices, both for compact graphs and for graphs with several semi-infinite branches. They have proven that the spectrum of the Schrödinger operator is discrete, provided that the potential is real, bounded from below and integrable, that the boundary conditions at the vertices are standard and that the graph is compact. At the same time, P. Exner and P. Šeba analysed numerous examples of quantum graphs [22; 23]. Besides the pure one dimensional case, they also studied more complicated structures: graphs with higher dimensional inclusions, such as a wire attached to a plane or graph superlattices [21]. Since then P. Exner has contributed to virtually all directions of research involving quantum graphs.

The above research was based on theory developed for the case of a finite interval, which can be seen as the simplest example of a geometric graph. The inverse spectral problem for the Schrödinger operator on a finite interval has been studied extensively in the middle of the last century. This problem consists of recovering the potential in the Schrödinger operator from its spectrum. One of the first mathematicians to study this problem was V. A. Ambarzumian, who proved in 1929 that in one exceptional case the spectrum of the Schrödinger operator *does* determine the potential uniquely [2]. In general, one needs two spectra in order to determine the potential, a fact shown by G. Borg [11]. Later on, I. M. Gelfand and B. M. Levitan [29] gave an explicit method for calculating the potential $q(x)$, known today as the Gelfand-Levitan equation. Studies of the inverse spectral problem were being developed in close connection with the investigations of the inverse scattering problem on the infinite interval. The latter problem has been considered by G. Borg and V. A. Marchenko [12; 53]. These results have to be taken into account while investigating the inverse problems for metric graphs.

In the nineties and at the beginning of this century the spectral theory of quantum graphs experienced renaissance due to many potential applications in modern technology. Therefore, properties of arbitrary quantum graphs and different inverse problems

have been investigated by numerous authors. These studies include not only conventional ”locally” one-dimensional graphs but graphs with inclusions in the form of billiards and manifolds.

V. Kostrykin and R. Schrader have given the most general mathematically rigorous definition for a Schrödinger operator on a metric graph [40]. Their paper plays an important role in the theory of quantum graphs since then. In particular, they have described the most general vertex boundary conditions. The question of how to parameterise the boundary conditions has also been discussed by M. Harmer and P. Kuchment [37; 44; 45]. A detailed analysis of this topic is presented in section 3.4. of this thesis. In particular, we present a slightly novel parameterisation of the boundary conditions via the vertex scattering matrix, which has an advantage of being unique and having a straightforward relation with the connectivity of the graph (see section 4.2.). Recently, there have appeared two volumes entirely devoted to quantum graphs and we refer the reader to these volumes for most state-of-the-art developments of this theory. They also contain excellent introductions written by P. Kuchment [45; 46]. In addition we would like to mention important studies of spectral problems for quantum graphs carried out in series of papers by Solomyak [55; 56; 68; 69; 70; 71] and interesting examples of the two-dimensional periodic square graph lattice studied by K. Pankrashkin, V. Geyler and J. Brüning in [60; 15].

This thesis focuses on inverse problems for quantum graphs. To solve such a problem, one has to reconstruct:

- the metric graph,
- the real potential on the edges,
- the boundary conditions at the vertices.

At this moment only the inverse problem for quantum trees is close to being fully solved.

The inverse spectral and scattering problems for trees have been studied intensively in recent years, among others, by S. Avdonin, M. Belishev, M. Brown, R. Carlson, G. Freiling, P. Kurasov, A. Vakulenko, R. Weikard and V. Yurko [3; 6; 7; 13; 14; 17; 26; 27; 74]. It has been shown 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 [27], but the whole family of boundary conditions has not been investigated yet. In general, the methods used in inverse spectral problems for quantum graphs resemble very much the methods developed for ordinary differential operators. In particular, we discuss the problem of recovering boundary conditions for the special case of the star graph in paper IV. We believe that combination of the methods developed there, together with the boundary control method applied to quantum graphs in [3], will lead to a complete solution of the inverse problem for quantum trees. This is the main topic of section 7.

The spectral problems for general quantum graphs (i. e. with cycles) are much more sophisticated than those for trees. Therefore, in the literature one can find many more papers dealing with trees than with arbitrary graphs. The main reason is that the Cauchy

problem, on a graph with cycles and for arbitrary Cauchy data, may possess infinitely many solutions or even cannot be solved at all. This is the main reason why differential equations on graphs have properties of both ordinary and partial differential equations. The corresponding inverse scattering problems were discussed in [52] by P. Kurasov and F. Stenberg. They have shown that, in general, the scattering matrix does not determine neither the topology of the graph, the potentials on the edges, nor the boundary conditions. Methods used in this work have been generalised by J. Boman and P. Kurasov in [10], where it is proven that operators on graphs with internal symmetries cannot be recovered from the scattering matrices. On the other hand, P. Kurasov has shown that the Euler characteristics of the graph can be calculated from the scattering matrix and discrete spectrum of Schrödinger operator with essentially bounded compactly supported potential [48; 49]. The method used in these latest papers is based on the trace formula first presented (without proof) by J.-P. Roth in [64]. The trace formula used was first given by T. Kottos and U. Smilansky [43], but without paying attention to the fact that the secular equation describing the spectrum in general does not determine the correct multiplicity of the eigenvalue zero.

B. Gutkin and U. Smilansky [36] have applied the trace formula to the inverse spectral problem for graphs with rationally independent lengths of the edges. Mathematically rigorous proof of the trace formula for the case of standard boundary conditions is given in paper I. In the same paper, we also present the rigorous algorithm of reconstructing the metric graph with rationally independent lengths of the edges from the spectrum of the Laplace operator. In paper II it is shown that the condition of rational independence can be weakened. Moreover, in paper III, the trace formula has been derived even for arbitrary vertex boundary conditions leading to energy independent vertex scattering matrices, so-called non-resonant boundary conditions (see section 5.)

The trace formula can be used to prove that the Euler characteristic of the underlying graph is determined by the spectrum of the Laplace operator [48; 49]. An explicit formula for the Euler characteristics has been derived for standard boundary conditions in the case of Schrödinger operator in [49]. The spectral properties of the Laplace operator for discrete graphs and the topological invariants have been also investigated by S. Novikov and Y. Colin de Verdière [19; 57].

Applications of quantum graphs arise in many fields of science, such as chemistry (free electron theory of conjugated molecules [34; 35; 66]), superconductivity (thin superconducting networks [1; 65]), nanotechnology (quantum wires circuits [22]), optics (photonic crystals [24; 47; 67]), scattering theory [31], averaging in dynamical systems [25], spectral theory of differential operators in singular domains [20] and others. Quantum graphs are also used as testing models for more realistic operators, since solving ordinary differential equations is in general easier than solving partial differential ones. Such quantum graphs are used in quantum chaos theory [55] and to model effects of electron propagation in non-simply-connected media [5]. Another example of practical application of quantum graphs in nanowires has been presented by M.-E. Pistol in [62; 63].

2. Isospectral graphs

In this section we present an example of two isospectral Laplace operators on graphs, which shows that already the problem to reconstruct the metric graph is not trivial. This example shows that the inverse spectral problem in general cannot be solved uniquely. It has served as a motivation for our research. This also explains the reason why only the Laplace operator is investigated in this thesis.

2.1. "Can one hear the shape of a drum?"

For two-dimensional manifolds, a corresponding inverse spectral problem was formulated in 1966 by M. Kac as "Can one hear the shape of a drum?" It turns out that methods developed for certain partial differential operators can be applied successfully to quantum graphs.

Mark Kac's question "Can one hear the shape of a drum?" mathematically means that, if D_1 and D_2 are two isospectral domains in the Euclidean plane, must D_1 and D_2 be actually isometric? In his paper M. Kac showed that the eigenvalues *do* determine certain properties of domain D, for example the area, the circumference and the number of connected components [39]. Two years earlier, in 1964, Milnor found two 16-dimensional tori that are not congruent but are nevertheless isospectral [54]. Later, it was proven that there exist non-isometric pairs of Riemannian manifolds that are, nevertheless, isospectral.

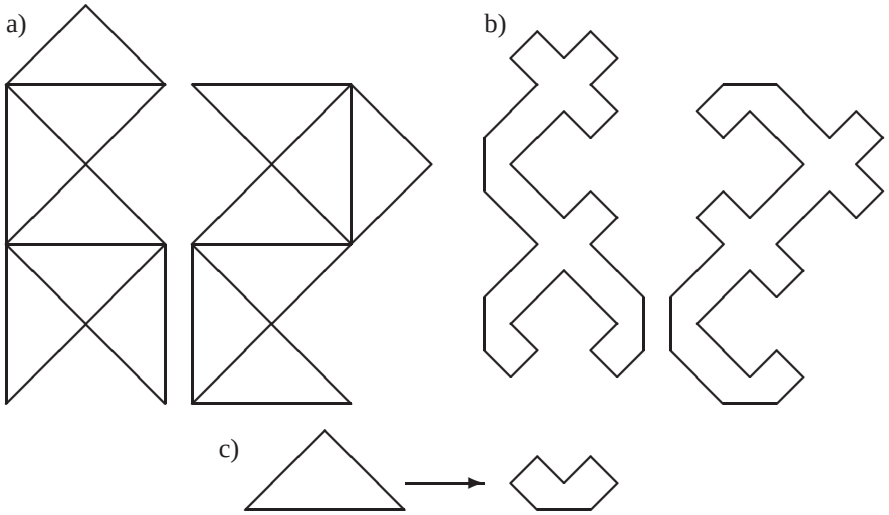


Figure 1: Two isospectral planar domains

Finally, in 1992, the M. Kac's question was answered, and this answer was negative (see [32] and [33]). Gordon, Webb and Wolpert, using the method developed by T. Sunada in [72], gave an explicit example of two non-isometric, simply-connected domains in the Euclidean plane which are both Dirichlet and Neumann isospectral. The Fig. 1b shows these two isospectral domains. Moreover, the authors of that pa-

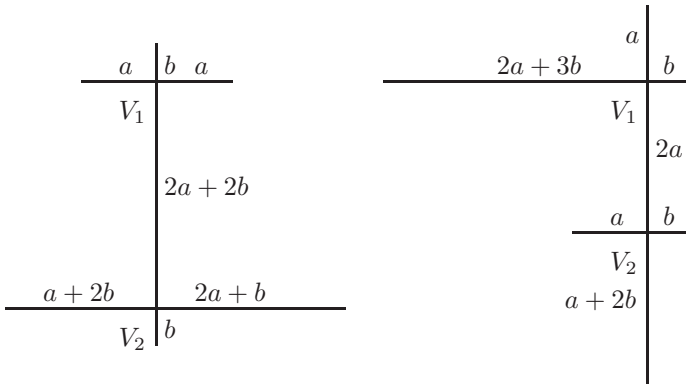


Figure 2: Two isospectral but non-isometric graphs. The edge lengths are expressed in terms of the two arbitrary lengths a and b.

per pointed out that one can make a simple geometric substitution (inverse mapping showed in Fig. 1c) to get another two isospectral domains shown in Fig. 1a.

2.2. "Can one hear the shape of a graph?"

We can follow Kac's question and ask "Can one hear the shape of the graph?" B. Gutkin and U. Smilansky in the paper [36] have shown that the answer is negative. Their counterexample was based on the ideas developed by C. Gordon, D. Webb and S. Wolpert [32] and by S. J. Chapman [18]. A similar problem for networks was analysed by J. von Below in [8].

Intuitively, one of the ways to construct isospectral graphs is to take two isospectral domains shown in Fig. 1a and to choose the subset of V-shape of each triangle as suggested on Fig. 1c in order to obtain the domains like those in Fig. 1b. Next, we shrink the width of the branches of V-shape in such a way that one branch has length a and the other has length b. We obtain graphs presented in Fig. 2. From this construction, it is clear that the two graphs have the same spectrum, provided the differential operator and the boundary conditions are chosen properly. It is natural to consider the Laplace operator with standard boundary conditions (see section 3.3.) at all internal vertices and at loose endpoints one can choose either Dirichlet or Neumann boundary conditions.

It is possible to calculate the spectra of corresponding Laplace operators explicitly and to compare them. Preliminary calculations were presented in [36], while complete analysis has been carried out by the author of this thesis in [58] and later by E. Wernersson in [73]. The cases of standard boundary conditions at all internal vertices and Dirichlet and Neumann conditions at loose endpoints were considered in [58] and [73], respectively.

3. Quantum graphs - definition

By **quantum graph** we mean a geometric graph Γ with symmetric differential expressions on the edges and with boundary conditions at the vertices, which guarantee the self-adjointness of the operator.

Let N be the total number of edges in Γ. We will identify each edge Δ_j, $j = 1, 2, \ldots, N$, of the graph with the interval of the real line $\Delta_j = [x_{2j-1}, x_{2j}] \subset \mathbb{R}$. We will denote the length of each edge by $d_j = |x_{2j} - x_{2j-1}|$. Furthermore, let us denote by M the number of vertices in the graph, where each vertex V_m is a set of equivalent endpoints from $\{x_k\}_{k=1}^{2N}$. The valence (degree) of the vertex, i.e. the number of endpoints joined at V_m, will be denoted by v_m.

A geometric graph Γ can be equipped with the natural metric $\rho(x, y)$ induced by the distances on the intervals Δ_j and thus can be considered as a metric space. Notice that the graph Γ, as a set, contains not only the vertices but all points on the edges. Therefore, one can define the Lebesgue measure $\mathrm{d}x$ on the graph in a natural way. Any function $f(x)$ on Γ is defined along each edge rather than only at the vertices as it would be in a discrete model.

In order to define a self-adjoint differential operator on Γ, let us consider the Hilbert space of square integrable functions on Γ:

$$\mathcal{H} \equiv L^2(\Gamma) = \oplus_{j=1}^{N} L^2(\Delta_j) = \oplus_{j=1}^{N} L^2[x_{2j-1}, x_{2j}]. \tag{1}$$

3.1. Differential operators

For quantum graphs, the most commonly used operator is the *Laplace operator*, which is equal to the negative second derivative:

$$L = \oplus_{j=1}^{N} \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} \right) . \tag{2}$$

An example of a more general operator is the *Schrödinger operator* with potential $q(x)$ on the edges

$$H = \oplus_{j=1}^{N} \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + q(x) \right) , \quad q(x) \in \mathbb{R},$$

where q belongs to the space of integrable functions L^1.

Finally, one can analyse an even more general *magnetic Schrödinger operator*, with real potentials $q(x)$ and $A(x)$ being sufficiently smooth

$$H_M = \oplus_{j=1}^{N} \left(\left(\frac{1}{\mathrm{i}} \frac{\mathrm{d}}{\mathrm{d}x_j} - A(x) \right)^2 + q(x) \right) .$$

Higher order differential and even pseudo-differential operators have been used by various researchers in studies of quantum graphs (see, for example, [45; 23] and references therein).

The problem of reconstructing the potential is very difficult in general case, therefore in this thesis, we will limit ourselves to the Laplace operator (2) only. This differential expression does not determine a self-adjoint operator uniquely and two differential operators in $L^2(\Gamma)$ are naturally associated with expression (2): the minimal operator $L_{\min}$ with the domain $\mathrm{Dom}\,(L_{\min}) = \oplus_{j=1}^{N} C_0^\infty(\Delta_j)$ and the maximal operator $L_{\max}$ with the domain $\mathrm{Dom}\,(L_{\max}) = \oplus_{j=1}^{N} W_2^2(\Delta_j)$, where W_2^2 denotes the Sobolev space:

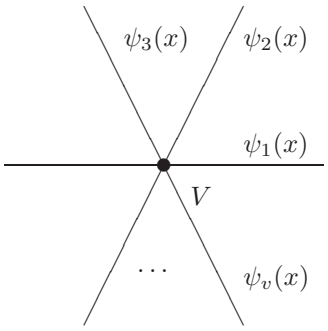
$$W_2^2(\Delta_j) = \{f \in L^2(\Delta_j) \mid f', f'' \in L^2(\Delta_j)\}.$$

The operator $L_{\max}$ is simply the adjoint operator to $L_{\min}$, $L_{\max} = L_{\min}^*$.

3.2. Self-adjoint boundary conditions for the Laplace operator

In this and following sections we are going to discuss how to define boundary conditions at a vertex in such a way that operator on the graph is self-adjoint and boundary conditions are consistent with the vertex structure. As we will see later, the boundary conditions also determine how the edges match each other. Thus, we will sometimes use the name *matching conditions*, instead of "boundary conditions". In order to make our presentation more readable, we will start by studying the star graph, having in mind to generalise our considerations later for the case of more complicated graphs.

Let us consider a star graph Γ_{star} with v semi-infinite nodes $\Delta_j = [0, \infty)$, $j = 1, 2, \ldots, v$, connected at one vertex V with valence v (equal to the number of edges connected at the vertex). In this case the Hilbert space of square integrable functions is



equal to

$$\mathcal{H} \equiv L^2(\Gamma) = \oplus_{j=1}^{v} L^2([0, \infty)). \tag{3}$$

The Laplace operator on Γ_{star} is the sum of the second derivative operators on each interval Δ_j,

$$\oplus_{j=1}^{v} \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} \right). \tag{4}$$

and the domains of the minimal and the maximal operator $L_{\min}$ and $L_{\max}$ are given as $\mathrm{Dom}\,(L_{\min}) = \oplus_{j=1}^{v} C_0^\infty((0, \infty))$ and $\mathrm{Dom}\,(L_{\max}) = \oplus_{j=1}^{v} W_2^2((0, \infty))$. Every self-adjoint operator L associated with the differential expression (4) can be obtained

by extending the minimal operator or by restricting the maximal one so that $L_{\min} \subset L \subset L_{\max}$. The domain of every such operator can be described using certain boundary conditions connecting boundary values of the functions on $\Gamma_{\rm star}$ at the vertex V.

Such self-adjoint extensions can be described using von Neumann formulae taking into account that $L_{\min}$ is symmetric and has deficiency indices (v, v), while parameterisation via boundary conditions appears more appropriate due to their local character.

Another parameterisation of extensions of $L_{\min}$ can be obtained using Lagrangian planes. Consider the boundary form of the maximal operator:

$$B[\varphi,\psi] = \langle L_{\max}\varphi,\psi\rangle - \langle\varphi, L_{\max}\psi\rangle = \sum_{j=1}^{v}(\partial_n\varphi_j(0)\overline{\psi_j}(0) - \varphi_j(0)\partial_n\overline{\psi_j}(0)),$$

where $\partial_n\psi$ denotes the normal derivative of the function ψ at the vertex V. Let us denote by $\boldsymbol{\psi}$ and $\partial_n\boldsymbol{\psi}$ the vectors of boundary values for φ and the values of its normal derivative at the vertex V, respectively. The boundary form gives a sesquilinear symplectic form in the finite dimensional space of boundary values $\mathbb{C}^{2v} = \{\boldsymbol{\psi}, \partial_n\boldsymbol{\psi}\}$. Then all Lagrangian planes π, i. e. all maximal subspaces in $\mathbb{C}^{2v}$ annulating the boundary form such that $\varphi, \psi \in \pi$ implies $B[\varphi, \psi] = 0$, describe all self-adjoint extensions of the minimal operator $L_{\min}$ to be denoted by L_π, so that $\mathrm{Dom}(L_\pi) = \{\varphi \in \mathrm{Dom}(L_{\max}) : (\boldsymbol{\varphi}(0), \partial_n\boldsymbol{\varphi}(0)) \in \pi\}$.

3.3. Boundary conditions via the vertex scattering matrix

In this section we are going to show that the boundary conditions at any vertex can be parameterised in a unique way by a certain unitary matrix. Our approach is a slight modification of that by M. Harmer [37], with the advantage of our parameterisation being that the parameter matrix S coincides with the value of the vertex scattering matrix at $k = 1$ (this explains our notation as well).

Theorem 1. *The family of self-adjoint extensions of the minimal operator $L_{\min}$ can be uniquely parameterised by an arbitrary $v \times v$ unitary matrix S, so that the operator $L(S)$ is the restriction of $L_{\max} = L^*_{\min}$ to the set of functions satisfying the boundary conditions*

$$i(S - I)\boldsymbol{\psi}(V) = (S + I)\partial_n\boldsymbol{\psi}(V). \tag{5}$$

The proof of this theorem can be found in paper III.

The advantage of parameterisation (5) is that there is one-to-one correspondence between S and self-adjoint extensions of $L_{\min}$ and the parameter has a clear meaning being the vertex scattering matrix for $E = 1$. Let us have a look at two intensively studied families of boundary conditions.

EXAMPLE 1. *Standard boundary conditions.* Let in this and the following example $\psi_n = \psi_n(0))$ for any $n = 1, \dots, v$. To get standard boundary conditions

$$\begin{cases} \psi_j = \psi_k, \quad j,k = 1,\dots,v, \\ \sum_{j=1}^{v}\partial_n\psi_j = 0, \end{cases} \tag{6}$$

the matrix S should be chosen equal to

$$S = \begin{pmatrix} \frac{2-v}{v} & \frac{2}{v} & \dots & \frac{2}{v} \\ \frac{2}{v} & \frac{2-v}{v} & & \frac{2}{v} \\ & & \dots & \\ \frac{2}{v} & \frac{2}{v} & & \frac{2-v}{v} \end{pmatrix}.$$

Then

$$S - I = \begin{pmatrix} \frac{2(1-v)}{v} & \frac{2}{v} & \frac{2}{v} \\ \frac{2}{v} & \frac{2(1-v)}{v} & \frac{2}{v} \\ & \dots & \\ \frac{2}{v} & \frac{2}{v} & \frac{2(1-v)}{v} \end{pmatrix}, \quad S + I = \begin{pmatrix} \frac{2}{v} & \frac{2}{v} & \frac{2}{v} \\ \frac{2}{v} & \frac{2}{v} & \frac{2}{v} \\ & \dots & \\ \frac{2}{v} & \frac{2}{v} & \frac{2}{v} \end{pmatrix}.$$

The boundary conditions (5) look as follows:

$$\begin{cases} i((1-v)\psi_1 + \psi_2 + \ldots + \psi_v) - (\partial_n\psi_1 + \ldots + \partial_n\psi_v) = 0, \\ i(\psi_1 + (1-v)\psi_2 + \ldots + \psi_v) - (\partial_n\psi_1 + \ldots + \partial_n\psi_v) = 0, \\ \vdots \\ i(\psi_1 + \psi_2 + \ldots + (1-v)\psi_v) - (\partial_n\psi_1 + \ldots + \partial_n\psi_v) = 0. \end{cases}$$

Subtracting the first equation from each of the other ones we obtain:

$$\begin{cases} i((1-v)\psi_1 + \psi_2 + \ldots + \psi_v) - (\partial_n\psi_1 + \ldots + \partial_n\psi_v) = 0, \\ i(v\psi_1 - v\psi_2) = 0, \\ \vdots \\ i(v\psi_1 - v\psi_v) = 0. \end{cases}$$

Finally we get $\psi_1 = \psi_2 = \ldots = \psi_v$ and $\partial_n\psi_1 + \ldots + \partial_n\psi_v = 0$, which are exactly the standard boundary conditions.

EXAMPLE 2. *Boundary conditions of δ-type.* To get boundary conditions of $\delta-$type:

$$\begin{cases} \psi_j = \psi_k, \quad j,k = 1,\ldots,v, \\ \sum_{j=1}^{v} \partial_n\psi_j = \alpha\psi_1, \end{cases} \tag{7}$$

the scattering matrix for $E = 1$ should be chosen equal to

$$S = \frac{1}{vi - \alpha} \begin{pmatrix} \alpha - (v-2)i & 2i & \dots & 2i \\ 2i & \alpha - (v-2)i & \dots & 2i \\ & & \ddots & \\ 2i & 2i & \dots & \alpha - (v-2)i \end{pmatrix},$$

where α is the real constant determining the strength of the δ-function at the vertex. Then

$$S - I = \frac{2}{vi - \alpha} \begin{pmatrix} \alpha - (v-1)i & i & \dots & i \\ i & \alpha - (v-1)i & \dots & i \\ & & \ddots & \\ i & i & \dots & \alpha - (v-1)i \end{pmatrix}$$

and

$$S + I = \frac{2i}{vi - \alpha} \begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & 1 & \dots & 1 \\ & & \ddots & \\ 1 & 1 & \dots & 1 \end{pmatrix}.$$

Therefore, the boundary conditions (5) look as follows:

$$\begin{cases} (\alpha - (v-1)i)\psi_1 + i\psi_2 + \ldots + i\psi_v - (\partial_n\psi_1 + \ldots + \partial_n\psi_v) = 0, \\ i\psi_1 + (\alpha - (v-1)i)\psi_2 + \ldots + i\psi_v - (\partial_n\psi_1 + \ldots + \partial_n\psi_v) = 0, \\ \vdots \\ i\psi_1 + i\psi_2 + \ldots + (\alpha - (v-1)i)\psi_v - (\partial_n\psi_1 + \ldots + \partial_n\psi_v) = 0. \end{cases}$$

Similarly as in the previous example, we subtract the first equation from every other one

$$\begin{cases} (\alpha - (v-1)i)\psi_1 + i\psi_2 + \ldots + i\psi_v - (\partial_n\psi_1 + \ldots + \partial_n\psi_v) = 0, \\ (\alpha - vi)\psi_1 + (vi - \alpha)\psi_2 = 0, \\ \vdots \\ (\alpha - vi)\psi_1 + (vi - \alpha)\psi_v = 0. \end{cases}$$

Thus $\psi_1 = \psi_2 = \ldots = \psi_v$, i. e. the functions ψ are continuous at the vertex V and from the first equation we obtain

$$(\alpha - (v-1)i)\psi_1 + (v-1)i\psi_1) - (\partial_n\psi_1 + \ldots + \partial_n\psi_v) = 0$$

and hence

$$\alpha\psi_1 = \partial_n\psi_1 + \ldots + \partial_n\psi_v.$$

Having considered these examples, let us establish the connection between the matrix S appearing in the boundary conditions and the vertex scattering matrix $S_v(k)$. Since S is a unitary matrix then it possesses the following spectral representation:

$$S\psi = \sum_{j=1}^{v} e^{i\theta_j} \langle \psi, \phi_j \rangle \phi_j, \tag{8}$$

where $e^{i\theta_j}$ is the eigenvalue and ϕ_j ($\theta_j \in \mathbb{R}, \langle \phi_i, \phi_j \rangle = \delta_{ij}, j = 1, \ldots, v$) is the corresponding eigenfunction.

In what follows the subspaces related to the eigenvalues 1 and -1

$$N_{\pm 1} = \ker\left(S - (\pm I)\right), \tag{9}$$

are going to play a very important role.

To introduce the vertex scattering matrix let us first consider the solutions to the differential equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) = k^2\psi(x), \quad x \in \Delta_j, \tag{10}$$

which satisfy the boundary conditions (5) at the vertex. Solution to the differential equation can be written in the basis of incoming and outgoing waves as shown below

$$\psi_j(x) = b_j e^{-ikx} + a_j e^{ikx}, \quad x \in \Delta_j. \tag{11}$$

The amplitudes $\mathbf{a}$ and $\mathbf{b}$ have to be chosen so that the function in (11) satisfies the boundary conditions at the vertex. The relation between the vectors of waves' amplitudes $\boldsymbol{a}$ and $\boldsymbol{b}$ is given by the vertex scattering matrix $S_v(k)$ as $\boldsymbol{a} = S_v(k)\boldsymbol{b}$. The values of the functions and of its normal derivatives at the vertex are:

$$\boldsymbol{\psi}(V) = \boldsymbol{b} + \boldsymbol{a} = \boldsymbol{b} + S_v(k)\boldsymbol{b}$$

and

$$\partial_n\boldsymbol{\psi}(V) = -ik\boldsymbol{b} + ik\boldsymbol{a} = -ik\boldsymbol{b} + ikS_v(k)\boldsymbol{b}.$$

After substitution into equation (5) we obtain

$$i(S - I)(I + S_v(k)) = ik(S + I)(-I + S_v(k))$$

and then

$$S_v(k) = \frac{k(S + I) + (S - I)}{k(S + I) - (S - I)}, \quad k \neq 0. \tag{12}$$

Thus $S_v(k)$ is a unitary vertex scattering matrix and S equals $S_v(1)$. In paper III we have shown that all boundary conditions at a vertex leading to self-adjoint extensions of $L_{\min}$ can be described by the matrix S. We would like to point out that in 2000 V. Kostrykin and R. Schrader ([41], Theorem 1) showed that the knowledge of $S_v(k_0)$ for some fixed energy parameter k_0 allows one to calculate $S_v(k)$ for any arbitrary k, and therefore determines the boundary conditions at the vertex.

3.4. Parameterisations of boundary conditions

Kostrykin-Schrader's parameterisation

In 1999, V. Kostrykin and R. Schrader [40] gave a full description of self-adjoint boundary conditions. Let A and B be $v \times v$ matrices. Then all boundary conditions at the vertex V can be described in the following way:

$$A\boldsymbol{\psi}(V) + B\partial_n\boldsymbol{\psi}(V) = 0, \tag{13}$$

where $\boldsymbol{\psi}$ is the v-dimensional vector of functions and $\partial_n\boldsymbol{\psi}$ - of normal derivatives defined on edges meeting at the vertex V.

Proposition 2 (Kostrykin, Schrader). *All self-adjoint extensions of the minimal operator $L_{\min}$ are described by the boundary conditions* (13) *where A and B are $v \times v$ matrices with the following properties:*

1. *the $v \times 2v$ matrix (A, B) has maximal rank v,*
2. *the matrix AB^* is Hermitian.*

Notice that parameterisation of boundary conditions in equation (13) with matrices A and B is not unique . One can take any arbitrary invertible matrix D and use matrices $A' = DA$ and $B' = DB$ instead of A and B. These matrices determine the same Lagrangian plane of boundary values.

The relation between the scattering matrix $S_v(k)$ and the matrices A and B (see [41]) can be written as

$$S_v(k) = -(A + ikB)^{-1}(A - ikB) \tag{14}$$

and, in particular,

$$S = S_v(1) = -(A + iB)^{-1}(A - iB). \tag{15}$$

Harmer's parameterisation

Another way to parameterise boundary conditions in a unique way and using only one unitary matrix U was proposed by M. Harmer in 2000 [37]

$$-i(U + I)\boldsymbol{\psi}(V) + (U - I)\partial_n\boldsymbol{\psi}(V) = 0. \tag{16}$$

In this parameterisation the unitary matrix again does not coincide with the unitary matrix appearing in von Neumann formulae. One may obtain this parameterisation from (5) simply by putting $S = -U$. The only advantage of the parameterisation via the matrix S is that it has a clear meaning, since it is the vertex scattering matrix for $k = 1$.

Kuchment's parameterisation

In 2004 P. Kuchment noticed that boundary condition (13) can be rewritten equivalently as two conditions which use orthogonal projection on $\ker B$. This makes Kostrykin-Schrader's parameterisation unique.

Proposition 3 (following Corollary 5 in [45]). *Let (A, B) has maximal rank and AB^* be Hermitian matrix. Then the boundary condition* (13) *is equivalent to the pair of conditions $P_{M^\perp}\boldsymbol{\psi} = 0$ and $LP_M\boldsymbol{\psi} + P_M\partial_n\boldsymbol{\psi} = 0$, where P_M is orthogonal projection onto space $M = (\mathrm{Ker}\ B)^\perp$, $P_{M^\perp}$ is the complementary projector, and L is the self-adjoint operator $B^{-1}A$.*

The operator $i\frac{\hat{S}-I}{\hat{S}+I}$, where $\hat{S} = P_{N_{-1}^\perp}SP_{N_{-1}^\perp}$, is hermitian in $N_{-1}^\perp$. Therefore, it can be shown that we obtain P. Kuchment's parameterisation by taking

$$M = N_{-1}^\perp \quad \text{and} \quad L = i\frac{P_{N_{-1}^\perp}SP_{N_{-1}^\perp} - I}{P_{N_{-1}^\perp}SP_{N_{-1}^\perp} + I}\ .$$

4. Boundary conditions and vertex scattering properties

In this section we shall describe how boundary conditions reflect the scattering properties of the vertex. We will start by looking at high energy asymptotics, showing that it is equal to some energy independent scattering matrix. Afterwards, we will discuss how does the vertex scattering matrix reflect connectivity of the vertex. Finally, we introduce and investigate in detail a new class of boundary conditions which we call hyperplanar matching conditions.

4.1. High energy asymptotics

In order to study the spectral asymptotics it is necessary to investigate the high energy behaviour of the vertex scattering matrix.

Let us remind that the unitary matrix S possesses the spectral representation (8) and that the vertex scattering matrix $S_v(k)$ is given by (12). We then obtain the following representation for the matrix $S_v(k)$:

$$\begin{aligned} S_v(k)\psi &= \sum_{j:\theta_j=\pi} (-1)\langle\psi,\phi_j\rangle\phi_j + \sum_{j:\theta_j=0} 1\langle\psi,\phi_j\rangle\phi_j \\ &+ \sum_{j:\theta_j\neq\pi,0} \frac{k(e^{i\theta_j}+1)+(e^{i\theta_j}-1)}{k(e^{i\theta_j}+1)-(e^{i\theta_j}-1)}\langle\psi,\phi_j\rangle\phi_j. \end{aligned} \tag{17}$$

Since S is unitary N_1 and N_{-1} are orthogonal to each other; if S has no other eigenvalues, then $N_1 \oplus N_{-1} = \mathbb{C}^v$. Formula (17) implies that the eigenvalues ± 1 are stable, whereas all other eigenvalues depend on k. The properties of this representation for $S_v(k)$ give us immediately the following two theorems.

Theorem 4. *The scattering matrix $S_v(k)$ is energy independent if and only if the parameter matrix S has just eigenvalues 1 and -1, i.e. iff boundary conditions* (5) *take the form*

$$P_{N_1}\partial_n\boldsymbol{\psi}(V) = 0, \quad P_{N_{-1}}\boldsymbol{\psi}(V) = 0, \tag{18}$$

where $N_1 \oplus N_{-1} = \mathbb{C}^v$.

Boundary conditions leading to energy independent vertex scattering matrices are going to play an important role in our studies, therefore we would like to introduce the following definition

Definition 5. *Vertex boundary conditions are called* **non-resonant** *iff the corresponding vertex scattering matrix is energy independent.*

The main motivation for this definition is that all other boundary conditions lead to vertex scattering matrices having singularities.

From spectral representation (8) we immediately obtain

Theorem 6. *As $k \to \infty$, the vertex scattering matrix tends to the energy independent vertex scattering matrix*

$$S_v^\infty = \sum_{j:\theta_j=\pi} (-1)\langle \cdot, \phi_j\rangle \phi_j + \sum_{j:\theta_j\neq\pi} \langle \cdot, \phi_j\rangle \phi_j \equiv -P_{N_{-1}} + P_{N_{-1}^\perp}, \tag{19}$$

where N_{-1} is the eigensubspace for S (and hence for all $S(k)$). In addition, the following holds

$$S_v(k) = S_v^\infty + \mathcal{O}(1/k), \quad \text{as } k \to \infty.$$

The above theorem is a modification of the result already given by M. Harmer in [37] and it implies, that for high energies, every vertex scattering matrix tends to a certain scattering matrix corresponding to non-resonant boundary conditions.

4.2. Vertex scattering matrix and connectivity

In this section we will discuss what additional conditions (beyond unitarity) are needed for the matrix S_v to connect all endpoints meeting at the vertex V. The only requirement we introduced so far is that the boundary conditions (5) connect together only boundary values corresponding to the vertex V. This alone is insufficient since it might happen that the endpoints can be divided into two classes $V = V_1 \cup V_2$ in such a way that the boundary conditions connect together the boundary values at V_1 and V_2 separately. Unfortunately, in a case like this, boundary conditions do not correspond to the vertex V but rather to two (independent) vertices V_1 and V_2 (see Fig. 3). In other

Figure 3: Boundary conditions and connectivity

words, if the vertex V can be chopped into two vertices in such a way that the boundary conditions are preserved, then those conditions are not properly connecting and should be excluded from our consideration if no special reason exists to do otherwise. This problem has been discussed in details in [52], [42], but we describe it using the parameterisation via the matrix S. Due to uniqueness of this parameterisation the discussion becomes much more transparent.

For energy dependent vertex scattering matrices, we are facing another interesting effect. It might happen that the corresponding boundary conditions are properly connecting, but the boundary conditions corresponding to the limit scattering matrix S_v^∞ are not. However, it is the limit scattering matrix that is important in calculating spectral asymptotics. Therefore, we also need to define asymptotically properly connecting boundary conditions, but let us consider one example first.

EXAMPLE 3. Let the graph Γ be a loop formed by just one edge $\Delta_1 = [-\pi, \pi]$ with the endpoints $-\pi$ and π connected at the vertex V_1. Consider the boundary conditions

$$\begin{cases} \psi(-\pi) &= -\partial_n\psi(+\pi), \\ \psi(\pi) &= -\partial_n\psi(-\pi), \end{cases}$$

which are clearly properly connecting and correspond to $S = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$. The vertex scattering matrix can be calculated using (12) to be

$$S_v^1(k) = \begin{pmatrix} \dfrac{k^2-1}{k^2+1} & \dfrac{2ik}{k^2+1} \\ \dfrac{2ik}{k^2+1} & \dfrac{k^2-1}{k^2+1} \end{pmatrix}.$$

Clearly, it tends to the unit matrix as $k \to \infty$. The boundary conditions corresponding to unit scattering matrix are simply Neumann boundary conditions $\partial_n\psi(-\pi) = \partial_n\psi(\pi) = 0$, which do not connect the values at $\pm\pi$ together.

Let us summarise our discussion by giving the following definition.

Definition 7. *Vertex boundary conditions are called* **properly connecting** *iff the vertex cannot be divided into two (or more) vertices in such a way that the boundary conditions connect together only boundary values belonging to each of the new vertices. Vertex boundary conditions are called* **asymptotically properly connecting** *iff the limit scattering matrix S_v^∞ corresponds to certain properly connecting boundary conditions.*

Characterisation of all properly connecting boundary conditions via the matrix S is rather straightforward, which again can be attributed to the uniqueness of our parameterisation of boundary conditions.

Theorem 8. *Boundary conditions* (5) *are properly connecting if and only if the unitary matrix S cannot be turned into block-diagonal form by any permutation of the basis vectors.*

We are now going to study the relation between the properly connecting boundary conditions and the space N_{-1} in more details. In order to do this, we need to introduce the notion of *coordinate subspace* — any subspace in $\mathbb{C}^n$ spanned by a certain number of basic vectors from the standard basis in $\mathbb{C}^n$, but does not coincide with $\mathbb{C}^n$. This is a straightforward generalisation of the notion of coordinate planes in $\mathbb{R}^3$. We say that a subspace N is *perpendicular* to a coordinate subspace K iff $P_K N \subset N \cap K$ and $P_N K \subset N \cap K$, where P denotes the orthogonal projection.

Theorem 9. *The non-resonant boundary conditions corresponding to the matrix S are properly connecting iff N_{-1} is not perpendicular to any coordinate subspace.*

This theorem can be generalised to describe all asymptotically properly connecting boundary conditions using the fact that the subspace N_{-1} is stable for $S_v(k)$.

Theorem 10. *The boundary conditions are asymptotically properly connecting iff N_{-1} is not perpendicular to any coordinate subspace.*

The energy independent scattering matrix S is not properly connecting for example in the following two cases:

1. $N_1 = \{0\}, N_{-1} = \mathbb{C}^v$, which corresponds to the Dirichlet boundary conditions at the endpoints forming the vertex;
2. $N_1 = \mathbb{C}^v, N_{-1} = \{0\}$, which corresponds to the Neumann boundary conditions at the endpoints forming the vertex.

Clearly, these boundary conditions are not properly connecting and they correspond to the case where the vertex V is maximally decomposed into v separate edges.

4.3. Hyperplanar matching conditions

Let $\boldsymbol{\psi}(V) = (\psi(x_1), \psi(x_3), \ldots, \psi(x_{2v-1}))$ and let us define the following two important families of properly connecting non-resonant boundary conditions:

1. **Hyperplanar Neumann conditions** — defined by a certain vector $\boldsymbol{w} \in \mathbb{C}^v$ with all components different from zero

$$\begin{cases} \boldsymbol{\psi}(V) \parallel \boldsymbol{w}, \\ \partial_n \boldsymbol{\psi}(V) \perp \boldsymbol{w}. \end{cases} \tag{20}$$

2. **Hyperplanar Dirichlet conditions** — defined by a certain vector $\boldsymbol{u} \in \mathbb{C}^v$ with all components different from zero

$$\begin{cases} \boldsymbol{\psi}(V) \perp \boldsymbol{u}, \\ \partial_n \boldsymbol{\psi}(V) \parallel \boldsymbol{u}. \end{cases} \tag{21}$$

These boundary conditions correspond to the case where one of the subspaces N_1 and N_{-1} is one dimensional. For hyperplanar Dirichlet conditions N_{-1} is spanned by $\boldsymbol{u}$ and, since all components of $\boldsymbol{u}$ are different from zero, N_{-1} is not perpendicular to any coordinate subspace. For Neumann conditions it is N_1 that is spanned by $\boldsymbol{w}$ and, again, N_1, and therefore N_{-1} as well, is not perpendicular to any coordinate subspace. It follows that both hyperplanar Neumann and Dirichlet conditions are non-resonant properly connecting boundary conditions. In the case of vertex formed by one endpoint, hyperplanar Neumann and Dirichlet conditions reduce to classical Neumann and Dirichlet conditions respectively, which is the motivation their names. The word "hyperplanar" reflects the fact that one of the corresponding subspaces (N_1 or N_{-1}) has codimension 1. Note that if the vector $\boldsymbol{w}$ is chosen equal to $(1, 1, ..., 1)$, then hyperplanar Neumann conditions coincide with the standard boundary conditions (which are sometimes called Neumann conditions in the literature).

For hyperplanar Neumann matching conditions (in particular, for standard boundary conditions) for the vertex of valence 2, it may happen that the reflection coefficient is equal to zero. It is easy to show that the other reflection coefficient is zero as well

and the transition coefficients are $e^{i\mu}$ and $e^{-i\mu}$ with a certain $\mu \in \mathbb{R}$. In such a case, one may apply the transformation (6) from paper IV, and as a result obtain a unitary equivalent Laplace operator with standard boundary conditions. Then the corresponding two edges can be substituted by one single edge with the length equal to the sum of the lengths of the removed edges. This procedure is called *cleaning* [52] and the graph without vertices of valence 2 is called *clean graph*.

5. Trace formula for non-resonant boundary conditions

This section is based on papers I and III.

Unlike in previous sections, from now on we consider an arbitrary graph Γ, consisting of N edges, M vertices and C connected components, as defined in section 3. We also assume that the graph Γ is clean, finite and simple, except in the case of standard boundary conditions, where we allow loops and multiple edges. A graph is called *simple* if it contains no loops and no multiple edges.

The theorems for a star graph can be easily generalised for any arbitrary graph Γ in the following way:

Theorem 11. *The family of self-adjoint restrictions of $L_{\max}$ can be described by boundary conditions connecting the boundary values $\boldsymbol{\psi} = (\boldsymbol{\psi}(V_1), \ldots, \boldsymbol{\psi}(V_M))$ and $\partial_n\boldsymbol{\psi} = (\partial_n\boldsymbol{\psi}(V_1), \ldots, \partial_n\boldsymbol{\psi}(V_M))$*

$$i(S - I)\boldsymbol{\psi} = (S + I)\partial_n\boldsymbol{\psi}. \tag{22}$$

These boundary conditions are properly connecting iff they have the form

$$i(S^m - I)\boldsymbol{\psi}(V_m) = (S^m + I)\partial_n\boldsymbol{\psi}(V_m), \tag{23}$$

where S^m is a unitary $v_m \times v_m$ matrix with $N_{-1}(S^m)$ not orthogonal to any coordinate subspace in $\mathbb{C}^{v_m}$.

The non-resonant boundary conditions are given by:

$$P_{N_1^m}\partial_n\boldsymbol{\psi}(V_m) = 0, \quad P_{N_{-1}^m}\boldsymbol{\psi}(V_m) = 0, \tag{24}$$

where $N_1^m \oplus N_{-1}^m = \mathbb{C}^{v_m}$.

Assume that the boundary conditions at the vertices are non-resonant. Every eigenfunction $\psi(x,k)$, corresponding to the energy $\lambda = k^2$, is a solution of the differential equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x,k) = k^2\psi(x,k), \tag{25}$$

on the edges, satisfying the boundary conditions (24) at the vertices. For $k \neq 0$ every solution to (25) can be written using either a basis of incoming or one of outgoing waves (see Fig. 5.)

$$\begin{aligned} \psi(x,k) &= a_{2j-1}e^{ik|x-x_{2j-1}|} + a_{2j}e^{ik|x-x_{2j}|} \qquad x \in \Delta_j = [x_{2j-1}, x_{2j}]. \\ &= b_{2j-1}e^{-ik|x-x_{2j-1}|} + b_{2j}e^{-ik|x-x_{2j}|} \end{aligned} \tag{26}$$

The amplitudes $\boldsymbol{a} = \{a_j\}_{j=1}^{2N}$ and $\boldsymbol{b} = \{b_j\}_{j=1}^{2N}$ are related to each other by the edge scattering matrix

$$\boldsymbol{b} = \mathbf{S}_e\boldsymbol{a}, \text{ where } \mathbf{S}_e(k) = \left(\begin{array}{c|c|c} S_e^1 & 0 & \dots \\ \hline 0 & S_e^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array}\right), \; S_e^j(k) = \begin{pmatrix} 0 & e^{ikd_j} \\ e^{ikd_j} & 0 \end{pmatrix}, \quad (27)$$

where d_j is the length of the edge Δ_j. The amplitudes are also connected by the vertex scattering matrices, which are obtained from the requirement that $\psi(x,k)$ satisfies (22).

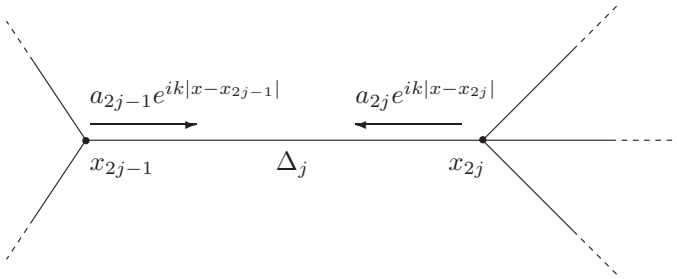


Figure 4: Incoming waves at the edge Δ_j

It is convenient to use the following representation for the solution to (25), using only amplitudes related to every endpoint x_i from V_m

$$\psi(x,k) = a_j e^{ik|x-x_j|} + b_j e^{-ik|x-x_j|}$$

and corresponding vectors $\boldsymbol{a}^m, \boldsymbol{b}^m \in \mathbb{C}^{v_m}$ of amplitudes. Then for all $k \neq 0$ the boundary conditions (24) are equivalent to

$$\begin{cases} P_{N_{-1}^m}(\boldsymbol{a}^m + \boldsymbol{b}^m) = 0, \\ P_{N_1^m}(\boldsymbol{a}^m - \boldsymbol{b}^m) = 0. \end{cases} \quad (28)$$

It follows that $\boldsymbol{a}^m$ and $\boldsymbol{b}^m$ are related by the corresponding vertex scattering matrix S_v^m as follows

$$\boldsymbol{a}^m = S_v^m \boldsymbol{b}_m, \; m = 1, 2, ..., M. \quad (29)$$

The last equation implies that

$$\begin{pmatrix} \boldsymbol{a}^1 \\ \boldsymbol{a}^2 \\ \vdots \\ \boldsymbol{a}^M \end{pmatrix} = \mathbf{S}_v \begin{pmatrix} \boldsymbol{b}^1 \\ \boldsymbol{b}^2 \\ \vdots \\ \boldsymbol{b}^M \end{pmatrix}, \text{ with } \mathbf{S}_v = \left(\begin{array}{c|c|c} S_v^1 & 0 & \dots \\ \hline 0 & S_v^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array}\right). \quad (30)$$

Note that the matrices $\mathbf{S}_e$ and $\mathbf{S}_v$ possess the block representations (27) and (30) in different bases. Clearly, vector $\boldsymbol{a}$ determines an eigenfunction of the Laplace operator if and only if the following equation holds:

$$\det\left(\mathbf{S}(k) - I\right) = 0, \text{ where } \mathbf{S}(k) = \mathbf{S}_v\mathbf{S}_e(k). \quad (31)$$

The matrix $\mathbf{S}(k)$ is unitary for real k since it is a product of two unitary matrices. It is easy to see that

$$\| \mathbf{S}(k) \| < 1 \text{ for } \mathrm{Im}k > 0, \text{ and } \| \mathbf{S}^{-1}(k) \| < 1 \text{ for } \mathrm{Im}k < 0, \tag{32}$$

since the (independent of k) matrix $\mathbf{S}_v$ is unitary and the matrix $\mathbf{S}_e(k)$ satisfies (32).

Equation (31) determines the spectrum of L with correct multiplicities for all non-zero values of the energy. On the other hand, the multiplicity $m_a(0)$ of the zero eigenvalue given by this equation (i. e. the dimension of $\ker(\mathbf{S}(k) - I)$), to be called *algebraic multiplicity*, may be different from the dimension $m_s(0)$ of the zero eigensubspace of L, to be called *spectral multiplicity*.

In paper III we have calculated explicitly the spectral and algebraic multiplicities of zero eigenvalue in case of hyperplanar Neumann and Dirichlet matching conditions.

For a graph Γ with cycles and with hyperplanar boundary conditions at the vertices it looks natural to impose an extra consistency condition. Consider a closed path p of discrete length $n(p)$. Every such path can uniquely be defined by a sequence of endpoints $(x_{l_1}, x_{l_2}, \ldots, x_{l_{2n(p)}})$ that the path comes across, where $x_{l_{2k}}$ and $x_{l_{2k+1}}$ (as well as $x_{l_{2n(p)}}$ and x_{l_1}) belong to the same vertex while $x_{l_{2k-1}}$ and $x_{l_{2k}}$ are different endpoints of the same edge.

Definition 12. *We say that the hyperplanar Neumann boundary conditions are consistent iff for every closed path $p = (x_{l_1}, x_{l_2}, \ldots, x_{l_{2n(p)}})$ the following holds*

$$\prod_{k=1}^{n(p)} w(x_{l_{2k}}) = \prod_{k=0}^{n(p)-1} w(x_{l_{2k+1}}). \tag{33}$$

Similarly, the hyperplanar Dirichlet boundary conditions are consistent iff

$$\prod_{k=1}^{n(p)} w(x_{l_{2k}}) = (-1)^{n(p)} \prod_{k=0}^{n(p)-1} w(x_{l_{2k+1}}). \tag{34}$$

These consistency conditions play an important role in calculating the multiplicities $m_s(0)$ and $m_a(0)$.

Theorem 13. *The spectral and algebraic multiplicities of the ground state eigenvalue $\lambda = 0$ for the Laplace operator with consistent hyperplanar Neumann and Dirichlet boundary conditions are equal to:*

$$\begin{array}{ll} m_s^N(0) = C, & m_a^N(0) = m_a^D(0) = 2C - \chi, \\ m_s^D(0) = C - \chi, & \end{array} \tag{35}$$

where C is the number of connected components and $\chi = M - N$ is the Euler characteristic.

We now introduce the distribution u connected with the spectral measure

$$u \equiv 2m_s(0)\delta(k) + \sum_{n=1}^{\infty} \left(\delta(k - k_n) + \delta(k + k_n)\right).$$

For any test function $\varphi \in C_0^\infty(\mathbb{R})$, the value of the distribution $u[\varphi]$ can be calculated, with the help of the function $f = \det(\mathbf{S}(k) - I)$ as follows

$$u[\varphi] = \lim_{\varepsilon \to 0} \frac{1}{2\pi i} \int_{-\infty}^{\infty} \left(\frac{f'(k - i\varepsilon)}{f(k - i\varepsilon)} - \frac{f'(k + i\varepsilon)}{f(k + i\varepsilon)} \right) \varphi(k) \mathrm{d}k + (2m_s(0) - m_a(0))\varphi(0). \tag{36}$$

Moreover we have the following relation

$$\begin{aligned} u[\varphi] \quad - \quad & (2m_s(0) - m_a(0))\varphi(0) = \\ &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \{(\ln \det(\mathbf{S}(k - i0) - I))' - (\ln \ \det(\mathbf{S}(k + i0) - I))'\} \varphi(k) \mathrm{d}k \\ &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \{(\mathrm{Tr} \ln(\mathbf{S}(k - i0) - I))' - (\mathrm{Tr} \ln(\mathbf{S}(k + i0) - I))'\} \varphi(k) \mathrm{d}k \\ &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \{\mathrm{Tr}(\ln(\mathbf{S}(k - i0) - I))' - \mathrm{Tr}(\ln(\mathbf{S}(k + i0) - I))'\} \varphi(k) \mathrm{d}k \\ &= \frac{1}{2\pi i} \int_{-\infty}^{\infty} \left\{ \mathrm{Tr} \frac{\mathbf{S}'(k - i0)}{\mathbf{S}(k - i0) - I} - \mathrm{Tr} \frac{\mathbf{S}'(k + i0)}{\mathbf{S}(k + i0) - I} \right\} \varphi(k) \mathrm{d}k. \end{aligned}$$

Taking into account that the matrix $\mathbf{S}_v$ is independent of the energy we obtain

$$\mathbf{S}(k)' = \mathbf{S}_v \mathbf{S}_e(k) i\mathcal{D} = i\mathbf{S}(k)\mathcal{D},$$

where $\mathcal{D} = \mathrm{diag}[d_1, d_1, d_2, d_2, d_3, d_3, \ldots]$ in the basis associated with the edges. This allows us to substitute $i\mathbf{S}(k)\mathcal{D}$ into the previous formula, leading to

$$\begin{aligned} u[\varphi] - (2m_s(0) - m_a(0))\varphi(0) & \\ = \frac{1}{2\pi i} \lim_{\varepsilon \to 0} \int_{-\infty}^{\infty} & [\mathrm{Tr}((I + \mathbf{S}(k + i\varepsilon) + \ldots)\mathbf{S}(k + i\varepsilon) i\mathcal{D}) \\ & + \mathrm{Tr}((\mathbf{S}^{-1}(k - i\varepsilon) + \mathbf{S}^{-2}(k - i\varepsilon) + \ldots)\mathbf{S}(k - i\varepsilon) i\mathcal{D})] \varphi(k) \mathrm{d}k. \end{aligned} \tag{37}$$

In the formula above we can exchange the $\lim_{\varepsilon \to 0}$ and the integral sign, since the sum under the integral is absolutely converging (see Paper I for details). Thus we obtain the following formula

$$u[\varphi] = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \mathrm{Tr}((\ldots + \mathbf{S}^{-1}(k) + I + \mathbf{S}(k) + \ldots) i\mathcal{D}) \varphi(k) \mathrm{d}k + (2m_s(0) - m_a(0))\varphi(0),$$

i. e.

$$u = \frac{1}{2\pi i} \mathrm{Tr} \left[(\ldots + \mathbf{S}^{-1}(k) + I + \mathbf{S}(k) + \ldots) i\mathcal{D} \right] + (2m_s(0) - m_a(0))\delta(k). \tag{38}$$

To calculate the trace, let us introduce the orthonormal basis of incoming waves to be $e_1 = (1, 0, 0, \ldots)$, $e_2 = (0, 1, 0, \ldots)$,..., $e_{2N} = (\ldots, 0, 0, 1)$. By a *periodic orbit* we understand any oriented closed path on Γ. It is not allowed for an orbit to turn back at any inner point of an edge, but it may turn back at a vertex. Note that the orbit so

defined does not have a starting point. With every such (continuous) periodic orbit, we can associate a *discrete periodic orbit*, consisting of all edges that the orbit p comes across.

Also let:

- $\mathcal{P}$ be the set of all periodic orbits for the graph Γ,
- $l(p)$ be the geometric length of a periodic orbit p,
- $n(p)$ be the discrete length of p — the number of edges that the orbit contains,
- $\mathcal{P}_m^n$ be the set of all periodic orbits passing through the point x_m into the interval $\Delta_{[\frac{m+1}{2}]}$ (where $[\,\cdot\,]$ denotes the integer part) and having discrete length n,
- $\mathrm{prim}(p)$ denote a primitive periodic orbit of p, i. e. the shortest orbit such that p is a multiple of $\mathrm{prim}(p)$,
- $d(p) = n(p)/n(\mathrm{prim}(p))$ be the degree of p.

The geometric length of an orbit is equal to the sum of lengths of the edges contained in the orbit (including multiplicities). When the orbit goes from one edge to another, passing through a vertex, we need to take into account the corresponding scattering coefficients.

The right-hand side of (38) can be divided into three parts: identity, all positive powers of $\mathbf{S}(k)$ and all negative powers of $\mathbf{S}(k)$. The contribution from the first part is equal to

$$\frac{1}{2\pi}\mathrm{Tr}(I\mathcal{D}) = \frac{2\mathcal{L}}{2\pi} = \frac{\mathcal{L}}{\pi},$$

where $\mathcal{L} = d_1 + d_2 + \ldots + d_N$ is the total length of the graph Γ.

The second part (all positive powers of $\mathbf{S}(k)$) is equal to

$$\begin{aligned}\frac{1}{2\pi}\mathrm{Tr}[(\mathbf{S}(k)^1 + \mathbf{S}(k)^2 + \ldots)\mathcal{D}] &= \frac{1}{2\pi}\sum_{r=1}^{\infty}\sum_{n=1}^{2N} < \mathbf{S}^r\mathcal{D}e_n, e_n > \\ &= \frac{1}{2\pi}\sum_{r=1}^{\infty}\sum_{n=1}^{2N} d_{[\frac{n+1}{2}]}\sum_{p\in\mathcal{P}_n^r} S(p)\; e^{ikl(p)} \\ &= \frac{1}{2\pi}\sum_{p\in\mathcal{P}} l(\mathrm{prim}(p))S(p)\; e^{ikl(p)},\end{aligned}$$

where $S(p)$ is the product of all vertex scattering coefficients along the path p. And the third part (all negative powers of $\mathbf{S}(k)$) is equal to

$$\frac{1}{2\pi}\mathrm{Tr}[(\ldots + \mathbf{S}^{-2}(k) + \mathbf{S}^{-1}(k))\mathcal{D}] = \frac{1}{2\pi}\sum_{p\in\mathcal{P}} l(\mathrm{prim}(p))S^*(p)\; e^{-ikl(p)}.$$

Theorem 14 (Trace formula). *Let Γ be a compact finite metric graph with the total length $\mathcal{L}$ and let L be the Laplace operator in $L_2(\Gamma)$ determined by properly connecting non-resonant boundary conditions at the vertices. Then, the following two trace formulae establish the relation between the spectrum $\{k_n^2\}$ of L and the set $\mathcal{P}$ of closed paths on the metric graph Γ*

$$u(k) \equiv 2m_s(0)\delta(k) + \sum_{k_n \neq 0} (\delta(k-k_n) + \delta(k+k_n)) \tag{39}$$

$$= (2m_s(0) - m_a(0))\delta(k) + \frac{\mathcal{L}}{\pi} + \frac{1}{2\pi}\sum_{p\in\mathcal{P}} l(\mathrm{prim}\,(p))\big(S(p)e^{ikl(p)} + S^*(p)e^{-ikl(p)}\big)$$

and

$$\sqrt{2\pi}\hat{u}(l) = 2m_s(0) + \sum_{k_n\neq 0} 2\cos k_n l \tag{40}$$

$$= 2m_s(0) - m_a(0) + 2\mathcal{L}\delta(l) + \sum_{p\in\mathcal{P}} l(\mathrm{prim}\,(p))\Big(S(p)\delta(l-l(p)) + S^*(p)\delta(l+l(p))\Big).$$

6. Uniqueness theorems for standard boundary conditions

In this section we will consider the conditions on Γ which guarantee that the spectrum of L determines Γ uniquely.

The set of lengths of all periodic orbits Λ is usually called the *length spectrum*. In some cases, formula (40) allows us to recover the whole length spectrum from the energy spectrum. On the other hand, there are known graphs for which some lengths of periodic orbits cannot be recovered. Formula (40) implies directly that the spectrum of a graph allows one to recover the lengths l of all periodic orbits from the *reduced length spectrum* $\Lambda' \subset \Lambda$ defined as

$$\Lambda' = \{l : \Big(\sum_{\substack{p\in\mathcal{P}\\ l(p)=l}} \mathcal{A}_p\Big) \neq 0\}. \tag{41}$$

The following example shows that sets Λ and Λ' can differ.

EXAMPLE 4. In this example we will show a case of a vanishing coefficient $\mathcal{A}_p$. Consider the graph presented at Fig. 5. There exist exactly three periodic orbits with the length equal to $2d_1 + d_2 + d_3 + d_4 + d_5$.

Assume that the degrees of the vertices V_2 and V_4 are arbitrary and $v_1 = v_3 = 3$. If $l = 2d_1 + d_2 + d_3 + d_4 + d_5$, then

$$\sum_{\substack{p\in\mathcal{P}\\ l(p)=l}} \mathcal{A}_p = \frac{16}{9v_2v_4}\left[\frac{-2}{9} + \frac{-2}{9} + \frac{4}{9}\right] l = 0.$$

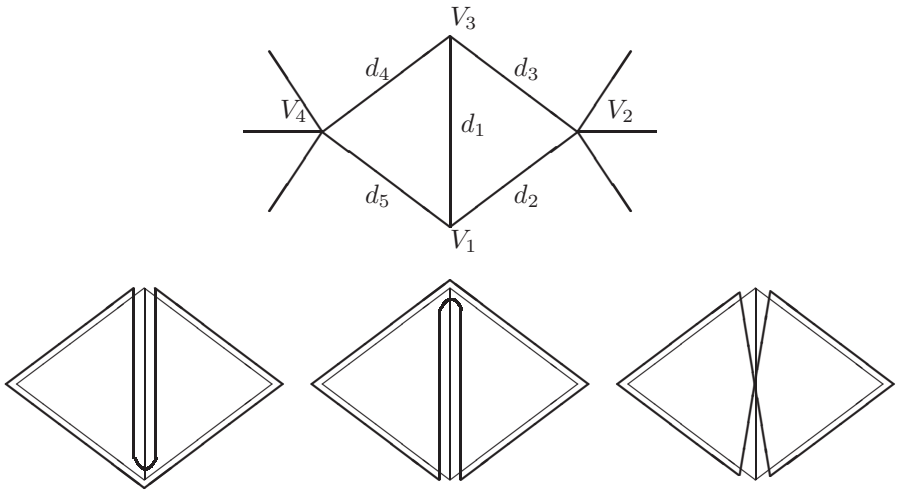


Figure 5: Periodic orbits of length $2d_1 + d_2 + d_3 + d_4 + d_5$

6.1. Graphs with rationally independent edges

In this section we are going to describe the main results from Paper I, where we have studied graphs with rationally independent lengths of edges.

As we have just shown, some periodic orbits do not appear in the length spectrum, but we can prove that at least some specific ones *do* appear in it.

Lemma 15. *Let Γ be a finite, clean and connected metric graph with rationally independent lengths of edges. The reduced length spectrum Λ' contains at least the following lengths:*

- *the shortest orbit formed by any interval Δ_j only (i. e. d_j or $2d_j$ depending on whether Δ_j is a loop or not);*
- *the shortest orbit formed by any two neighbouring edges Δ_j and Δ_k only (i. e. $2(d_j + d_k)$, $d_j + 2d_k$, $2d_j + d_k$, $d_j + d_k$ depending on how these edges are connected to each other).*

The first step in the reconstruction of Γ is to recover the set of lengths of the edges from the total length of the graph and the set of reduced length spectrum Λ'.

Lemma 16. *Let the lengths of the edges of a clean, finite and connected metric graph Γ be rationally independent. Then the total length $\mathcal{L}$ of the graph and the reduced length spectrum Λ' (defined by (41)), determine the lengths of all edges and whether these edges form loops or not.*

Once the lengths of all edges are known the graph can be reconstructed from the reduced length spectrum. Lemma 15 implies that by looking at the reduced length spectrum Λ', one can determine whether any two edges Δ_j and Δ_k are neighbours or

not (i. e. whether they have at least one common endpoint): the edges Δ_j and Δ_k are neighbours if and only if Λ' contains at least one of the lengths $d_j + d_k$, $2d_j + d_k$, $d_j + 2d_k$ or $2(d_j + d_k)$.

Lemma 17. *Every clean, finite and connected metric graph Γ can be reconstructed from the set $D = \{d_j\}$ of the lengths of all edges and the reduced length spectrum Λ' — the subset of all periodic orbits defined by (41), provided that d_j are rationally independent.*

Any graph Γ can be reduced to a simple subgraph Γ^* by deleting all loops and removing all but one of the edges connecting the same two vertices.

We have, in Paper I, proven the following theorem in a constructive way, by first reconstructing a simple subgraph Γ^* and then by adding all multiple edges and loops.

Theorem 18. *The spectrum of a Laplace operator on a metric graph determines the graph uniquely, provided that:*

- *the graph is clean, finite and connected,*
- *the lengths of edges are rationally independent.*

6.2. Graphs with rationally dependent edges

In this section we are going to describe the main results from Paper II, in which we analysed graphs with rationally dependent lengths of edges.

Graphs with trivially rationally dependent edges

We say that the lengths of the edges are *trivially rationally dependent* if they are equal. We will now discuss graphs where the set of all lengths of edges is rationally independent, but where some edges can have equal lengths. We will call such entities *graphs with trivially rationally dependent edges*. We shall prove that even such graphs can be uniquely reconstructed from the length spectrum and total length of the graph — and, therefore, can be uniquely reconstructed from spectrum of Laplace operator on this graph — provided that the edges with the same length are separated by "sufficiently" many edges with rationally independent lengths. We restrict our considerations to graphs that are finite, clean, connected and simple (i. e. without loops or multiple edges).

We shall begin by generalising Lemma 15 to the case of graphs with trivially rationally dependent edges.

Lemma 19. *Let Γ be a finite, clean, connected and simple graph with trivially rationally dependent edges. Assume that the edges of the same length are not neighbours to each other. Then the reduced length spectrum Λ' contains at least the following lengths:*

- *$4d_j$, for all $j = 1, \ldots, N$;*
- *$2d_j$ if there exist exactly one edge of length d_j;*

- $2(d_j + d_k)$ *iff the edges having lengths* d_j *and* d_k *are neighbours;*
- $2(d_i + d_j + d_k)$ *if* Δ_i, Δ_j *and* Δ_k *form a path but do not form a cycle.*

As before, from the reduced length spectrum, we can obtain the lengths of all the edges. However, we can also get the exact number of edges with the same length, that exist in the graph Γ.

Lemma 20. *Assume that* Γ *is a finite, clean, connected and simple metric graph with trivially rationally dependent edges. Let us denote the number of edges of length* d_1 *by* β_1*, number of edges of length* d_2 *by* $\beta_2, \ldots$*, number of edges of length* d_n *by* β_n *(where* $\beta_i \geq 1$ *for* $i = 1 \ldots n$*).*

Then the total length $\mathcal{L}$ *of the graph and the reduced length spectrum* Λ' *determine the lengths of all edges (*d_j*), as well as the number of edges having these particular lengths (*β_j*).*

Lemma 21. *Assume that* Γ *is a finite, clean, connected and simple metric graph with trivially rationally dependent edges. Also assume that any two edges* Δ, Δ' *with lengths* d_i, d_j *(where* i *can be equal to* j*), for which* $\beta_i \geq 2$ *and* $\beta_j \geq 2$ *(i. e. they are both repeating edges), are separated by at least two non-repeating edges (i. e. edges for which* $\beta = 1$*).*

Then the graph Γ *can be reconstructed from the set* $D = \{d_j\}$ *of the lengths of all edges and the reduced length spectrum* Λ'*.*

Now, using these three lemmata, we can prove the following theorem

Theorem 22. *The spectrum of a Laplace operator on a metric graph determines the graph uniquely, provided that:*

- *the graph is clean, finite, simple and connected,*
- *the edges are trivially rationally dependent,*
- *any two repeating edges are separated by at least two non-repeating edges (i. e. ones having rationally independent lengths).*

Graphs with weakly rationally dependent edges

In the last part we shall consider a special class of graphs with rationally dependent edges and we will prove that for those graphs the unique reconstruction from the spectrum of the Laplace operator is still possible. We shall use, as before, the trace formula and some properties of mutually prime numbers.

Definition 23. *Assume that the metric graph* Γ *is finite, clean, connected and simple. We say that the lengths of the edges are weakly rationally dependent if the lengths of edges belong to the set*

$$\left\{d_1, \frac{p_{12}}{q_{12}}d_1, \frac{p_{13}}{q_{13}}d_1, \ldots \frac{p_{1r_1}}{q_{1r_1}}d_1, d_2, \frac{p_{22}}{q_{22}}d_2, \ldots \frac{p_{2r_2}}{q_{2r_2}}d_2, \ldots d_n, \frac{p_{n2}}{q_{n2}}d_n, \ldots \frac{p_{nr_n}}{q_{nr_n}}d_n\right\},$$

where $p_{ij}/q_{ij} > 1$ *are proper fractions,* $q_{i2}, q_{i3}, \ldots, q_{ir_i}$ *are mutually prime for all* $i = 1, \ldots, n$ *and* $d_1, d_2, \ldots, d_n$ *are rationally independent.*

Observe that if $n = 1$ then all edges in the graph are rationally dependent. On the other hand, if all $p_{ij} = 0$ for $j \geq 2$ and all i, then all edges in the graph are rationally independent. Note that the denominators q_{ij} are mutually prime but it does not immediately indicate that they are prime numbers.

Lemma 24. *Assume that Γ is a finite, clean, connected and simple metric graph with weakly rationally dependent edges. Then the total length $\mathcal{L}$ of the graph and the reduced length spectrum Λ' determine the lengths of all edges.*

Lemma 25. *Assume that Γ is a finite, clean, connected and simple metric graph with weakly rationally dependent edges. Then the graph Γ can be reconstructed from the sets $D = \{d_j\}$ and the reduced length spectrum Λ'.*

From the two above lemmata we can easily prove the following theorem

Theorem 26. *The spectrum of the Laplace operator L on a metric graph Γ determines the graph uniquely, provided that the graph is clean, finite, simple and connected, and the edges are weakly rationally dependent.*

7. Reconstruction of the boundary conditions of star graphs

In paper [3] S. Avdonin and P. Kurasov have considered three data sets: (1) reduced by one dimension Titchmarsh-Weyl matrix, (2) reduced by one dimension the scattering matrix and (3) reduced by one dimension response operator for sufficiently large time parameter. They have shown that any one of those sets allows one to reconstruct uniquely the connectivity of the tree, the lengths of edges and the potential q for Schrödinger operator on a tree with m boundary points (equal to the dimension of the scattering matrix).

Similar inverse problem is described in this section and has been investigated in paper IV. We will show that for a star graph with the vertex V of valence v and for *asymptotically properly connecting* 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). Explicit interpretation of this free parameter is given using unitary equivalent operators. Later we will also show 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.

Let us remind that the vertex scattering matrix $S_v(k)$ is given, after (12), as

$$S_v(k) = \frac{(k+1)S + k - 1}{(k-1)S + k + 1},\ k \neq 0. \tag{42}$$

This formula allows one to establish explicit connection between vertex scattering matrices for different values of the energy parameter

$$S_v(k) = \frac{(k+k_0)S_v(k_0) + k - k_0}{(k-k_0)S_v(k_0) + k + k_0},\ k, k_0 \neq 0. \tag{43}$$

7.1. 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 $L_2(\Gamma_{\rm star})$

$$(T_\theta f)(x)=\begin{cases} f(x), & x\in\Delta_j, j=1,2,...,v-1;\\ e^{i\theta}f(x), & x\in\Delta_v. \end{cases} \tag{44}$$

This transformation does not change the differential operator but do change the matching conditions at the vertex. The corresponding unitary matrix S^θ is changed as follows

$$S^\theta = R_\theta S^0 R_{-\theta}, \tag{45}$$

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

$$R_\theta = \mathrm{diag}\,\{1,1,...,1,e^{i\theta}\} = \begin{pmatrix} 1 & 0 & \dots & 0 & 0\\ 0 & 1 & \dots & 0 & 0\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & \dots & 1 & 0\\ 0 & 0 & \dots & 0 & e^{i\theta} \end{pmatrix}. \tag{46}$$

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 (42) implies that

$$S_v^\theta(k) = R_\theta S_v^0(k) R_{-\theta}, \tag{47}$$

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

Theorem 27. *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*

$$S_v^\theta(k) = R_\theta S_v^0(k) R_{-\theta}, \tag{48}$$

where R_θ is given by (46) and $S_v^0(k)$ is a certain particular member of the family.

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 (47) (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 [41], 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.

7.2. Properly connecting matching conditions

In what follows, 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 only 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 (45) and (46).

Theorem 28. *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*

$$S_v^{\theta}(k)=R_{\theta}S_v^0(k)R_{-\theta}, \tag{49}$$

where R_θ is given by (46) and $S_v^0(k)$ is a certain particular member of the family.

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

$$S_v^{\alpha,\beta}(k_0)=R_{\alpha}S_v^0(k_0)R_{\beta}, \tag{50}$$

where $S_v^0(k_0)$ is a certain particular member of the family. Then the scattering matrix for all values of the energy parameter k can be calculated using (43)

$$S_v^{\alpha,\beta}(k)=\frac{(k+k_0)S_v^{\alpha,\beta}(k_0)+k-k_0}{(k-k_0)S_v^{\alpha,\beta}(k_0)+k+k_0}. \tag{51}$$

The proof of this theorem is based on the analysis of the diagonal elements of the matrix $S_v^{\alpha,\beta}(k)$ and their dependence on the parameter $\gamma=\alpha+\beta$. It appears that if all those diagonal elements are independent of γ then $S_v^0(k_0)$ has a block diagonal form and hence the corresponding boundary conditions are not properly connecting.

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Paper I

Inverse Spectral Problem for Quantum Graphs*

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Abstract
The inverse spectral problem for the Laplace operator on a finite metric graph is investigated. It is shown that this problem has a unique solution for graphs with rationally independent edges and without vertices having valence 2. To prove the result trace formula connecting the spectrum of the Laplace operator with the set of periodic orbits for the metric graph is established.

1. Introduction

Differential operators on metric graphs (quantum graphs) is a rather new and rapidly developing area of modern mathematical physics. Such operators can be used to model the motion of quantum particles confined to certain low dimensional structures. This explains recent interest to such problems due to possible applications to quantum computing and design of nanoelectronic devices [1].

Quantum graphs are differential (self-adjoint) operators on metric graphs determined on the functions satisfying certain boundary conditions at the vertices. Therefore these operators combine features of both ordinary and partial differential equations. On every edge the differential equation to solve is an ordinary differential equation which includes the spectral parameter. On the other hand the Cauchy problem on the whole graph is not solvable but for special values of the spectral parameter and Cauchy data only. The main mathematical tool used in this article - the trace formula - supports this point of view. This formula establishes the connection between the spectrum of the Laplace operator on a metric graph and *the length spectrum* - the set of all periodic orbits on the graph. This is in complete analogy with the semiclassical approach due to V. Guillemin and R. Melrose [19; 20] and the relations between the spectrum of a

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Laplace operator on certain two-dimensional domains and operators on graphs established in [6; 7]. J.P. Roth [31] has proven trace formula for quantum graphs using the heat kernel approach. An independent way to derive trace formula using scattering approach was suggested by B. Gutkin, T. Kottos and U. Smilansky [21; 24]. We provide mathematically rigorous proof of this result. The trace formula is applied to reconstruct the graph from the spectrum of the corresponding Laplace operator. This procedure can be carried out in the case when the lengths of the edges are rationally independent and the graph has no vertices having valence 2. A rigorous proof of this fact is also provided in the current paper (Theorem 2). We decided to restrict our consideration to the case of the so-called Laplace operator on metric graphs - the second derivative operator with natural or free boundary conditions at the vertices. The results proven in the current paper are stronger than those proposed in [21]: it is not required that the graph is simple i.e. graphs with loops and multiple edges are allowed. We believe that our methods can now be extended to prove similar results for arbitrary quantum graphs with rationally independent edges.

Explicit examples constructed in [21; 27; 3] show that the inverse spectral and scattering problems for quantum graphs in general do not have a unique solution (if no restriction on the lengths of the edges is imposed).

The notion of quantum graphs was introduced in the 80-ies by B. Pavlov and N. Gerasimenko [17; 18; 30]. Many important examples including graphs with higher dimensional inclusions were considered by P. Exner and P. Šeba [13; 16] (see also two conference proceedings volumes [14; 15] collecting articles on this subject). The extension theory used in the current article is similar to one developed for multi-interval problems in [8; 9; 10; 11; 12]. One can find recent reference list with historical remarks in the book [2] and volumes [25; 26] devoted entirely to quantum graphs.

The spectral problem for quantum graphs has been investigated recently by K. Naimark, A. Sobolev and M. Solomyak [28; 29; 32; 33; 34; 35]. The inverse spectral problem was investigated by B. Gutkin and U. Smilansky [21] and for a special class of operators in [5]. Borg-Levison theorem for Sturm-Louville operator on trees was proven in [4]. The direct scattering problem was investigated by V. Kostrykin and R. Schrader [23]. The inverse scattering problem is discussed in [27] and [22].

2. Basic definitions

Consider arbitrary finite metric graph Γ consisting of N edges. The edges will be identified with the intervals of the real line $\Delta_j = [x_{2j-1}, x_{2j}] \subset \mathbb{R}$, $j = 1, 2, \ldots, N$. Their length will be denoted by $d_j = |x_{2j} - x_{2j-1}|$. Let us denote by M the number of vertices that can be obtained by dividing the set $\{x_k\}_{k=1}^{2N}$ of endpoints into equivalence classes $V_m, m = 1, 2, \ldots, M$. The coordinate parametrization of the edges does not play any important role, therefore we are going to identify metric graphs having the same topological structure and the same lengths of the edges. More precisely this equivalence is described in [27; 3]. A graph Γ is called *clean* if it contains no vertices of valence 2. In what follows we are going to consider clean graphs only, since vertices of valence 2 can easily be removed by substituting the two edges joined at the vertex by one edge with the length equal to the sum of the lengths of the two edges. This

procedure is called *cleaning* [27].

To define the self-adjoint differential operator on Γ consider the Hilbert space of square integrable functions on Γ

$$\mathcal{H} \equiv L^2(\Gamma) = \oplus \sum_{j=1}^{N} L^2(\Delta_j) = \oplus \sum_{n=1}^{N} L^2[x_{2j-1}, x_{2j}]. \tag{1}$$

The Laplace operator on Γ is the sum of second derivative operators in each space $L^2(\Delta_j)$,

$$H = \oplus \sum_{j=1}^{N} \left(-\frac{d^2}{dx^2} \right). \tag{2}$$

This differential expression does not determine the self-adjoint operator uniquely. Two differential operators in $L^2(\Gamma)$ are naturally associated with the differential expression (2): the minimal operator with domain $\mathrm{Dom}\,(H_{\min}) = \oplus \sum_{j=1}^{N} C_0^\infty(\Delta_j)$ the maximal operator $H_{\max}$ with the domain $\mathrm{Dom}\,(H_{\max}) = \oplus \sum_{j=1}^{N} W_2^2(\Delta_j)$, where W_2^2 denotes the Sobolev space.

All self-adjoint operators associated with (2) can be obtained by restricting the maximal operator to a subspace using certain boundary conditions connecting boundary values of the functions on Γ associated with the same vertex.

The functions from the domain $\mathrm{Dom}\,(H_{\max})$ are continuous and have continuous first derivatives on each edge Δ_j. The Hilbert space $\mathcal{H}$ introduced above does not reflect the connectivity of the graph. It is the boundary conditions that connect values of the function on different edges. Therefore these conditions have to be chosen in a special way so that they reflect the connectivity of the graph. See [27] for the discussion how the most general boundary conditions can be chosen. In the current article we restrict our consideration to the case of natural, or free boundary conditions given by

$$\begin{cases} f(x_j) = f(x_k), \;\; x_j, x_k \in V_m, \\ \sum_{x_j \in V_m} \partial_n f(x_j) = 0, \end{cases} \qquad m = 1, 2, \ldots, M, \tag{3}$$

where $\partial_n f(x_j)$ denotes the normal derivative of the function f at the endpoint x_j. The functions satisfying these conditions are continuous at the vertices. In the case of the vertex with valence 2 conditions (3) imply that the function and its first derivative are continuous at the vertex, i.e. the vertex can be removed as described above.

The Laplace operator $H(\Gamma)$ on the metric graph Γ is the operator $H_{\max}$ given by (2) restricted to the set of functions satisfying boundary conditions (3). This operator is self-adjoint [27] and uniquely determined by the graph Γ. Therefore the inverse spectral problem for $H(\Gamma)$ is to reconstruct the graph Γ from the set of eigenvalues.

The Laplace operator $H(\Gamma)$ can be considered as a finite rank (in the resolvent sense) perturbation of the operator $H_{\max}$ restricted to the set of functions satisfying Dirichlet boundary conditions at the vertices. This operator is equal to the orthogonal sum of the second derivative operators on the disjoined intervals and therefore has pure discrete spectrum. Hence the spectrum of the operator $H(\Gamma)$ is also pure discrete with

unique accumulation point at $+\infty$. The quadratic form of the operator

$$\langle Hf, f\rangle = \sum_{j=1}^{N} \int_{x_{2j-1}}^{x_{2j}} (-f''(x))\overline{f(x)}dx = \sum_{j=1}^{N} \int_{x_{2j-1}}^{x_{2j}} |f'(x)|^2 dx \geq 0$$

is nonnegative and therefore the operator H is nonnegative. Thus the spectrum of H contains of an infinite sequence of nonnegative real numbers accumulating to $+\infty$. The kernel of the operator contains only constant functions on Γ (see Lemma 1).

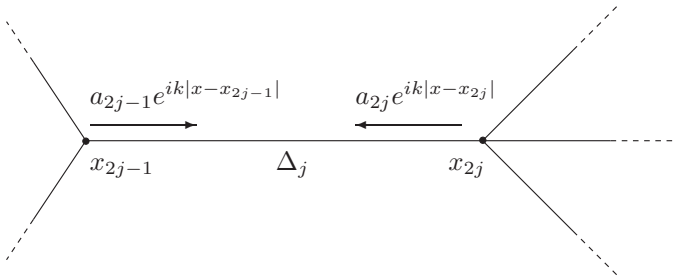
3. Trace formula

In this section we establish the correspondence between the positive spectrum of the operator $H(\Gamma)$ and *the length spectrum* of the metric graph Γ - the set L of lengths of all periodic orbits of Γ. Our presentation follows essentially [21; 24], but we were able to correct few minor mistakes making presentation mathematically rigorous.

Let us establish the secular equation determining all positive eigenvalues of the operator H. Suppose that ψ is an eigenfunction for the operator corresponding to the positive spectral parameter $E = k^2 > 0$. Then this function is a solution to the one-dimensional Schrödinger equation on the edges $-\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = k^2\psi$. The general solution to the differential equation on the edge $\Delta_j = [x_{2j-1}, x_{2j}]$ with the length $d_j = |x_{2j} - x_{2j-1}|$ can be written in the basis of incoming waves as follows

$$\psi(x) = a_{2j-1}e^{ik|x-x_{2j-1}|} + a_{2j}e^{ik|x-x_{2j}|}, \tag{4}$$

where a_m is the amplitude of the wave coming in from the end point x_m.



The same solution in the basis of outgoing waves possesses a similar representation

$$\psi(x) = b_{2j}e^{-ik|x-x_{2j}|} + b_{2j-1}e^{-ik|x-x_{2j-1}|},$$

where

$$\begin{pmatrix} b_{2j-1} \\ b_{2j} \end{pmatrix} = \begin{pmatrix} 0 & e^{ikd_j} \\ e^{ikd_j} & 0 \end{pmatrix} \begin{pmatrix} a_{2j-1} \\ a_{2j} \end{pmatrix}. \tag{5}$$

The following notation will be useful

$$e^j = \begin{pmatrix} 0 & e^{ikd_j} \\ e^{ikd_j} & 0 \end{pmatrix}.$$

If one introduces the $2N$ dimensional vectors of amplitudes of incoming and outgoing waves

$$\mathbf{a} = \left\{ \begin{pmatrix} a_{2j-1} \\ a_{2j} \end{pmatrix} \right\}_{j=1}^{N}; \quad \mathbf{b} = \left\{ \begin{pmatrix} b_{2j-1} \\ b_{2j} \end{pmatrix} \right\}_{j=1}^{N},$$

the relation (5) can be written as

$$\mathbf{b} = \mathcal{E}\mathbf{a}, \quad \text{where} \quad \mathcal{E} = \left(\begin{array}{c|c|c} e^1 & 0 & \dots \\ \hline 0 & e^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array} \right) \tag{6}$$

is a block matrix composed of matrices e^j on the diagonal.

Consider any vertex $V_m = \{x_{l_1}, x_{l_2}, ..., x_{l_{v_m}}\}$ of valence $v_m = \mathrm{val}\,(V_m)$ connecting exactly v_m edges (counting multiplicities). Then knowing the amplitudes $b_{l_j}, j = 1, 2, ..., v_m$ of all waves $b_{l_j} e^{-ik|x-x_{l_j}|}$ approaching the vertex V_m, the amplitudes $a_{l_j}, j = 1, 2, ..., v_m$ of all waves $a_{l_j} e^{ik|x-x_{l_j}|}$ going out from the vertex can be calculated from the boundary conditions (3).

We introduce the notations

$$\mathbf{a}^m = \begin{pmatrix} a_{l_1} \\ a_{l_2} \\ \vdots \\ a_{l_{v_m}} \end{pmatrix}, \quad \mathbf{b}^m = \begin{pmatrix} b_{l_1} \\ b_{l_2} \\ \vdots \\ b_{l_{v_m}} \end{pmatrix}.$$

Then the relation between the vector $\mathbf{a^m}$ and $\mathbf{b^m}$ is described by a certain vertex scattering matrix σ^m determined by the boundary condition

$$\mathbf{a^m} = \sigma^{\mathbf{m}} \mathbf{b^m}. \tag{7}$$

For natural boundary conditions the vertex scattering matrix does not depend on the energy

$$\sigma^m_{jk} = \begin{cases} \frac{2}{v_m}, & j \neq k, \\ \frac{2-v_m}{v_m}, & j = k, \end{cases} \qquad v_m \neq 1. \tag{8}$$

Observe that for $v_m = 2$ and $v_m = 1$ the scattering matrices are trivial and equal to $\sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$[†] and $\sigma = 1$, respectively, which explains the reason to call the boundary conditions (3) free or natural (and the operator H the Laplace operator). For the same reason we have to exclude vertices with valence 2 from our consideration and consider clean graphs only, since one cannot "distinguish" vertices of valence 2 with natural boundary conditions from the other internal points of the edges. In the case $v_m = 1$ (loose endpoint) the boundary condition coincides with Neumann condition.

[†]Observe that in our parametrization the scattering matrix $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ corresponds to zero reflection coefficient and unit transition coefficient — no scattering occurs in that case.

The connection between the amplitudes $\mathbf{b}$ and $\mathbf{a}$ given by the vertex scattering matrices appears in a simple way if one considers the basis associated with the vertices

$$\begin{pmatrix} \mathbf{a}^1 \\ \mathbf{a}^2 \\ \vdots \\ \mathbf{a}^M \end{pmatrix} = \Sigma \begin{pmatrix} \mathbf{b}^1 \\ \mathbf{b}^2 \\ \vdots \\ \mathbf{b}^M \end{pmatrix}, \quad \text{where } \Sigma = \left(\begin{array}{c|c|c} \sigma^1 & 0 & \dots \\ \hline 0 & \sigma^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array}\right). \tag{9}$$

Then formulae (6) and (9) imply that the amplitudes $\mathbf{a}$ determine an eigenfunction of $H(\Gamma)$ for $E > 0$ if and only if $\mathbf{a} = \Sigma\mathcal{E}\mathbf{a}$, i.e. the matrix

$$U(k) = \Sigma\mathcal{E}(k) \tag{10}$$

has eigenvalue 1 and $\mathbf{a}$ is the corresponding eigenvector. Observe that the matrices Σ and $\mathcal{E}$ have simple representations in different bases associated with the vertices and edges respectively. Thus the nonzero spectrum of the operator H can be calculated as zeroes of the following function:

$$f(k) = \det(U(k) - I) = 0 \tag{11}$$

on the positive axis. Let us denote the eigenvalues of the Laplace operator H in non-decreasing order as follows

$$E_0 = k_0^2 = 0 < E_1 = k_1^2 \le E_2 = k_2^2 \le ....$$

Then the zeroes of the function $f(k)$ are situated at the points

$$k = 0, \pm\sqrt{E_1}, \pm\sqrt{E_2}, ...$$

(Lemma 1 see below, implies that $E_0 = 0$ has multiplicity 1). Together with the secular equation (11) we are going to consider the corresponding linear system

$$(U(k) - I)\mathbf{a} = 0, \tag{12}$$

which has nontrivial solutions if and only if (12) is satisfied.

Let us call by *spectral multiplicity* the multiplicity of the eigenvalue E of the operator H and by *algebraic multiplicity* the dimension of the linear space of solutions to the equation (11).

The spectral and algebraic multiplicities of all non-zero eigenvalues of H coincide, since for $E \neq 0$ there is a one to one correspondence between $\mathbf{a}$ and $\psi(x)$ (see (4)).

Let us study the point $E = 0$ in more details.

Lemma 1. *Let Γ be a connected metric graph with N edges and M vertices. Then the point $E = 0$ is an eigenvalue for the Laplace operator H with the spectral multiplicity 1 and algebraic multiplicity $N - M + 2$.*

PROOF. If $E = 0$ then the corresponding eigenfunction should satisfy the following equation $-\frac{d^2\psi}{dx^2} = 0$ on each edge. The solution to this equation is just a linear

function. In addition the function should satisfy the boundary conditions (3). To prove the first part of the lemma it is enough to show that the unique eigenfunction is constant (having equal values on all edges). Assume that there is an eigenfunction which is not constant. Since such function is linear on the edges it attains its maximum and minimum at the end points of the edges, i.e. at the vertices. Consider the vertex being the global maximum point for the function. Then the sum of the normal derivatives at this vertex is a sum of non-positive numbers but it is equal to zero. Therefore all normal derivatives are equal to zero and the function is constant on all edges meeting at the vertex in question. It follows that the eigenfunction attains maximum at all neighbouring vertices. Proceeding with the same argument and taking into account the continuity condition we conclude that the function is constant on the whole graph since it is connected.

The general solutions to the equation (12) are given by (4) on each edge. Now if $E = 0$ then $k = 0$ and using continuity of the eigenfunction at the vertices, the amplitudes a_j have to fulfill the relation $a_{2j-1} + a_{2j} = a_{2k-1} + a_{2k}$ where j, k are indices such that the edges Δ_j and Δ_k are connected. When the graph is connected there is always a path from Δ_1 to any other edge Δ_j. This system of equations is equivalent t the following system of $N - 1$ linearly independent equations: $a_1 + a_2 = a_{2j-1} + a_{2j}$, where $j = 2, \ldots, N$.

Moreover, the second boundary condition provides an additional $M - 1$ linearly independent relations among elements a_j. Thus the number of linearly independent solutions to (12) is equal to $2N - (N - 1) - (M - 1) = N - M + 2$. Hence the algebraic multiplicity is $N - M + 2$. □

Thus the secular equation (11)gives all nonnegative eigenvalues of $H(\Gamma)$ with correct multiplicities except for the point $E = 0$.

The function f is analytic in $\mathbb{C}$, because all elements of the finite matrix $U(k)$ are analytic functions of the variable k. Zeroes of this function cannot accumulate to any finite point, since f is analytic and it is not identically equal to zero. This gives another proof for the fact that the spectrum of the operator H is discrete.

Let us introduce the distribution u connected with the spectral measure

$$u \equiv \delta(k) + \sum_{n=1}^{\infty} \left(\delta(k - k_n) + \delta(k + k_n)\right).$$

For any test function $\varphi \in C_0^\infty(\mathbb{R})$ the value of the distribution $u[\varphi]$ can be calculated using the function f as follows

$$u[\varphi] = \lim_{\varepsilon \to 0} \frac{1}{2\pi i} \int_{-\infty}^{\infty} \left(\frac{f'(k - i\varepsilon)}{f(k - i\varepsilon)} - \frac{f'(k + i\varepsilon)}{f(k + i\varepsilon)} \right) \varphi(k) \mathrm{d}k - (N - M + 1)\varphi(0), \quad (13)$$

where the correction term $-(N - M + 1)\varphi(0)$ appears due to the difference between the spectral and algebraic multiplicities at $E = 0$.

Since the function φ has compact support, say the interval $[a, b]$, the sum is in fact finite and thus it is sufficient to study the case when the support of φ contains only one zero of f, say a simple zero k_j. In this case we have

$$\int_{-\infty}^{\infty} \delta(k - k_j)\varphi(k)\mathrm{d}k \quad = \quad \lim_{\varepsilon \to 0} \frac{1}{2\pi i} \int_a^b \left(\frac{f'(k - i\varepsilon)}{f(k - i\varepsilon)} - \frac{f'(k + i\varepsilon)}{f(k + i\varepsilon)} \right) \varphi(k)\mathrm{d}k$$

$$= \lim_{\varepsilon\to 0}\frac{1}{2\pi i}\left(\int_a^{k_j-\chi}+\int_{k_j-\chi}^{k_j+\chi}+\int_{k_j+\chi}^{b}\right)(\ \dots\ )\varphi(k)\mathrm{d}k,$$

where $\chi \ll 1$. The first and the third integrals have trivial limits

$$\lim_{\varepsilon\to 0}\left(\int_a^{k_j-\chi}+\int_{k_j+\chi}^{b}\right)(\ \dots\ )\varphi(k)\mathrm{d}k = 0,$$

since $\frac{f'(k)}{f(k)}\varphi(k)$ is a continuous function outside $(k_j-\chi, k_j+\chi)$. We can split the middle integral into two as follows

$$\lim_{\varepsilon\to 0}\frac{1}{2\pi i}\varphi(k_j)\int_{k_j-\chi}^{k_j+\chi}(\ \dots\ )\mathrm{d}k + \lim_{\varepsilon\to 0}\frac{1}{2\pi i}\int_{k_j-\chi}^{k_j+\chi}(\ \dots\ )(\varphi(k)-\varphi(k_j))\mathrm{d}k.$$

The integrand in the second integral is uniformly bounded, and therefore its absolute value is less than a constant times χ. The first integral can be transformed to the integral over a small circle around k_j, due to residue calculus equal to $\varphi(k_j)$. Therefore we have

$$\lim_{\varepsilon\to 0}\frac{1}{2\pi i}\varphi(k_j)\int_{-\infty}^{\infty}\left(\frac{f'(k-i\varepsilon)}{f(k-i\varepsilon)}-\frac{f'(k+i\varepsilon)}{f(k+i\varepsilon)}\right)\mathrm{d}k = \varphi(k_j) = \delta(k-k_j)[\varphi].$$

If the support of φ contains several zeroes of f, then the following formula holds

$$u[\varphi] = \frac{1}{2\pi i}\int_{-\infty}^{\infty}[(\ln f(k-i0))' - (\ln f(k+i0))']\varphi(k)\mathrm{d}k - (N-M+1)\varphi(0). \quad (14)$$

For any diagonalizable nonsingular matrix A the following equation holds modulo $2\pi i$:

$$\ln\det A = \mathrm{Tr}\ln A. \quad (15)$$

In the case when all entries of the matrix function $A = A(k)$ are differentiable we get the equality:

$$(\ln\det A(k))' = (\mathrm{Tr}\ln A(k))'. \quad (16)$$

The matrix $A(k) = U(k) - I$ is diagonalizable for real k, since $U(k) = \Sigma\mathcal{E}(k)$ is unitary there. This property holds true in a certain neighbourhood of the real line, since the entries of $\mathcal{E}(k)$ are analytic functions.

Moreover the matrix $U(k) - I = \Sigma\mathcal{E}(k) - I$ is nonsingular outside the real axis because

1. for $\mathrm{Im}k > 0$, $||U(k)|| = ||\mathcal{E}(k)|| < 1$, this implies that $\det(U-I) \neq 0$,
2. for $\mathrm{Im}k < 0$, $||U^{-1}(k)|| = ||\mathcal{E}^{-1}(k)|| < 1$, this implies that $\det(U-I) = \det(U(I-U^{-1})) = \det U \cdot \det(I-U^{-1}) \neq 0$.

Formula (16) holds for $A(k) = U(k) - I$ and for $k \neq k_n$ from the neighbourhood of the real line.

With the function $f(k) = \det(U(k) - I)$ we have then

$$\begin{aligned} u[\varphi] \quad + \quad & (N - M + 1)\varphi(0) = \\ & = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \{(\ln\det(U(k - i0) - I))' - (\ln\ \det(U(k + i0) - I))'\}\varphi(k)\mathrm{d}k \\ & = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \{(\mathrm{Tr}\ln(U(k - i0) - I))' - (\mathrm{Tr}\ln(U(k + i0) - I))'\}\varphi(k)\mathrm{d}k \\ & = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \{\mathrm{Tr}(\ln(U(k - i0) - I))' - \mathrm{Tr}(\ln(U(k + i0) - I))'\}\varphi(k)\mathrm{d}k \\ & = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \left\{\mathrm{Tr}\frac{U'(k - i0)}{U(k - i0) - I} - \mathrm{Tr}\frac{U'(k + i0)}{U(k + i0) - I}\right\}\varphi(k)\mathrm{d}k. \end{aligned}$$

Since $||\mathcal{E}(k+i\varepsilon)|| < 1$, the norm $||U(k+i\varepsilon)||$ is also less than 1 and the geometric expansion can be used

$$\mathrm{Tr}\frac{U'(k + i\varepsilon)}{I - U(k + i\varepsilon)} = \mathrm{Tr}\big((I + U(k + i\varepsilon) + U^2(k + i\varepsilon) + \ldots)U'(k + i\varepsilon)\big)$$

In the lower half-plane $\mathrm{Im}(k - i\varepsilon) < 0$, $||U^{-1}(k - i\varepsilon)|| < 1$ and we get:

$$\begin{aligned} \mathrm{Tr}\ \frac{U'(k - i\varepsilon)}{U(k - i\varepsilon) - I} &= \mathrm{Tr}\frac{1}{U(k - i\varepsilon)} \quad \frac{U'(k - i\varepsilon)}{I - U^{-1}(k - i\varepsilon)} \\ &= \mathrm{Tr}U(k - i\varepsilon)^{-1}\big((I + U^{-1}(k - i\varepsilon) + U^{-2}(k - i\varepsilon) + \ldots)U'(k - i\varepsilon)\big) \\ &= \mathrm{Tr}\big((U^{-1}(k - i\varepsilon) + U^{-2}(k - i\varepsilon) + \ldots)U'(k - i\varepsilon)\big). \end{aligned}$$

Putting together the last two expansions we have

$$\begin{aligned} u[\varphi] + (N - M + 1)\varphi(0) = \frac{1}{2\pi i}\lim_{\varepsilon\to 0}\int_{-\infty}^{\infty} [\mathrm{Tr}((I + U(k + i\varepsilon) + \ldots)U'(k + i\varepsilon)) \\ + \mathrm{Tr}((U^{-1}(k - i\varepsilon) + U^{-2}(k - i\varepsilon) + \ldots)U'(k - i\varepsilon))]\varphi(k)\mathrm{d}k. \end{aligned}$$

Taking into account that the matrix Σ is independent of the energy one gets

$$U' = \Sigma\mathcal{E}i\mathcal{D} = iU\mathcal{D},$$

where $\mathcal{D} = \mathrm{diag}[d_1, d_1, d_2, d_2, d_3, d_3, \ldots]$ (in the basis associated with the edges). Substitution into the previous formula implies

$$\begin{aligned} u[\varphi] + (N - M + 1)\varphi(0) = \frac{1}{2\pi i}\lim_{\varepsilon\to 0}\int_{-\infty}^{\infty} [\mathrm{Tr}((I + U(k + i\varepsilon) + \ldots)U(k + i\varepsilon)i\mathcal{D}) \\ + \mathrm{Tr}((U^{-1}(k - i\varepsilon) + U^{-2}(k - i\varepsilon) + \ldots)U(k - i\varepsilon)i\mathcal{D})]\varphi(k)\mathrm{d}k \end{aligned} \tag{17}$$

In the last formula one can exchange the $\lim_{\varepsilon\to 0}$ and the integral sign, since the sum under the integral is absolutely converging. To prove that one can use the fact that the test function φ has compact support and is infinitely many times differentiable and

therefore its Fourier transform decays faster than any polynomial, i.e. in particular the following estimate holds

$$\left|\int_{-\infty}^{\infty} e^{i(k+i\varepsilon)d}\varphi(k)\mathrm{d}k\right| \leq \frac{C}{d^{N+1}}, \qquad |d|>1$$

where C is a certain positive constant. Entries of the matrices $U(k)$ are exponential functions $e^{i(k+i\varepsilon)d_j}$. Therefore the entries of the matrix $U^m(k+i\varepsilon)$ are equal to sums of exponentials $e^{i(k+i\varepsilon)\sum_{j=1}^m d_{\alpha_j}}$, where $\vec{\alpha}=(\alpha_1,\alpha_2,...,\alpha_m)$ is an m-dimensional vector with nonnegative integer coordinates less or equal to N. The number of all such vectors is less than m^{N-1}. Then the product of matrices $U^m(k)\mathcal{D}$ can be written as a finite sum with less than m^{N-1} items

$$U^m(k+i\varepsilon)\mathcal{D}=\sum_{\vec{\alpha}} B_{\vec{\alpha}} e^{i(k+i\varepsilon)\sum_{j=1}^m d_{\alpha_j}},$$

where the norms of the constant matrices $B_{\vec{\alpha}}$ are not greater than the norm of the matrix $U^m(k+i\varepsilon)\mathcal{D}$ equal to $\max\{d_j\}$. Therefore the traces $|\mathrm{Tr}\, B_{\vec{\alpha}}|$ are less than $2N\max\{d_j\}$. Then every item containing positive powers of U can be estimated as

$$\begin{aligned}\left|\int_{-\infty}^{\infty}\mathrm{Tr}[U^m(k+i\varepsilon)\mathcal{D}]\varphi(k)\mathrm{d}k\right| &= \left|\int_{-\infty}^{\infty}\mathrm{Tr}\left[\sum_{\vec{\alpha}} B_{\vec{\alpha}} e^{i(k+i\varepsilon)\sum_{j=1}^m d_{\alpha_j}}\right]\varphi(k)\mathrm{d}k\right| \\ &\leq \sum_{\vec{\alpha}} 2N\max\{d_j\}\left|\int_{-\infty}^{\infty} e^{i(k+i\varepsilon)\sum_{j=1}^m d_{\alpha_j}}\varphi(k)\mathrm{d}k\right| \\ &\leq m^{N-1}2N\max\{d_j\}\,\frac{C}{m^{N+1}(\min\{d_j\})^{N+1}} \leq \frac{K}{m^2},\end{aligned} \tag{18}$$

where K is another constant. Estimating the sum of negative powers of U in a similar way the following formula is now proven

$$u[\varphi]=\frac{1}{2\pi i}\int_{-\infty}^{\infty}\mathrm{Tr}((\ldots+U^{-1}(k)+I+U(k)+\ldots)i\mathcal{D})\varphi(k)\mathrm{d}k-(N-M+1)\varphi(0),$$

i.e.

$$u=\frac{1}{2\pi i}\mathrm{Tr}\left[(\ldots+U^{-1}(k)+I+U(k)+\ldots)i\mathcal{D}\right]-N\delta(k). \tag{19}$$

To calculate the trace, let us introduce the orthonormal basis of incoming waves to be $e_1=(1,0,0,\ldots)$, $e_2=(0,1,0,\ldots)$,..., $e_{2N}=(\ldots,0,0,1)$. By a *periodic orbit* we understand any oriented closed path on Γ. Note that the orbit so defined does not have any starting point. To any such (continuous) periodic orbit p one can associate the *discrete periodic orbit* consisting of all edges that the orbit comes across. Also let:

- $\mathcal{P}$ be the set of all periodic orbits for the graph Γ,
- $l(p)$ be the geometric length of a periodic orbit p,
- $n(p)$ be the discrete length of p - the number of edges that the orbit comes across,

- $\mathcal{P}_m^n$ be the set of all periodic orbits going through the point x_m into the interval $\Delta_{[\frac{m+1}{2}]}$, where $[\,\cdot\,]$ denotes the integer part, and having discrete length n,
- $\mathrm{prim}(p)$ denotes a primitive periodic orbit, i.e. such that p is a multiple of $\mathrm{prim}(p)$
- $d(p) = n(p)/n(\mathrm{prim}(p))$ is the degree of p.

The geometric length of an orbit is equal to the sum of lengths of the edges composing the orbit (with multiplicities of course).When the orbit goes from one edge to another it passes through a vertex and we will need to take into account the corresponding scattering coefficients. Then let us denote by $\mathcal{T}(p)$ the set of all scattering coefficients along the orbit p.

The right-hand side of (19) can be divided in three parts: identity, all positive powers of U and all negative powers of U. The first part gives

$$\frac{1}{2\pi}\mathrm{Tr}(I\mathcal{D}) = \frac{2\mathcal{L}}{2\pi} = \frac{\mathcal{L}}{\pi},$$

where $\mathcal{L} = d_1 + d_2 + \ldots + d_N$ is the total length of the graph Γ.

Contribution from all other terms can be calculated using corresponding periodic orbits. Let us consider for example the contribution from U^4 :

$$\frac{1}{2\pi}\mathrm{Tr}(U^4\mathcal{D}) = \frac{1}{2\pi}\sum_{n=1}^{2N} < U^4\mathcal{D}e_n, e_n > .$$

Using that $\mathcal{D}e_n = d_{[\frac{n+1}{2}]}e_n$ and definition (10), the trace can be calculated

$$\begin{aligned}\frac{1}{2\pi}\mathrm{Tr}(U^4\mathcal{D}) &= \frac{1}{2\pi}\sum_{n=1}^{2N} d_{[\frac{n+1}{2}]} < U^4 e_n, e_n > \\ &= \frac{1}{2\pi}\sum_{n=1}^{2N} d_{[\frac{n+1}{2}]} \sum_{p\in\mathcal{P}_n^4} \Big(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \sigma_{(ij)}^m \Big)\, e^{ikl(p)}.\end{aligned}$$

Now we will sum all positive powers

$$\begin{aligned}\frac{1}{2\pi}\mathrm{Tr}[(U^1 + U^2 + U^3 + \ldots)\mathcal{D}] &= \frac{1}{2\pi}\sum_{s=1}^{\infty}\sum_{n=1}^{2N} < U^s\mathcal{D}e_n, e_n > \\ &= \frac{1}{2\pi}\sum_{s=1}^{\infty}\sum_{n=1}^{2N} d_{[\frac{n+1}{2}]} \sum_{p\in\mathcal{P}_n^s} \Big(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \sigma_{ij}^m \Big)\, e^{ikl(p)} \\ &= \frac{1}{2\pi}\sum_{p\in\mathcal{P}} l(\mathrm{prim}(p)) \Big(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \sigma_{ij}^m \Big)\, e^{ikl(p)}\end{aligned}$$

Similarly we have for negative powers

$$\frac{1}{2\pi}\mathrm{Tr}[(\ldots + U^{-3} + U^{-2} + U^{-1})\mathcal{D}] = \frac{1}{2\pi}\sum_{p\in\mathcal{P}} l(\mathrm{prim}(p)) \Big(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \overline{\sigma_{ij}^m} \Big)\, e^{-ikl(p)}.$$

For the sake of simplicity one can introduce:

$$\mathcal{A}_p = l(\mathrm{prim}(p))\Big(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \sigma_{ij}^m\Big), \qquad \mathcal{A}_p^* = l(\mathrm{prim}(p))\Big(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \overline{\sigma_{ij}^m}\Big). \tag{20}$$

Thus we have proved the following trace formula (21), which is a rigorous counterpart of the formula derived by B. Gutkin, T. Kottos and U. Smilansky in [21; 24].

Theorem 1 (Trace formula). *Let $H(\Gamma)$ be the Laplace operator on a finite connected metric graph Γ, then the following two trace formulae establishes the relation between the spectrum $\{k_j^2\}$ of $H(\Gamma)$ and the set of periodic orbits $\mathcal{P}$, the number of edges N and the total length $\mathcal{L}$:*

$$u(k) \equiv \delta(k) + \sum_{n=1}^{\infty} (\delta(k-k_n) + \delta(k+k_n)) \tag{21}$$

$$= -(N-M+1)\delta(k) + \frac{\mathcal{L}}{\pi} + \frac{1}{2\pi}\sum_{p\in\mathcal{P}} \Big(\mathcal{A}_p\, e^{ikl(p)} + \mathcal{A}_p^*\, e^{-ikl(p)}\Big),$$

and

$$\hat{u}(l) \equiv 1 + \sum_{n=1}^{\infty} \big(e^{-ik_n l} + e^{ik_n l}\big) \tag{22}$$

$$= -(N-M+1) + 2\mathcal{L}\delta(l) + \sum_{p\in\mathcal{P}} \Big(\mathcal{A}_p\delta(l-l(p)) + \mathcal{A}_p^*\delta(l+l(p))\Big)$$

where $\mathcal{A}_p$, $\mathcal{A}_p^*$ are independent of the energy complex numbers given by (20).

The second formula (22) is just a Fourier transform of (21). If the graph is not clean, then the coefficients $\mathcal{A}_p$ containing reflections from the vertices of valence 2 are equal to zero. If the graph is clean, then (8) implies that all coefficients $\mathcal{A}_p$ are different from zero, but it may happen that the singular support of $\hat{u}(l)$ does not contain lengths of all periodic orbits (see the following section).

4. The inverse spectral problem

In this section we are going to apply formula (22) to prove that the inverse spectral problem has unique solution for clean finite connected metric graphs, provided the lengths of the edges are rationally independent.

The set L of lengths of all periodic orbits is usually called the length spectrum. In principle formula (22) allows one to recover the length spectrum (of periodic orbits) from the energy spectrum (of the Laplace operator H). But this relation is not straightforward and we are able to prove it in certain special cases only (see the following section). Formula (22) implies directly that the spectrum of a graph allows one to recover the lengths l of all periodic orbits from the *reduced length spectrum* $L' \subset L$ defined as

$$L' = \{l : \Big(\sum_{\substack{p\,\in\,\mathcal{P}\\ l(p)\,=\,l}} \mathcal{A}_p\Big) \neq 0\}. \tag{23}$$

Lemma 2. *Let Γ be a connected finite clean metric graph with rationally independent lengths of edges. The reduced length spectrum L' contains at least the following lengths:*

- *the shortest orbit formed by any interval Δ_j only (i.e. d_j or $2d_j$ depending on whether Δ_j forms a loop or not);*
- *the shortest orbit formed by any two neighbouring edges Δ_j and Δ_k only (i.e. $2(d_j + d_k)$, $d_j + 2d_k$, $2d_j + d_k$, $d_j + d_k$ depending on how do these edges are connected to each other).*

PROOF. Note that if the graph is clean and there is a unique periodic orbit p_0 of a certain length $l(p_0)$ then the corresponding sum degenerates and is different from zero:

$$\sum_{\substack{p \in \mathcal{P} \\ l(p) = l(p_0)}} \mathcal{A}_p = \mathcal{A}_{p_0} \neq 0. \tag{24}$$

If there are several, say r, orbits having the same length as p_0 and all $\mathcal{A}$ - coefficients are equal, then the sum is different from zero:

$$\sum_{\substack{p \in \mathcal{P} \\ l(p) = l(p_0)}} \mathcal{A}_p = r\mathcal{A}_{p_0} \neq 0. \tag{25}$$

- In the case Δ_j is a loop, there are two orbits of length d_j with equal coefficients $\mathcal{A}$. If Δ_j does not form a loop, then the shortest orbit is unique and has length $2d_j$.
- Suppose that neither Δ_j nor Δ_k forms a loop and they do not form a double edge. Then the shortest possible length of an orbit formed by Δ_j and Δ_k is $2(d_j + d_k)$ and such orbit is unique.

  Suppose that exactly one of the two neighbouring edges, say Δ_j, forms a loop. Then there are two orbits having the shortest possible length $d_j + 2d_k$ and the corresponding $\mathcal{A}$ - coefficients are equal.

  Suppose that Δ_j and Δ_k form a double edge. Then there are two orbits with the shortest possible length $d_j + d_k$ and the corresponding $\mathcal{A}$ - coefficients are equal.

  Suppose that both Δ_j and Δ_k form loops. Then the number of orbits having the shortest length $d_j + d_k$ is four and the $\mathcal{A}$ - coefficients are equal.

All possible cases have been considered. □

We are going to show now that the knowledge of the reduced length spectrum together with the total length of the graph is enough to reconstruct the graph. The first step in this direction is to recover the lengths of the edges from the total length of the graphs and the set L'. The following result can be proven by refining the method of B. Gutkin-U. Smilansky [21].

Lemma 3. *Let the lengths of the edges of a clean finite connected metric graph Γ be rationally independent. Then the total length $\mathcal{L}$ of the graph and the reduced length spectrum L' (defined by (23)) determine the lengths of all edges and whether these edges form loops or not.*

PROOF. Consider the finite subset L'' of $L' \subset L$ consisting of all lengths less than or equal to $2\mathcal{L}$

$$L'' = \{l \in L' : l \leq 2\mathcal{L}\}.$$

This finite set contains at least one of the numbers d_j or $2d_j$. Therefore there exists a basis $s_1, s_2, \ldots, s_N$, such that every length $l \in L''$ (as well as from L) can be written as a half-integer combination of s_j

$$l = \frac{1}{2}\sum_{j=1}^{N} n_j s_j, \quad n_j \in \mathbb{N}.$$

Such basis is not unique especially if the graph has loops. Any two bases $\{s_j\}$ and $\{s'_j\}$ are related as follows $s_j = n_j s'_{i_j},\ n_j = \frac{1}{2}, 1, 2$, where $i_1, i_2, \ldots, i_N$ is a permutation of $1, 2, \ldots, N$. Then among all possible bases consider a basis with the shortest total length $\sum_{j=1}^{N} s_j$.

The total length of the graph $\mathcal{L}$ can also be written as a sum of s_j with the coefficients equal to 1 or $1/2$

$$\mathcal{L} = \sum_{j=1}^{N} \alpha_j s_j, \quad \alpha_j = 1, 1/2. \tag{26}$$

The coefficients in this sum are equal to 1 if s_j is equal to the length of a certain edge Δ_j, i.e. when the edge forms a loop. The coefficient $1/2$ appears if s_j is equal to double the length of an edge. In this case the edge does not form a loop. Therefore the lengths of the edges up to permutation can be recovered from (26) using the formula $d_j = \alpha_j s_j,\ j = 1, 2, \ldots, N$. To check whether an edge Δ_j forms a loop or not it is enough to check whether d_j belongs to L' or not. □

Once the lengths of all edges are known the graph can be reconstructed from the reduced length spectrum. Lemma 2 implies that looking at the reduced length spectrum L' one can determine whether any two edges Δ_j and Δ_k are neighbours or not (have at least one common end point): the edges Δ_j and Δ_k are neighbours if and only if L' contains at least one of the lengths $d_j + d_k, 2d_j + d_k, d_j + 2d_k$, or $2(d_j + d_k)$.

Lemma 4. *Every clean finite connected metric graph Γ can be reconstructed from the set $D = \{d_j\}$ of the lengths of all edges and the reduced length spectrum L' - the subset of all periodic orbits determined by (23), provided that d_j are rationally independent.*

PROOF. Let us introduce the set of edges $E = \{\Delta_j\}_{j=1}^{N}$ uniquely determined by $D = \{d_j\}$. We shall prove lemma for simple graphs first. A graph is called *simple* if it contains no loops and no multiple edges. From an arbitrary graph one can obtain a simple graph by cancelling all loops and choosing only one edge from every multiple one:

1. If $d_k \in L'$ then the corresponding edge is a loop. Then remove Δ_k from E and all lengths containing d_k from L'.

2. If $d_k + d_j \in L'$ then there exists a double edge composed of Δ_j and Δ_k (since the loops have already been removed). Then remove either Δ_j or Δ_k from E and also all lengths containing the chosen length from L.

The new subsets $E^* \subset E$ containing $N^* \leq N$ elements and $L^* \subset L'$ obtained in this way correspond to a simple subgraph $\Gamma^* \subset \Gamma$ which can be obtained from Γ by removing all loops and reducing all multiple edges. One obtains different Γ^* by choosing different edges to be left during the reduction.

The reconstruction will be done iteratively and we will construct an increasing finite sequence of subgraphs such that $\Gamma_1 \subset \Gamma_2 \subset \ldots \Gamma_{N^*} = \Gamma^*$. The corresponding subsets of edges will be denoted by E_k.

For $k = 1$ take the graph Γ_1 consisting of one edge, say Δ_1. By looking at L' pick up any edge, say Δ_2, which is a neighbour of Δ_1. Attach it to any endpoint of Δ_1 to get the graph Γ_2.

Suppose that connected subgraph Γ_k consisting of k edges ($k \geq 2$) is reconstructed. Pick up any edge, say Δ_{k+1}, which is a neighbour of at least one of the edges in Γ_k. Let us denote by $E_k^{\rm nbh}$ the subset of E_k of all edges which are neighbours of Δ_{k+1}. We have to identify one or two vertices in Γ_k to which the new Δ_{k+1} is attached. Every such vertex is uniquely determined by listing the edges joined at this vertex, since the subgraph Γ_k is simple, connected and contains at least two edges. Therefore we have to separate $E_k^{\rm nbh}$ into two classes of edges attached to each endpoint of Δ_{k+1}. (One of the two sets can be empty, which corresponds to the case the edge Δ_{k+1} is attached to Γ_k at one vertex only.)

Take any two edges from $E_k^{\rm nbh}$, say Δ' and Δ''. The edges Δ' and Δ'' belong to the same class if and only if:

- Δ' and Δ'' are neighbours themselves and
- $d' + d'' + d_{k+1} \notin L'$ i.e. the edges Δ', Δ'' and Δ_{k+1} do not build a cycle. Note that if Δ', Δ'' and Δ_{k+1} form a cycle, then there are two periodic orbits having with the length $d' + d'' + d_{k+1}$ and the corresponding $\mathcal{A}$-coefficients are equal, which implies that $d' + d'' + d_{k+1} \in L'$.

In this way we either separate $E_k^{\rm nbh}$ into two classes of edges or $E_k^{\rm nbh}$ consists of edges joined at one vertex. In the first case the new edge Δ_{k+1} connects the two unique vertices determined by the subclasses. In the second case Δ_{k+1} is attached by one endpoint to Γ_k at the vertex uniquely determined by $E_k^{\rm nbh}$. It does not play any role which of the two end points of Δ_{k+1} is attached to the chosen vertex of Γ_k, since the two possible graphs are equivalent.

Denote the graph obtained in this way by Γ_{k+1}.

Since the graph Γ^* is connected and finite, after N^* steps one arrives at $\Gamma_{N^*} = \Gamma^*$.

It remains to add all loops and multiple edges to reconstruct the initial graph Γ. Suppose that the reconstructed subgraph Γ^* is not trivial, i.e. consists of more than one edge. Then every vertex is uniquely determined by listing all edges joined at it. Check first to which vertex the loop Δ_n is connected by checking if periodic orbits of the length $d_n + 2d_j$ belongs to L' or not. All such edges Δ_j determine the unique vertex to which Δ_n should be adjusted. To reconstruct multiple edges check whether $d_m + d_j$ is from L', where $\Delta_j \in E^*$. Substitute all such edges Δ_j with corresponding multiple edges.

In the case Γ^* is trivial, the proof is an easy exercise. $\square$

Our main result can be obtained as a straightforward implication of Lemma 3 and Lemma 4.

Theorem 2. *The spectrum of a Laplace operator on a metric graph determines the graph uniquely, provided that:*

- *the graph is clean, finite and connected,*
- *the edge lengths are rationally independent.*

PROOF. The spectrum of the operator determines the left-hand side of the trace formula (21). Formula (22) shows that the spectrum of the graph determines the total length of the graph and the reduced length spectrum. Lemma 3 implies that the lengths of all edges can be extracted from this quantities under the conditions of the theorem. It follows from Lemma 4 that the whole graph can be reconstructed provided that its edges are rationally independent and it is clean, finite and connected. □

One can easily remove the condition that the graph is connected. The result can be generalized to include more general differential operators on the edges and boundary conditions at the vertices. Rigorous proofs of these results will be a subject of one of forthcoming publications.

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Paper II

Inverse spectral problem for quantum graphs with rationally dependent edges*

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Abstract. In this paper we study the problem of unique reconstruction of the quantum graphs. The idea is based on the trace formula which establishes the relation between the spectrum of Laplace operator and the set of periodic orbits, the number of edges and the total length of the graph. We analyse conditions under which is it possible to reconstruct simple graphs containing edges with rationally dependent lengths.

1. Introduction

Differential operators on metric graphs (quantum graphs) is a rather new and rapidly developing area of modern mathematical physics. Such operators can be used to model the motion of quantum particles confined to certain low dimensional structures. This has many possible applications to quantum computing and design of nanoelectronic devices [1], which explains recent interest in the area.

The main mathematical tool used in this article is the trace formula, which establishes the connection between the spectrum of the Laplace operator on a metric graph and *the length spectrum* (the set of all periodic orbits on the graph), the number of edges and the total length of the graph.

J.P. Roth [12] proved trace formula for quantum graphs using the heat kernel approach. An independent way to derive trace formula using scattering approach was suggested by B. Gutkin, T. Kottos and U. Smilansky [6; 8] and mathematically rigorous proof of this result was provided by P. Kurasov and M. Nowaczyk [10]. The trace formula is applied in order to reconstruct the graph from the spectrum of the corresponding Laplace operator. It has been proven that this procedure can be carried out in the case when the lengths of the edges are rationally independent and the graph has no vertices of valence 2. In current paper we go further and consider graphs with trivially and weakly rationally dependent edges. We have decided to restrict our considerations

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to the case of the so-called Laplace operator on metric graphs — the second derivative operator with natural (free, standard, Kirchhoff) boundary conditions at vertices.

Explicit examples constructed in [6; 11; 2] show that the inverse spectral and scattering problems for quantum graphs do not have, in general, unique solutions.

For a historical background on quantum graphs, their applications and theory development see Introduction and References in our previous paper [10].

2. Basic definitions

All notations and definitions in this paper will follow those used in [10]. We are not going to repeat the rigorous derivation of the trace formula presented there, but in this section we will introduce the definitions which we are going to use.

Consider arbitrary finite metric graph Γ consisting of N edges. The edges will be identified with the intervals of the real line $\Delta_j = [x_{2j-1}, x_{2j}] \subset \mathbb{R}$, $j = 1, 2, \ldots, N$ and the set of all edges will be denoted by $E = \{\Delta_j\}_{j=1}^N$. Their lengths will be denoted by $d_j = |x_{2j} - x_{2j-1}|$ and corresponding set of all lengths by $D = \{d_j\}$. Let us denote by M the number of vertices in the graph Γ. Vertices can be obtained by dividing the set $\{x_k\}_{k=1}^{2N}$ of endpoints into equivalence classes $V_m, m = 1, 2, \ldots, M$. The coordinate parameterization of the edges does not play any important role, therefore we are going to identify metric graphs having the same topological structure and the same lengths of the edges. This equivalence is more precisely described in [11; 2].

Consider the Hilbert space of square integrable functions on Γ

$$\mathcal{H} \equiv L^2(\Gamma) = \oplus \sum_{j=1}^{N} L^2(\Delta_j) = \oplus \sum_{n=1}^{N} L^2[x_{2j-1}, x_{2j}]. \tag{1}$$

The Laplace operator H on Γ is the sum of second derivative operators acting in each space $L^2(\Delta_j)$,

$$H = \oplus \sum_{j=1}^{N} \left(-\frac{d^2}{dx^2} \right). \tag{2}$$

This differential expression does not uniquely determine the self-adjoint operator. Two differential operators in $L^2(\Gamma)$ are naturally associated with the differential expression (2), namely the minimal operator with the domain $\mathrm{Dom}\,(H_{\min}) = \oplus \sum_{j=1}^{N} C_0^\infty(\Delta_j)$ and the maximal operator $H_{\max}$ with the domain $\mathrm{Dom}\,(H_{\max}) = \oplus \sum_{j=1}^{N} W_2^2(\Delta_j)$, where W_2^2 denotes the Sobolev space.

The Hilbert space $\mathcal{H}$ introduced above does not reflect the connectivity of the graph. It is the boundary conditions that connect values of the function on different edges. Therefore these conditions have to be chosen in a special way so that they reflect the connectivity of the graph. See [11] for the discussion how the most general boundary conditions can be chosen. In the current paper we restrict our consideration to the case of natural (free, standard, Kirchhoff) boundary conditions given by

$$\begin{cases} f(x_j) = f(x_k), \quad x_j, x_k \in V_m, \\ \sum_{x_j \in V_m} \partial_n f(x_j) = 0, \end{cases} \qquad m = 1, 2, \ldots, M, \tag{3}$$

where $\partial_n f(x_j)$ denotes the normal derivative of the function f at the endpoint x_j. The functions satisfying these conditions are continuous at the vertices. In the case of the vertex with valence 2 conditions (3) imply that the function and its first derivative are continuous at the vertex, i.e. the vertex can be removed by substituting the two edges joined at the vertex by one edge with the length equal to the sum of the lengths of the two edges. This procedure is called *cleaning* [11] and a graph Γ with no vertices of valence 2 is called *clean*.

The Laplace operator $H(\Gamma)$ on the metric graph Γ is the operator $H_{\max}$ given by (2) restricted to the set of functions satisfying boundary conditions (3). This operator is self-adjoint [11] and uniquely determined by the graph Γ. The spectrum of the operator $H(\Gamma)$ is discrete and consists of positive eigenvalues accumulating at $+\infty$. Therefore the inverse spectral problem for $H(\Gamma)$ is to reconstruct the graph Γ from the set of eigenvalues.

3. Trace Formula

Let us establish the secular equation determining all positive eigenvalues of the operator H. Suppose that ψ is an eigenfunction for the operator corresponding to the positive spectral parameter $E = k^2 > 0$. Then this function is a solution to the one-dimensional Schrödinger equation on the edges $-\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = k^2\psi$. The general solution to the differential equation on the edge $\Delta_j = [x_{2j-1}, x_{2j}]$ with the length $d_j = |x_{2j} - x_{2j-1}|$ can be written in the basis of incoming waves as follows

$$\psi(x) = a_{2j-1}e^{ik|x-x_{2j-1}|} + a_{2j}e^{ik|x-x_{2j}|}, \tag{4}$$

where a_m is the amplitude of the wave coming in from the endpoint x_m.

Now let us introduce two matrices $\mathcal{E}$ and Σ corresponding to evaluation of amplitudes through edges and vertices respectively. First matrix

$$\mathcal{E} = \left(\begin{array}{c|c|c} e^1 & 0 & \dots \\ \hline 0 & e^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array}\right), \qquad \text{where} \quad e^j = \begin{pmatrix} 0 & e^{ikd_j} \\ e^{ikd_j} & 0 \end{pmatrix}. \tag{5}$$

The second matrix is formed by blocks of vertex scattering matrices

$$\Sigma = \left(\begin{array}{c|c|c} \sigma^1 & 0 & \dots \\ \hline 0 & \sigma^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array}\right), \tag{6}$$

where for natural boundary conditions the vertex scattering matrices do not depend on the energy and elements are given by

$$\sigma^m_{jk} = \begin{cases} \frac{2}{v_m}, & j \neq k, \\ \frac{2-v_m}{v_m}, & j = k, \end{cases} \quad \text{for } v_m \neq 1 \qquad \text{and} \qquad \sigma = 1 \quad \text{for } v_m = 1. \tag{7}$$

After evaluation of the amplitudes through edges and then through vertices we arrive to the same incoming amplitudes. Therefore the amplitudes $\mathbf{a}$ determine an eigenfunction of $H(\Gamma)$ for $E > 0$ if and only if $\mathbf{a} = \Sigma\mathcal{E}\mathbf{a}$, i.e. when the matrix

$$U(k) = \Sigma\mathcal{E}(k) \tag{8}$$

has eigenvalue 1 and $\mathbf{a}$ is the corresponding eigenvector.

Let us denote the eigenvalues of the Laplace operator H in nondecreasing order as follows

$$E_0 = k_0^2 = 0 < E_1 = k_1^2 \leq E_2 = k_2^2 \leq ...$$

and we will introduce the distribution u connected with the spectral measure

$$u \equiv \delta(k) + \sum_{n=1}^{\infty} \left(\delta(k - k_n) + \delta(k + k_n)\right).$$

Now we are going to present the relation between spectrum of Laplace operator H and lengths of periodic orbits, number of edges and total length of the graph. Before we do this, however, we need to give a few definitions related to periodic orbits of a graph.

By a *periodic orbit* we understand any oriented closed path on Γ. We do not allow to turn back at any internal point of the edge, but walking the same edge multiple times is allowed. Note that so defined orbit does not have any starting point. With any such (continuous) periodic orbit p one can associate the *discrete periodic orbit* consisting of all edges forming that orbit. Also let:

- $\mathcal{P}$ be the set of all periodic orbits for the graph Γ,
- $l(p)$ be the geometric length of a periodic orbit p,
- $\mathrm{prim}(p)$ denote a primitive periodic orbit, i.e. such that p is a multiple of $\mathrm{prim}(p)$,
- $\mathcal{L} = d_1 + d_2 + \ldots + d_N$ be the total length of the graph Γ,
- $\mathcal{T}(p)$ be the set of all scattering coefficients along the orbit p.

Let us introduce coefficients which are independent of the energy:

$$\mathcal{A}_p = l(\mathrm{prim}(p))\Big(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \sigma_{ij}^m\Big), \qquad \mathcal{A}_p^* = l(\mathrm{prim}(p))\Big(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \overline{\sigma_{ij}^m}\Big). \tag{9}$$

The following theorem has been proven in [10], following the ideas of B. Gutkin and U. Smilansky [6].

Proposition 1 (Theorem 1 from [10]). *Let $H(\Gamma)$ be the Laplace operator on a finite connected metric graph Γ, then the following two trace formulae establishes the relation between the spectrum $\{k_j^2\}$ of $H(\Gamma)$ and the set of periodic orbits $\mathcal{P}$, the number of edges N and the total length $\mathcal{L}$ of the graph:*

$$u(k) \equiv \delta(k) + \sum_{n=1}^{\infty} \left(\delta(k - k_n) + \delta(k + k_n)\right) \tag{10}$$

$$= -(N-M+1)\delta(k) + \frac{\mathcal{L}}{\pi} + \frac{1}{2\pi}\sum_{p\in\mathcal{P}}\Big(\mathcal{A}_p\, e^{ikl(p)} + \mathcal{A}_p^*\, e^{-ikl(p)}\Big),$$

and

$$\hat{u}(l) \equiv 1 + \sum_{n=1}^{\infty}\big(e^{-ik_n l} + e^{ik_n l}\big) \tag{11}$$

$$= -(N-M+1) + 2\mathcal{L}\delta(l) + \sum_{p\in\mathcal{P}}\Big(\mathcal{A}_p\delta(l-l(p)) + \mathcal{A}_p^*\delta(l+l(p))\Big)$$

where $\mathcal{A}_p$, $\mathcal{A}_p^*$ are independent of the energy complex numbers given by (9).

The formula (11) converges in the sense of distributions (see [10] p. 4908–4909 for explicit calculations).

4. The inverse spectral problem

In this section we are going to apply formula (11) to prove that the inverse spectral problem has unique solution for certain simple (i.e. without loops or multiple edges), clean, finite connected metric graphs with rationally dependent lengths of edges.

The set L of lengths of all periodic orbits is usually called the length spectrum. In some cases, formula (11) allows us to recover the length spectrum (of periodic orbits) from the energy spectrum (of the Laplace operator H). On the other hand, there are known graphs for which some lengths of periodic orbits cannot be recovered. Formula (11) implies directly that the spectrum of a graph allows one to recover the lengths l of all periodic orbits from the *reduced length spectrum* $L' \subset L$ defined as

$$L' = \{l : \Big(\sum_{\substack{p\,\in\,\mathcal{P}\\ l(p)\,=\,l}} \mathcal{A}_p\Big) \neq 0\}. \tag{12}$$

Although for any periodic orbit p the coefficient $\mathcal{A}_p$ defined in (9) is non-zero it can happen that the sum of all coefficients in front of $\delta(l-l(p))$ is zero. This is the reason why we use reduced length spectrum instead of more common length spectrum.

4.1. Graphs with trivially rationally dependent edges

In this subsection we will discuss graphs where the set of all lengths of edges is rationally independent, while some edges can have equal lengths (we will call such case a graph with *trivially rationally dependent* edges). One can prove that such graphs can be uniquely reconstructed from length spectrum and total length of the graph — and, therefore, can be uniquely reconstructed from spectrum of Laplace operator on this graph.

We shall now remind Lemma 2 from paper [10] and we will re-state this lemma for graphs with trivially rationally dependent edges.

Lemma 2. *Let Γ be a graph with trivially rationally dependent edges. Assume that the edges of the same length are not neighbours to each other. Then the reduced length spectrum L' contains at least the following lengths:*

- $4d_j$*, for all* $j = 1, \ldots, N$*;*
- $2d_j$ *if there exist exactly one edge of length* d_j*;*
- $2(d_j + d_k)$ *iff the edges having lengths* d_j *and* d_k *are neighbours;*
- $2(d_i + d_j + d_k)$ *if* Δ_i*,* Δ_j *and* Δ_k *form a path but do not form a cycle.*

PROOF. Consider any orbit p of the length $4d_j$. Then the coefficient $\mathcal{A}_p$ product consists of exactly two squared reflection coefficients and therefore is strictly positive. The coefficient in front of $\delta(l - 4d_j)$ in the sum (11): $\sum_{p:l(p)=4d_j}$ is also strictly positive. Thus $4d_j$ belongs to the reduced length spectrum L'.

The other three parts of this proof follow from the Lemma 2 and its proof in [10] □

Lemma 3. *Assume that Γ is a finite, clean, connected and simple metric graph with trivially rationally dependent edges. Let us denote number of edges of length d_1 by β_1, number of edges of length d_2 by β_2, ..., number of edges of length d_n by β_n (where $\beta_i \geq 1$ for $i = 1 \ldots n$).*

Then the total length $\mathcal{L}$ of the graph and the reduced length spectrum L' determine the lengths of all edges (d_j), as well as the number of edges having these particular lengths (β_j).

PROOF. Consider the finite subset L'' of $L' \subset L$, consisting of all lengths less than or equal to $4\mathcal{L}$

$$L'' = \{l \in L' : l \leq 4\mathcal{L}\}.$$

This finite set contains at least the numbers $4d_j$ and those numbers form a basis for a set of all lengths of periodic orbits, i.e. every length $l \in L''$ (as well as in L) can be written as a combination of $4d_j$

$$l = \frac{1}{4}\sum_{j=1}^{n} n_j 4d_j, \quad n_j \in \mathbb{N},$$

where n_j are the smallest possible non-negative integers. Since all d_j are rationally independent then this combination is unique. Such a basis is not unique but any two bases $\{4d_j\}$ and $\{4d'_j\}$ are equal with respect to a permutations of its elements.

The total length of the graph $\mathcal{L}$ can also be written as

$$\mathcal{L} = \frac{1}{4}\sum_{j=1}^{n} \beta_j 4d_j, \quad \beta_j \in \mathbb{N}. \tag{13}$$

Because the graph Γ is simple (i.e. without loops or multiple edges), the coefficients β_j indicate the total number of edges of length d_j. □

Lemma 4. *Assume that Γ is a finite, clean, connected and simple metric graph with trivially rationally dependent edges. Also assume that any two edges Δ, Δ' with lengths d_i, d_j (where i can be equal j), for which $\beta_i \geq 2$ and $\beta_j \geq 2$ (i.e. they are both repeating edges), are separated by at least two non-repeating edges (i.e. edges for which $\beta = 1$).*

Then the graph Γ can be reconstructed from the set $D = \{d_j\}$ of the lengths of all edges and the reduced length spectrum L'.

PROOF. At the beginning we are going to reconstruct the graph Γ without repeating edges. In order to do this, we shall use the idea of reconstructing the simple subgraph in the proof of Lemma 4 in the paper [10].

Let us denote by Γ^* the subgraph of Γ which can be obtained by deleting all edges with $\beta_j \geq 2$. Γ^* does not have to be a connected graph, so let us denote its components by $\Gamma^{(1)}$, $\Gamma^{(2)}$, ..., $\Gamma^{(s)}$. The reconstruction will be done iteratively and we will construct an increasing finite sequence of subgraphs such that $\Gamma_1 \subset \Gamma_2 \subset \ldots \subset \Gamma_{N^*} = \Gamma^*$. The corresponding subsets of edges will be denoted by E_k for $k = 1, \ldots, N^*$.

The reconstruction of any component $\Gamma^{(j)}$ is done in the following way. For $k = 1$ take the graph $\Gamma_1^{(j)}$, consisting of an arbitrary non-repeating edge, say Δ_1. In order to get $\Gamma_2^{(j)}$, pick any neighbour of Δ_1, say Δ_2, and attach it to any of the endpoints of Δ_1 (the set of neighbours of Δ_1 can be easily obtained from the reduced length spectrum L').

Suppose that connected subgraph $\Gamma_k^{(j)}$ consisting of k edges ($k \geq 2$) is already reconstructed. Pick any edge, say Δ_{k+1}, which is a neighbour of at least one of the edges in $\Gamma_k^{(j)}$. Let us denote by E_k^{nbh} the subset of E_k consisting of all edges which are neighbours of Δ_{k+1}. We have to identify (one or two) vertices in $\Gamma_k^{(j)}$ to which the new Δ_{k+1} is attached – every such vertex is uniquely determined by listing of the edges joined at this vertex (since the subgraph $\Gamma_k^{(j)}$ is simple, connected and contains at least two edges). Therefore we have to separate E_k^{nbh} into two classes of edges, each attached to one endpoint of Δ_{k+1}. Observe that one of the two sets can be empty, which corresponds to the case the edge Δ_{k+1} is attached to $\Gamma_k^{(j)}$ at one vertex only.

Take any two edges from E_k^{nbh}, say Δ' and Δ''. The edges Δ' and Δ'' belong to the same class if and only if:

- Δ' and Δ'' are neighbours themselves and
- $d' + d'' + d_{k+1} \notin L'$ i.e. the edges Δ', Δ'' and Δ_{k+1} do not form a cycle (note that if Δ', Δ'' and Δ_{k+1} form a cycle, then there are two periodic orbits of length $d' + d'' + d_{k+1}$ and the corresponding $\mathcal{A}$-coefficients are equal — which implies that $d' + d'' + d_{k+1} \in L'$).

In this way we either separate the set E_k^{nbh} into two classes of edges or E_k^{nbh} consists of edges joined at one vertex. In the first case, the new edge Δ_{k+1} connects the two vertices uniquely determined by those two subclasses. In the second case, the edge Δ_{k+1} is attached at one end point to $\Gamma_k^{(j)}$ at the vertex uniquely determined by E_k^{nbh}. It does not matter which of the two end points of Δ_{k+1} is attached to the chosen vertex of $\Gamma_k^{(j)}$, since the two possible resulting graphs are equivalent.

Denote the graph created this way by $\Gamma^{(j)}_{k+1}$.

When there are no more edges left which are neighbours of $\Gamma^{(j)}_{k}$, then pick any new non-repeating edge from E and start the reconstruction procedure for new component of graph Γ^*, say $\Gamma^{(j')}$. After a finite number of steps one arrives at the graph Γ^*.

It remains now to add the repeating edges. Since each repeating edge of length d_n is separated from any other repeating edge of length d_m by at least two non-repeating edges, then there is no interference between adding edges d_n and d_m to Γ^*. Following previous lemma, from reduced length spectrum L' and total length of the graph $\mathcal{L}$ we know that we have exactly β_n edges of length d_n.

As the first step we want to split all neighbours of all d_n edges into $2\beta_n$ classes (some of which can be empty). The set of all neighbours of d_n from graph Γ^* will be denoted by $\mathbb{E}_n$. We say that Δ_j and Δ_k from $\mathbb{E}_n$ are in the same class if:

- Δ_j and Δ_k are neighbours to each other,
- they do not build a cycle of length $d_n + d_j + d_k$,
- if there is an edge Δ_m which is a neighbour to Δ_j and to Δ_k but is not a neighbour to any edge of length d_n, then there is a cycle of length $d_m + d_j + d_k$.

In that way we obtain non-empty sets $\mathbb{E}^1_n, \mathbb{E}^2_n, \ldots, \mathbb{E}^{\alpha_n}_n$ which correspond to vertices $v_1, v_2, \ldots, v_{\alpha_n}$ where $\alpha_n \leq 2\beta_n$.

As the second step we have to identify, for any edge of length d_n, two vertices (or only one) to which this particular edge is attached. We are going to check all pairs of vertices v_i and v_j from the list above. An edge of length d_n is attached to those two vertices if

- v_i and v_j are connected by a path of two edges d' and d'' where $d' \in \mathbb{E}^i_n$ and $d'' \in \mathbb{E}^j_n$ and there exist a periodic orbit of length $d' + d'' + d_n$ in L', or
- v_i and v_j are not connected by any path of two edges and for each pair $d' \in \mathbb{E}^i_n$ and $d'' \in \mathbb{E}^j_n$ there exist a periodic orbits of length $2(d' + d'' + d_n)$ in L'.

For each of those vertices $v_1, v_2, \ldots, v_{\alpha_n}$ for which neither of the above conditions are satisfied, we attach a loose edge of length d_n.

We repeat this procedure for all edges of repeating lengths. Since the graph is finite, after finite number of steps we arrive at reconstruct the whole graph Γ. □

Theorem 5. *The spectrum of a Laplace operator on a metric graph determines the graph uniquely, provided that:*

- *the graph is clean, finite, simple and connected,*
- *the edges are trivially rationally dependent,*
- *any two repeating edges are separated by at least two non-repeating edges (i.e. ones having rationally independent lengths).*

PROOF. The spectrum of the operator determines the left-hand side of the trace formula (10). Formula (11) shows that the spectrum of the graph determines the total length of the graph and the reduced length spectrum. Lemma 3 implies that the lengths of all edges and their multiplicities can be extracted from this quantities under the conditions of the theorem. It follows from Lemma 4 that the whole graph can be reconstructed. □

4.2. Graphs with weakly rationally dependent edges

In the last part of this paper we shall consider some special kind of graph with rationally dependent edges and we will prove that for those graphs the unique reconstruction from the spectrum of Laplace operator is still possible. We shall use, as before, the trace formula and some properties of mutually prime numbers.

Definition 6. *Assume that the metric graph Γ is finite, clean, connected and simple. We say that the edge lengths are weakly rationally dependent if the lengths of edges belong to the set*

$$\left\{ d_1, \frac{p_{12}}{q_{12}}d_1, \dots, \frac{p_{1r_1}}{q_{1r_1}}d_1, d_2, \frac{p_{22}}{q_{22}}d_2, \dots, \frac{p_{2r_2}}{q_{2r_2}}d_2, \dots, d_n, \frac{p_{n2}}{q_{n2}}d_n, \dots, \frac{p_{nr_n}}{q_{nr_n}}d_n \right\},$$

where $p_{ij}/q_{ij} > 1$ are proper fractions, $q_{i2}, q_{i3}, \dots, q_{ir_i}$ are mutually prime for all $i = 1, \dots, n$ and $d_1, d_2, \dots, d_n$ are rationally independent.

Observe that if $n = 1$ then all edges in the graph are rationally dependent. On the other hand, if all $p_{ij} = 0$ for $j \geq 2$ and all i, then all edges in the graph are rationally independent. Note that the denominators q_{ij} are mutually prime but it does not immediately indicate that they are prime numbers.

Lemma 7. *Assume that the metric graph Γ has weakly rationally dependent edges. Then the total length $\mathcal{L}$ of the graph and the reduced length spectrum L' determine the lengths of all edges.*

PROOF. As in Lemma 3 we will use an approach of finding a basis for all periodic orbits. We claim that the set $\{2s_j\}$, where s_j is length of any edge in the graph, is a basis for all periodic orbits. Consider as before the finite subset L'' of $L' \subset L$ consisting of all lengths less than or equal to $2\mathcal{L}$

$$L'' = \{l \in L' : l \leq 2\mathcal{L}\}.$$

It is obvious that any periodic orbit can be written as a half-integer combination of $2s_j$ elements

$$l = \frac{1}{2}\sum_{j=1}^{N} \alpha_j 2s_j, \quad \alpha_j \in \mathbb{N}.$$

We shall prove that for graph with weakly rationally dependent edges this combination is unique.

Among all periodic orbits there exist periodic orbits of length $2s_j$. Assume that for some arbitrary j such orbit is a linear combination of the other edges and since

$d_1, d_2, \ldots, d_n$ are rationally independent it is enough to consider only rationally dependent edges. For sake of notation clearness we will omit the first index in numbers p_{ij} and q_{ij} as well as index at d_i. Thus we have the following equation

$$2\frac{p_j}{q_j}d = \alpha_1\frac{p_1}{q_1}d + \alpha_2\frac{p_2}{q_2}d + \ldots + \alpha_{j-1}\frac{p_{j-1}}{q_{j-1}}d + \alpha_{j+1}\frac{p_{j+1}}{q_{j+1}}d + \ldots + \alpha_n\frac{p_n}{q_n}d \quad (14)$$

$$2\frac{p_j}{q_j} = \frac{\alpha_1 p_1 q_2 \ldots q_{j-1}q_{j+1}\ldots q_n + \ldots + \alpha_n q_1 q_2 \ldots q_{j-1}q_{j+1}\ldots q_{n-1}p_n}{q_1 q_2 \ldots q_{j-1}q_{j+1}\ldots q_n}$$

$$\begin{aligned} 2p_j q_1 \ldots q_{j-1}q_{j+1}\ldots q_n &= \alpha_1 p_1 q_2 \ldots q_n + \ldots \alpha_{j-1} q_1 q_2 \ldots p_{j-1} q_j \ldots q_n \\ &+ \alpha_{j+1} q_1 q_2 \ldots q_j p_{j+1} \ldots q_n + \ldots \alpha_n q_1 q_2 \ldots q_{n-1} p_n. \end{aligned}$$

Let us compare both sides of the previous equation, one by one, modulo each of $q_1, q_2, \ldots, q_{j-1}, q_{j+1}, \ldots, q_n$, thus giving the following system of equations

$$\begin{cases} 0 = \alpha_1 p_1 q_2 \ldots q_n & (\mathrm{mod}\ q_1) \\ \quad\vdots & \\ 0 = \alpha_{j-1} q_1 q_2 \ldots p_{j-1} q_j \ldots q_n & (\mathrm{mod}\ q_{j-1}) \\ 0 = \alpha_{j+1} q_1 q_2 \ldots q_j p_{j+1} \ldots q_n & (\mathrm{mod}\ q_{j+1}) \\ \quad\vdots & \\ 0 = \alpha_n q_1 q_2 \ldots q_{n-1} p_n & (\mathrm{mod}\ q_n) \end{cases}$$

Since all q_i are mutually prime and p_i/q_i are proper fractions, the only solution to this system of equations is $\alpha_i = 0 \pmod{q_i}$ for all $i = 1, 2, \ldots, j-1, j+1, \ldots, n$. It means that all elements on the right hand side of (14) are nonnegative integers, while the left hand side of the same equation is an integer if and only if $j = 1$ or $j = 2$ (then $p_1 = q_1 = 1$ or, respectively, $q_2 = 2$ and $p_2 = 3$).

In the first case, the left hand side is equal 2, while at the same time the right hand side is either 0 or is strictly greater than 2. In the second case, the left hand side is equal to 3, while the right hand side is equal to $\alpha_1 + r$, where r is either 0 or is strictly greater than 3. Thus, to fulfill equation (14), r has to be 0 and α_1 has to be 3. This is, however, impossible — since there is exactly one periodic orbit of length 3 (consisting of double edge of length $\frac{p_2}{q_2} = \frac{3}{2}$).

Thus we have proven that the set $\{2s_j\}$ where s_j are lengths of all edges in the graph Γ form the basis for all lengths of periodic orbits.

Hence we have determined all lengths of edges if these edges are weakly rationally dependent. □

Lemma 8. *Assume that the metric graph Γ has weakly rationally dependent edges. Then the graph Γ can be reconstructed from the sets $D = \{d_j\}$ and the reduced length spectrum L'.*

PROOF. As we have just shown in Lemma 7, from reduced length spectrum L' one can obtain lengths of all edges in graph Γ with weakly rationally dependent edges. Following Lemma 2 we can deduce that the reduced length spectrum L' contains at least the shortest orbit formed by any two neighbouring edges Δ_j and Δ_k i.e. $2(d_j + d_k)$. Thus we can identify all neighbours of each edge. The algorithm of reconstruction the graph Γ will be the same as in proof of Lemma 4 in part where we reconstruct components of Γ^*. □

Theorem 9. *The spectrum of a Laplace operator on a metric graph determines the graph uniquely, provided that:*

- *the graph is clean, finite, simple and connected,*
- *the edges are weakly rationally dependent.*

PROOF. The spectrum of the operator determines the left-hand side of the trace formula (10). Formula (11) shows that the spectrum of the graph determines the total length of the graph and the reduced length spectrum. Lemma 7 implies that the lengths of all edges can be extracted from this quantities under the conditions of the theorem. It follows from Lemma 8 that the whole graph can be reconstructed. □

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Paper III

Geometric properties of quantum graphs and vertex scattering matrices*

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ABSTRACT. Differential operators on metric graphs are investigated. It is proven that vertex boundary conditions can be successfully parameterized by the vertex scattering matrix at the energy equal to 1. Connectivity and high energy asymptotics are investigated in detail. The trace formula is proven for energy independent vertex scattering matrices. Two new families of boundary conditions are investigated: hyperplanar Neumann and Dirichlet conditions. It is proven that the Euler characteristic of the metric graph can be determined from the spectrum of the Laplace operator with the boundary conditions from any one of these classes.

1. Introduction

Quantum graphs is a rapidly developing area of research in mathematical physics with important prospective applications in nanotechnology and modern engineering, which was started in the 80-ies [4; 3]. Probably there is no necessity to explain the importance of such studies for the readers of the current volume. From the mathematical point of view this is exactly the area of research where ordinary and partial differential equations meet each other, in other words where methods developed originally for ordinary and partial differential equations are used simultaneously. In the current article we study differential operators on metric graphs coupled by boundary conditions at the vertices. These operators are studied using methods of spectral analysis of self-adjoint operators concentrating on the relations between their spectral properties and geometric structure of the underlying graph. To calculate an eigenfunction of such an operator one needs to solve first a certain ordinary differential equation on every edge separately, but solutions on different edges are connected through the boundary conditions and thus remind us about partial differential equations.

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In a series of papers [13; 11; 12] it was proven that the spectrum in the case of a compact graph determines the Euler characteristic of the underlying graph as well as the number of connected components in the special case of so-called standard boundary conditions at the vertices. The main analytic tool developed there is celebrated trace formula proposed independently by J.-P. Roth [15] and B. Gutkin and U. Smilansky [5]. The aim of the current article is to develop this approach further in order to include most general boundary conditions at the vertices. Therefore the first part of the article is devoted to the discussion of most general boundary conditions at the vertices including studies of their high-energy asymptotics. In order to make our presentation clear only a star graph is considered in the first part. During these studies we found it useful to use a new parametrization of such boundary conditions by the matrix S, which is nothing else than the vertex scattering matrix for the energy equal to 1. The advantage of this parametrization is that it is unique and that the parameter has clear physical interpretation. This parametrization reminds very much of Harmer's parametrization, which is unique as well, but the parameter used there has not been given clear interpretation so far. We establish connection with classical (for the area of quantum graphs) Kostrykin-Schrader's and Kuchment's parameterizations of boundary conditions. We investigate the high energy asymptotics of the corresponding vertex scattering matrix proving that the limit always exists and coincides with a certain matrix which may be obtained by choosing the boundary conditions in a special way, so that the corresponding vertex scattering matrix does not depend on the energy. The set of all such energy independent vertex scattering matrices is characterized and relations with known parameterizations are established. The corresponding boundary conditions we call non-resonant.

In section 6. all properly connecting boundary conditions are classified which allows us to establish the correspondence between the families of boundary conditions and connectivity of the underlying graph. Studies of the high energy asymptotics lead us to the notion of asymptotically properly connecting boundary conditions - the boundary conditions leading to scattering matrices with proper limit at high energies. As we have already mentioned the high energy limit of every vertex scattering matrix coincides with a certain energy independent vertex scattering matrix. It might happen that even if the original boundary conditions are properly connecting, the boundary conditions corresponding to the limit (energy independent) matrix are not, which leads to spectral asymptotics reminding of the graphs with different connectivity than the underlying graph. The family of boundary conditions leading to asymptotically connecting boundary conditions is characterized. In particular we select two families of boundary conditions: hyperplanar Neumann and Dirichlet conditions (see Definitions 18 and 19). The first family is a direct generalization of standard boundary conditions. The second family generalizes the so-called δ'_s boundary conditions considered by P. Exner [2] and P. Kuchment [10].

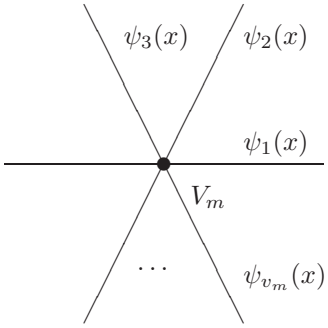
In the second part of the article arbitrary finite compact graphs are considered. The corresponding Laplace operator is defined on the domain of functions satisfying boundary conditions at the vertices that are properly connecting and lead to energy independent vertex scattering matrices. These operators have pure discrete spectrum consisting of eigenvalues tending to $+\infty$. Following methods developed in [15; 5; 13; 12] we prove the trace formula for arbitrary boundary conditions leading to energy independent vertex scattering matrices. This formula connect the set of eigenvalues

(the energy spectrum) with the set of periodic orbits on the metric graph (the length spectrum), but includes so-called spectral and algebraic multiplicities of the eigenvalue zero. The first number is just the multiplicity of the eigenvalue zero whereas the second number is the multiplicity of the eigenvalue given by the characteristic equation used in the derivation of the trace formula. These numbers may be different and the Section 8. is devoted to calculation of these numbers for the special case of hyperplanar Neumann and Dirichlet conditions at the vertices. Both the spectral and algebraic multiplicities of the eigenvalue zero can be calculated from the spectrum. The first number is trivially given as multiplicity of $\lambda = 0$, the second number is determined by the asymptotics of the spectrum. It appears that for connected graphs these two numbers determine the Euler characteristic of the metric graph and therefore makes it possible to determine which sort of boundary conditions (hyperplanar Neumann or Dirichlet conditions) at the vertices is used to define the operator.

2. Star graph

In this and following sections we are going to discuss how to write boundary conditions at a vertex so that they connect properly together different edges meeting at this vertex. In order to make our presentation clear we study the star graph having in mind to generalize our consideration later for more complicated graphs.

Let us consider a star graph Γ with v_m semi-infinite nodes $\Delta_j = [0, \infty)$, $j = 1, 2, \ldots, v_m$, connected at one vertex V_m with valence v_m (equal to the number of edges connected at the vertex). Consider the Hilbert space of square integrable func-



tions on Γ

$$\mathcal{H} \equiv L^2(\Gamma) = \oplus_{n=1}^{v_m} L^2([0, \infty)). \tag{1}$$

The Laplace operator on Γ is the sum of second derivative operators on each interval Δ_j,

$$L = \oplus_{j=1}^{v_m} \left(-\frac{d^2}{dx^2} \right). \tag{2}$$

This differential expression does not determine the self-adjoint operator uniquely. Two differential operators in $L^2(\Gamma)$ are naturally associated with the differential expression (2): the minimal operator with the domain $\mathrm{Dom}\,(L_{\min}) = \oplus_{j=1}^{v_m} C_0^\infty((0, \infty))$ and the

maximal operator $L_{\max}$ with the domain $\mathrm{Dom}\,(L_{\max}) = \oplus_{j=1}^{v_m} W_2^2((0,\infty))$, where W_2^2 denotes the Sobolev space. The operator $L_{\min}$ is symmetric and $L_{\max}$ is its adjoint: $L_{\max} = L_{\min}^*$.

All self-adjoint operators associated with (2) can be obtained by extending the minimal operator to a subspace in the domain of $L_{\max}$. Every such subspace can be described using certain boundary conditions connecting boundary values of the functions on Γ at the vertex.

Such self-adjoint extensions can be described using von Neumann formulas taking into account that $L_{\min}$ is symmetric and has deficiency indices (v_m, v_m). But parametrization via boundary conditions appears more appropriate due to its local character.

Another parametrization of extensions of $L_{\min}$ can be obtained using Lagrangian planes. Consider the boundary form:

$$B[\varphi,\psi] = \langle L_{\max}\varphi,\psi\rangle - \langle \varphi, L_{\max}\psi\rangle = \sum_{j=1}^{v_m}(\partial_n\varphi_j(0)\overline{\psi_j}(0) - \varphi_j(0)\partial_n\overline{\psi_j}(0))$$

which gives a sesquilinear symplectic form in the finite dimensional space of boundary values $\mathbb{C}^{2v_m}$. Then all Lagrangian planes ϖ i.e. subspaces of $\mathbb{C}^{2v_m}$ such that $\varphi,\psi\in\pi$, $B[\varphi,\psi]=0$ and are maximal, describe all extensions of $L_{\min}$ to self-adjoint operator L_ϖ, so that $\mathrm{Dom}(L_\varpi) = \{\varphi\in\mathrm{Dom}(L_{\max}) : (\boldsymbol{\varphi}(0),\partial_n\boldsymbol{\varphi}(0))\in\varpi\}$, where $\boldsymbol{\varphi},\partial_n\boldsymbol{\varphi}$ denote the vectors of boundary values for φ and its normal derivative at the vertex V_m.

3. Boundary conditions via the vertex scattering matrix

In the current section we are going to show that the boundary conditions at any vertex can be parameterized in the unique way by a certain unitary matrix. Our approach is a slight modification of that by M. Harmer [6], the advantage of our parametrization is that the parameter matrix S coincides with the value of the vertex scattering matrix at $k=1$ (this explains our notation as well).

Theorem 1. *The family of self-adjoint extensions of the minimal operator $L_{\min}$ can uniquely be parameterized by an arbitrary $v_m\times v_m$ unitary matrix S, so that the operator $L(S)$ is the restriction of $L_{\max}=L_{\min}^*$ to the set of functions satisfying the boundary conditions*

$$i(S-I)\boldsymbol{\psi}(V_m) = (S+I)\partial_n\boldsymbol{\psi}(V_m) \tag{3}$$

Proof. As a first step we will determine the deficiency indices for the operator $L_{\min}$. Let λ be an arbitrary parameter in the upper half-plane, i.e. $\mathrm{Im}\,\lambda>0$. Every deficiency element $g(\lambda)$ is a solution to $(L_{\max}-\lambda)g(\lambda)=0$. It is easy to see that the deficiency subspace $\mathcal{N}_{\bar\lambda}$ is spanned by $\{g_j(\lambda)\}$ given by:

$$g_j(\lambda) = \begin{cases} e^{i\sqrt{\lambda}x} & \text{for } x\in\Delta_j,\\ 0 & \text{otherwise.}\end{cases}$$

Similarly we can introduce a function $g_j(\bar{\lambda}) = \overline{g_j(\lambda)}$ as a solution to the equation $(L_{\max} - \bar{\lambda})g(\lambda) = 0$ and the deficiency subspace $\mathcal{N}_\lambda = span\{g_j(\bar{\lambda})\}$. As we can see from the form of solutions $g_j(\lambda)$ each of the spaces $\mathcal{N}_\lambda$ and $\mathcal{N}_{\bar{\lambda}}$ is spanned by exactly v_m functions, thus the deficiency indices are (v_m, v_m). Moreover any element $\psi_{\bar{\lambda}} \in \mathcal{N}_{\bar{\lambda}}$ can be written as $\psi_{\bar{\lambda}} = \sum_{j=1}^{v_m} \psi_j g_j(\lambda)$ and similarly $\psi_\lambda \in \mathcal{N}_\lambda$ as $\psi_\lambda = \sum_{j=1}^{v_m} \psi_j g_j(\bar{\lambda})$.

Every function ψ from $\mathrm{Dom}(L_{\max})$ can be written in the form:

$$\psi = \tilde{\psi} + \psi_\lambda + \psi_{\bar{\lambda}}, \quad \text{where } \tilde{\psi} \in \mathrm{Dom}(\overline{L_{\min}}), \psi_\lambda \in \mathcal{N}_\lambda, \psi_{\bar{\lambda}} \in \mathcal{N}_{\bar{\lambda}}$$

and the sum is direct.

Consider a unitary operator $\mathbb{W}$ mapping $\mathcal{N}_{\bar{\lambda}}$ onto $\mathcal{N}_\lambda$; $\mathbb{W} : \mathcal{N}_{\bar{\lambda}} \to \mathcal{N}_\lambda$ and the matrix W representing the operator $\mathbb{W}$ in the bases $\{g_j(\lambda)\} \subset \mathcal{N}_{\bar{\lambda}}$ and $\{g_j(\bar{\lambda})\} \subset \mathcal{N}_\lambda$. Then any self-adjoint extension of $\overline{L_{\min}}$ can be described as a restriction of $L_{\max}$ to the set of functions possessing the following representation

$$\psi = \tilde{\psi} + (\mathbb{W} - I)\psi_{\bar{\lambda}},$$

where $\tilde{\psi} \in \mathrm{Dom}(\overline{L_{\min}})$ and $\psi_{\bar{\lambda}} \in \mathcal{N}_{\bar{\lambda}}$. In other words

$$\mathrm{Dom}(L(\mathbb{W})) = \mathrm{Dom}(\overline{L_{\min}}) \dot{+} (\mathbb{W} - I)\mathcal{N}_{\bar{\lambda}}.$$

Then the boundary values at the vertex of any such function can be calculated

$$\begin{array}{rcl} \boldsymbol{\psi}(V_m) & = & (W - I)\boldsymbol{\psi}_{\bar{\lambda}}(V_m), \\ \partial_n\boldsymbol{\psi}(V_m) & = & i(\sqrt{\lambda}W + \sqrt{\bar{\lambda}}I)\boldsymbol{\psi}_{\bar{\lambda}}(V_m). \end{array} \tag{4}$$

Comparing (4) and (3) we conclude that the matrix S has to satisfy the equation

$$(S - I)(W - I) = (S + I)(\sqrt{\lambda}W + \sqrt{\bar{\lambda}}I).$$

Therefore the relation between the matrix S describing the boundary conditions and the unitary matrix W used in von Neumann parametrization is

$$S = \frac{W - I + (\sqrt{\lambda}W + \sqrt{\bar{\lambda}}I)}{W - I - (\sqrt{\lambda}W + \sqrt{\bar{\lambda}}I)}.$$

Note that the matrix $W - I - (\sqrt{\lambda}W + \sqrt{\bar{\lambda}}I)$ is invertible. Suppose that

$$(W - I - (\sqrt{\lambda}W + \sqrt{\bar{\lambda}}I))\varphi = 0$$

for some $\varphi \in \mathcal{N}_{\bar{\lambda}}$. Then

$$(1 - \sqrt{\lambda})W\varphi = (1 + \sqrt{\bar{\lambda}})\varphi.$$

Since W is unitary and φ in nonzero then $||W\varphi|| = ||\varphi|| \neq 0$. Thus comparing the norm on both sides of the last equation we obtain

$$|1 - \sqrt{\lambda}| = |1 + \sqrt{\bar{\lambda}}|$$

which is false since $\operatorname{Im}\lambda > 0$.

Moreover the matrix S is unitary, since W is unitary

$$S^* = \frac{W^{-1} - I + (\sqrt{\lambda}W^{-1} + \sqrt{\lambda}I)}{W^{-1} - I - (\sqrt{\lambda}W^{-1} + \sqrt{\lambda}I)} = \frac{I - W + (\sqrt{\lambda}I + \sqrt{\lambda}W)}{I - W - (\sqrt{\lambda}I + \sqrt{\lambda}W)} = S^{-1}.$$

We have proven that any self-adjoint extension can be described by (3) with a unitary S. Let us show that S can be chosen arbitrarily. Really we have that

$$W = \frac{S - I + \sqrt{\lambda}(S + I)}{S - I - \sqrt{\lambda}(S + I)}$$

and every such W is unitary, provided that S is unitary. This parametrization is obviously unique. □

As we already mentioned the advantage of parametrization (3) is that there is a one-to-one correspondence between the unitary matrices S and self-adjoint extensions of $L_{\min}$. Let us have a look at few intensively used families of boundary conditions.
EXAMPLE 1.Standard boundary conditions. For standard boundary conditions the matrix S should be chosen equal to

$$S = \begin{pmatrix} \frac{2-v_m}{v_m} & \frac{2}{v_m} & \cdots & \frac{2}{v_m} \\ \frac{2}{v_m} & \frac{2-v_m}{v_m} & & \frac{2}{v_m} \\ & \cdots & & \\ \frac{2}{v_m} & \frac{2}{v_m} & & \frac{2-v_m}{v_m} \end{pmatrix}.$$

Then

$$S - I = \begin{pmatrix} \frac{2(1-v_m)}{v_m} & \frac{2}{v_m} & \frac{2}{v_m} \\ \frac{2}{v_m} & \frac{2(1-v_m)}{v_m} & \frac{2}{v_m} \\ & \cdots & \\ \frac{2}{v_m} & \frac{2}{v_m} & \frac{2(1-v_m)}{v_m} \end{pmatrix}, \quad S + I = \begin{pmatrix} \frac{2}{v_m} & \frac{2}{v_m} & \frac{2}{v_m} \\ \frac{2}{v_m} & \frac{2}{v_m} & \frac{2}{v_m} \\ & \cdots & \\ \frac{2}{v_m} & \frac{2}{v_m} & \frac{2}{v_m} \end{pmatrix}$$

Subtracting the first equation in (3) from other ones we obtain that the functions ψ is continuous and the sum of its normal derivatives is equal to zero.

Let us establish the connection between the matrix S appearing in the boundary conditions and the vertex scattering matrix $S_v(k)$. Since S is an unitary matrix let us denote its eigenvalues and eigenvectors by $e^{i\theta_j}$ and ϕ_j respectively ($\theta_j \in \mathbb{R}, \langle \phi_i, \phi_j \rangle = \delta_{ij}, j = 1, \ldots, v_m$). Then S possesses the following spectral representation:

$$S\psi = \sum_{j=1}^{v_m} e^{i\theta_j} \langle \psi, \phi_j \rangle \phi_j. \tag{5}$$

In what follows the subspaces

$$N_{\pm 1} = \ker (S - (\pm I)), \tag{6}$$

are going to play very important role.

To introduce the vertex scattering matrix let us first consider the solutions to the differential equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x) = k^2\psi(x),$$

which satisfy conditions (3) at the vertex. Solution to the differential equation can be written in the basis of incoming and outgoing waves as follows

$$\psi_j(x) = b_j e^{-ikx} + a_j e^{ikx}, \quad x \in \Delta_j. \tag{7}$$

The relation between the vectors of waves' amplitudes $\boldsymbol{a}$ and $\boldsymbol{b}$ is given by the vertex scattering matrix $S_v(k)$: $\boldsymbol{a} = S_v(k)\boldsymbol{b}$. The scattering matrix has to be chosen so that the function in (7) satisfies the boundary conditions at the vertex. The values of the functions and of normal derivatives at the vertex are:

$$\boldsymbol{\psi}(V_m) = \boldsymbol{b} + \boldsymbol{a} = \boldsymbol{b} + S_v(k)\boldsymbol{b}$$

and

$$\partial_n\boldsymbol{\psi}(V_m) = -ik\boldsymbol{b} + ik\boldsymbol{a} = -ik\boldsymbol{b} + ikS_v(k)\boldsymbol{b}.$$

After substitution into equation (3) we obtain

$$i(S-I)(I+S_v(k)) = ik(S+I)(-I+S_v(k))$$

and then

$$S_v(k) = \frac{k(S+I)+(S-I)}{k(S+I)-(S-I)}, \quad k \neq 0. \tag{8}$$

Similarly as in the last proof we can show that the matrix appearing in the denominator is invertible, so $S_v(k)$ is well defined. From equation (8) we can easily observe that $S_v(1) = S$. This is the reason for us to choose parametrization (3).

Let us show that the matrix $S_v(k)$ is unitary for any real $k \neq 0$:

$$S_v(k)S_v^*(k) = \frac{k(S+I)+(S-I)}{k(S+I)-(S-I)} \cdot \frac{k(S^*+I)+(S^*-I)}{k(S^*+I)-(S^*-I)} = I$$

Hence we have shown that all boundary conditions at a vertex leading to self-adjoint extensions of $L_{\min}$ can be described by the matrix S equal to $S_v(1)$, where $S_v(k)$ is a unitary vertex scattering matrix. We would like to point out that in 2000 Kostrykin and Schrader ([8], Theorem 1.) showed that the knowledge of $S_v(k_0)$ for some fixed energy parameter k_0 allows one to calculate $S_v(k)$ for any arbitrary k, and therefore determines the boundary conditions at the vertex.

4. Different parameterizations of boundary conditions

The research on boundary conditions and self-adjoint operators on graphs goes back to 80-ies to works of B. Pavlov and N. Gerasimenko [4] and of P. Exner and P. Šeba [3] and is described in details by P. Kuchment in [10]

4.1. Kostrykin-Schrader's parametrization

In 1999 Kostrykin and Schrader [7] gave a full description how all self-adjoint extensions can be obtained from local boundary conditions. Let A and B be $v_m \times v_m$ matrices then all boundary conditions at the vertex can be described in the following way:

$$A\boldsymbol{\psi}(V_m) + B\partial_n\boldsymbol{\psi}(V_m) = 0 \tag{9}$$

where $\boldsymbol{\psi}$ is the v_m-dimensional vector of functions and $\partial_n\boldsymbol{\psi}$ - of normal derivatives defined on edges of the graph Γ.

Proposition 2 (Kostrykin, Schrader). *All self-adjoint extensions of the minimal operator $L_{\min}$ are described by the boundary conditions (9) where A and B are $v_m \times v_m$ matrices with the following properties:*

1. *the $v_m \times 2v_m$ matrix (A, B) has maximal rank v_m,*
2. *the matrix AB^* is Hermitian.*

Notice that parametrization of boundary conditions in equation (9) with matrices A and B is not unique . One can take any arbitrary invertible matrix D and use matrices $A' = DA$ and $B' = DB$ instead of A and B. These matrices determine the same Lagrangian plane of boundary values.

The parametrization via vertex scattering matrix $S_v(k)$ presented in the previous section is unique. Moreover to describe properties of boundary conditions and therefore self-adjoint extensions we will investigate properties of only one matrix $S_v(k)$.

The boundary conditions (9) can be rewritten as:

$$A(\boldsymbol{b} + S_v\boldsymbol{b}) + B(-ik\boldsymbol{b} + ikS_v\boldsymbol{b}) = 0.$$

Hence the relation between the scattering matrix $S_v(k)$ and the matrices A and B (see [8]) is

$$S_v(k) = -(A + ikB)^{-1}(A - ikB) \tag{10}$$

and in particular

$$S = S_v(1) = -(A + iB)^{-1}(A - iB). \tag{11}$$

4.2. Harmer's parametrization

Another parametrization of boundary conditions using only one unitary matrix U and which is unique was proposed by Harmer in 2000 [6]

$$-i(U + I)\boldsymbol{\psi}(V_m) + (U - I)\partial_n\boldsymbol{\psi}(V_m) = 0. \tag{12}$$

In this parametrization the unitary matrix again does not coincide with the unitary matrix appearing in von Neumann formulas. One may obtain this parametrization from (3) just by putting

$$S = -U.$$

The only advantage of the parametrization via the matrix S is that it has clear meaning being the vertex scattering matrix for $k = 1$.

4.3. Kuchment's parametrization

In 2004 Kuchment has noticed that boundary condition (9) can be rewritten equivalently as two conditions which use orthogonal projection on $\ker B$. This makes Kostrykin-Schrader's parametrization unique.

Proposition 3 (following Corollary 5 in [10]). *Let (A, B) has maximal rank and AB^* be Hermitian matrix. Then the boundary condition (9) is equivalent to the pair of conditions $P_{M^\perp}\boldsymbol{\psi} = 0$ and $LP_M\boldsymbol{\psi} + P_M\partial_n\boldsymbol{\psi} = 0$, where P_M is orthogonal projection onto space $M = (\mathrm{Ker}\ B)^\perp$, $P_{M^\perp}$ is the complementary projector, and L is the self-adjoint operator $B^{-1}A$.*

The operator $i\frac{\hat{S}-I}{\hat{S}+I}$, where $\hat{S} = P_{N_{-1}^\perp}SP_{N_{-1}^\perp}$, in $N_{-1}^\perp$ is hermitian. It follows that we get Kuchment's parametrization by taking

$$M = N_{-1}^\perp \quad \text{and} \quad L = i\frac{P_{N_{-1}^\perp}SP_{N_{-1}^\perp} - I}{P_{N_{-1}^\perp}SP_{N_{-1}^\perp} + I}.$$

5. High energy asymptotics and energy independent scattering matrices

For the studies of spectral asymptotics it is necessary to investigate the high energy behavior of the vertex scattering matrix.

Let us remind that the unitary matrix S possesses the spectral representation (5) and that the vertex scattering matrix $S_v(k)$ is given by (8). Then we obtain the following representation for the matrix $S_v(k)$:

$$\begin{aligned} S_v(k)\psi &= \sum_{j=1}^{v_m} \frac{k(e^{i\theta_j}+1)+(e^{i\theta_j}-1)}{k(e^{i\theta_j}+1)-(e^{i\theta_j}-1)}\langle\psi,\phi_j\rangle\phi_j \\ &= \sum_{j:\theta_j=\pi}(-1)\langle\psi,\phi_j\rangle\phi_j + \sum_{j:\theta_j=0}1\langle\psi,\phi_j\rangle\phi_j + \sum_{j:\theta_j\neq\pi,0}\frac{k(e^{i\theta_j}+1)+(e^{i\theta_j}-1)}{k(e^{i\theta_j}+1)-(e^{i\theta_j}-1)}\langle\psi,\phi_j\rangle\phi_j. \end{aligned} \tag{13}$$

Since S is unitary N_1 and N_{-1} are orthogonal to each other; if S has no other eigenvalues, then $N_1 \oplus N_{-1} = \mathbb{C}^{v_m}$. Formula (13) implies that the eigenvalues ± 1 are stable, whereas all other eigenvalues depend on k. The properties of this representation for $S_v(k)$ gives us immediately the following two theorems.

Theorem 4. *The scattering matrix $S_v(k)$ is energy independent if and only if the parameter matrix S has just eigenvalues 1 and -1, i.e. iff boundary conditions (3) take the form*

$$P_{N_1}\partial_n\boldsymbol{\psi}(V_m) = 0, \quad P_{N_{-1}}\boldsymbol{\psi}(V_m) = 0, \tag{14}$$

where $N_1 \oplus N_{-1} = \mathbb{C}^{v_m}$.

Proof. Observe that when $\theta_j \neq \pi$ and $\theta_j \neq 0$, the eigenvalues given by the fraction $\frac{k(e^{i\theta_j}+1)+(e^{i\theta_j}-1)}{k(e^{i\theta_j}+1)-(e^{i\theta_j}-1)}$ do depend on k. Therefore $S(k)$ does not depend on k if and only if the unitary matrix S has eigenvalues 1 and -1 only. □

Compare the conditions (14) with Kuchment's parametrization in Proposition 3. Notice also the connection between $S + I$ and B (take into account equation (3) and (9)).

We would like to mention here Datta [1] and Taniguchi and Büttiker [16] who at the beginning of 90-ies solved one explicit example of energy independent scattering matrix for junction of 3 wires. The Theorem 4 has been proven by Kostrykin and Schrader in [9].

Boundary conditions leading to energy independent vertex scattering matrices are going to play an important role in our studies.

Definition 5. *Vertex boundary conditions are called* **non-resonant** *iff the corresponding vertex scattering matrix is energy independent.*

The main motivation for this definition is that all other boundary conditions lead to vertex scattering matrices having singularities.

Theorem 6. *As $k \to \infty$ the vertex scattering matrix tends to the energy independent vertex scattering matrix*

$$S_v^{m,\infty} = \sum_{j:\theta_j=\pi} (-1)\langle\cdot,\phi_j\rangle\phi_j + \sum_{j:\theta_j\neq\pi} \langle\cdot,\phi_j\rangle\phi_j \equiv -P_{N_{-1}} + P_{N_{-1}^{\perp}}, \qquad (15)$$

where N_{-1} is the eigensubspace for S (and hence for all $S(k)$). In addition it holds

$$S_v^m(k) = S_v^{m,\infty} + \mathcal{O}(1/k), \quad \text{as } k \to \infty.$$

Proof. Notice that for $\theta_j \neq \pi$ each of the eigenvalues $\frac{k(e^{i\theta_j}+1)+(e^{i\theta_j}-1)}{k(e^{i\theta_j}+1)-(e^{i\theta_j}-1)}$ tends to 1 as k tends to infinity. Moreover it holds

$$\frac{k(e^{i\theta_j}+1)+(e^{i\theta_j}-1)}{k(e^{i\theta_j}+1)-(e^{i\theta_j}-1)} = 1 + \mathcal{O}(1/k), \text{ as } k \to \infty.$$

Hence the limit of $S_v^m(k)$ is the matrix $S_v^{m,\infty}$ with eigenvalues 1 and -1 only. By preceding theorem, $S_v^{m,\infty}$ is an energy independent vertex scattering matrix. □

This theorem is a modification of the result already proved by Harmer in [6] and implies that for high energies every vertex scattering matrix tends to a certain scattering matrix corresponding to non-resonant boundary conditions.

6. Vertex scattering matrix and connectivity

In this section we will discuss under which additional conditions (beyond unitarity) the matrix S do connect all end points meeting at the vertex V_m. The only requirement we introduced so far is that the boundary conditions (3) connect together only boundary values corresponding to the same vertex. But it might happen that the end points meeting at certain vertex V_m can be divided into two nonintersecting classes $V_m = V_{m_1} \cup V_{m_2}$ so that boundary conditions (3) connect together the boundary values at V_{m_1} and V_{m_2} separately. Such boundary conditions do not correspond to the

vertex V_m but rather to two (independent) vertices V_{m_1} and V_{m_2}. In other words, if the vertex V_m can be chopped into two vertices so that the boundary conditions are preserved, then such conditions are not properly connecting and should be excluded from our consideration if no special reason exists. This problem has been discussed in details in [14], [8], but we describe this problem using the parametrization via the matrix S. Due to uniqueness of this parametrization the discussion becomes much more transparent.

For energy dependent vertex scattering matrices we are meeting another interesting effect. It might happen that the corresponding boundary conditions are properly connecting, but the boundary conditions corresponding to the limit scattering matrix $S_v^{m,\infty}$ are not, but it is the limit scattering matrix that is important in calculating spectral asymptotics. Therefore we shall also define asymptotically properly connecting boundary conditions, but let us consider one example first.

EXAMPLE 2. Let the graph Γ be a loop formed by just one edge $\Delta_1 = [-\pi, \pi]$ with the endpoints $-\pi$ and π connected at the vertex V_1. Consider the boundary conditions

$$\left\{ \begin{array}{rcl} \psi(-\pi) & = & -\partial_n\psi(+\pi) \\ \psi(\pi) & = & -\partial_n\psi(-\pi) \end{array} \right. ,$$

which are clearly properly connecting and correspond to $S = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix}$. The vertex scattering matrix can be calculated using (8)

$$S_v^1(k) = \begin{pmatrix} \frac{k^2-1}{k^2+1} & \frac{2ik}{k^2+1} \\ \frac{2ik}{k^2+1} & \frac{k^2-1}{k^2+1} \end{pmatrix}$$

and it tends to the unit matrix as $k \to \infty$. The boundary conditions corresponding to unit scattering matrix are just Neumann boundary conditions $\partial_n\psi(-\pi) = \partial_n\psi(\pi) = 0$, which do not connect the values at $\pm\pi$ together.

Let us summarize our discussion by giving the following definition

Definition 7. *Vertex boundary conditions are called* **properly connecting** *iff 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** *iff the limit scattering matrix S_v^∞ corresponds to certain properly connecting boundary conditions.*

Characterization of all properly connecting boundary conditions via the matrix S is rather straightforward, which is due to the uniqueness of our parametrization of boundary conditions.

Theorem 8. *Boundary conditions (3) are properly connecting iff the unitary matrix S cannot be turned into block-diagonal form by permutation of the basis vectors.*

Proof. Assume that S is block-diagonal after some permutation σ,

$$\sigma S \sigma^{-1} = \begin{pmatrix} S^1 & 0 \\ 0 & S^2 \end{pmatrix} \tag{16}$$

where S^1 and S^2 are unitary matrices in $\mathbb{C}^{v_1}$ and $\mathbb{C}^{v_2}$ respectively, $v_1 + v_2 = v_m$. Let us separate the end points forming the vertex $V_m = \{x_{j_l}\}_{l=1}^{v_m}$ into two classes V_1 and V_2 : $V_m = V_1 \cup V_2$. The permutation σ can be considered acting on the end points from V_m. Let us denote by V_1 the union of end-points that after permutation σ occupy the first v_1 positions, and by V_2 - the union of all other end-points. Then it is natural to consider the vectors of boundary values at V_1 and V_2 separately, since the boundary conditions (16) can be written as

$$\begin{cases} i(S^1 - I)\boldsymbol{\psi}(V_1) = (S^1 + I)\partial_n\boldsymbol{\psi}(V_1), \\ i(S^2 - I)\boldsymbol{\psi}(V_2) = (S^2 + I)\partial_n\boldsymbol{\psi}(V_2), \end{cases} \tag{17}$$

and obviously connect only values of $\boldsymbol{\psi}(V_1)$ with $\partial_n\boldsymbol{\psi}(V_1)$ and separately $\boldsymbol{\psi}(V_2)$ with $\partial_n\boldsymbol{\psi}(V_2)$.

Assume now that boundary conditions at a certain vertex V_m are not properly connecting. Then the vertex V_m can be divided into two vertices V_1 and V_2 and the boundary conditions connect together only boundary values corresponding to each new vertex. Therefore boundary conditions can be written in the form (17), which leads to block diagonal form of the matrix S corresponding to the original vertex V_m. □

We are going to study in more details the relation between the properly connecting boundary conditions and the space N_{-1}. In order to do this we will need the notion of *coordinate subspace* - any subspace in $\mathbb{C}^n$ spanned by a certain number of basic vectors from the standard basis in $\mathbb{C}^n$, but does not coincide with $\mathbb{C}^n$. This is a straightforward generalization of the notion of coordinate planes in $\mathbb{R}^3$. We say that a subspace N is *perpendicular* to a coordinate subspace K iff $P_K N \subset N \cap K$ and $P_N K \subset N \cap K$, where P denotes the orthogonal projection.

Theorem 9. *The non-resonant boundary conditions corresponding to the matrix S are properly connecting iff N_{-1} is not perpendicular to any coordinate subspace.*

Proof. Let K denote some coordinate subspace of $\mathbb{C}^{v_m}$ and $K^\perp$ - its orthogonal complement. Assume that N_{-1} is perpendicular to K. Consider $P_K N_{-1} \equiv N_{-1}^1 \subset K$ and similarly $P_{K^\perp} N_{-1} \equiv N_{-1}^2 \subset K^\perp$ (where $K^\perp$ is also a coordinate subspace). Take $S^1 = I_K - 2P_{N_{-1}^1}$ a unitary matrix in K and $S^2 = I_{K^\perp} - 2P_{N_{-1}^2}$ a unitary matrix in $K^\perp$. Then we have that $\mathbb{C}^{v_m} = K \oplus K^\perp$ and $S = S^1 \oplus S^2$, i. e. S is a block-diagonal matrix after certain permutation of coordinates. Thus S is not properly connecting.

Assume that S is not properly connecting then it has a block-diagonal structure after a certain permutation of coordinates, i. e. $S = S^1 \oplus S^2$ where S^1 is a unitary matrix in a certain coordinate subspace K and S^2 is a unitary matrix in $K^\perp$. Then N_{-1} possesses the representation: $N_{-1} = N_{-1}(S^1) \oplus N_{-1}(S^2)$. And hence $P_K N_{-1} = N_{-1}(S^1)$, *i.e.* N_{-1} is perpendicular to K. □

This theorem can be generalized to describe all asymptotically properly connecting boundary conditions using the fact that the subspace N_{-1} is stable for $S_v(k)$.

Theorem 10. *The boundary conditions are asymptotically properly connecting iff N_{-1} is not perpendicular to any coordinate subspace.*

Proof. By Theorem (6) the limit of the scattering matrix $S_v(k)$ is a certain energy independent scattering matrix S_v^∞, which has the same eigensubspace N_{-1}. Then current theorem follows from Theorem (9). □

The energy independent scattering matrix S_{V_m} is not properly connecting for example in the following two cases:

1. $N_1 = \{0\}, N_{-1} = \mathbb{C}^{v_m}$, which corresponds to Dirichlet boundary conditions at the endpoints forming the vertex;
2. $N_1 = \mathbb{C}^{v_m}, N_{-1} = \{0\}$, which leads to the Neumann boundary conditions at the endpoints forming the vertex.

Clearly these boundary conditions are not properly connecting and correspond to the case where the vertex V_m is maximally decomposed.

On the other hand it is possible to define the following two important families of properly connecting non-resonant boundary conditions:

1. **Hyperplanar Neumann conditions** - defined by a certain vector $\boldsymbol{w}^m \in \mathbb{C}^{v_m}$ with all components different from zero
$$\begin{cases} \boldsymbol{\psi}(V_m) \parallel \boldsymbol{w}^m, \\ \partial_n \boldsymbol{\psi}(V_m) \perp \boldsymbol{w}^m \end{cases} . \tag{18}$$
2. **Hyperplanar Dirichlet conditions** - defined by a certain vector $\boldsymbol{u}^m \in \mathbb{C}^{v_m}$ with all components different from zero
$$\begin{cases} \boldsymbol{\psi}(V_m) \perp \boldsymbol{u}^m, \\ \partial_n \boldsymbol{\psi}(V_m) \parallel \boldsymbol{u}^m \end{cases} . \tag{19}$$

These boundary conditions correspond to the case where one of the subspaces N_1 and N_{-1} is one dimensional. For hyperplanar Dirichlet conditions N_{-1} is spanned by $\boldsymbol{u}^m$ and, since all components of $\boldsymbol{u}^m$ are different from zero, N_{-1} is not perpendicular to any coordinate subspace. For Neumann conditions it is N_1 that is spanned by $\boldsymbol{w}^m$ and again N_1, and therefore N_{-1} as well, is not perpendicular to any coordinate subspace. It follows that both hyperplanar Neumann and Dirichlet conditions are non-resonant properly connecting boundary conditions. In the case of vertex formed by one end point hyperplanar Neumann and Dirichlet conditions reduce to classical Neumann and Dirichlet conditions respectively, which motivates their name. The word "hyperplanar" reflects the fact that one of the corresponding subspaces N_1 or N_{-1} has codimension 1. Note that if the vector $\boldsymbol{w}^m$ is chosen equal to $(1, 1, ..., 1)$, then hyperplanar Neumann conditions coincide with the standard boundary conditions (which are sometimes called Neumann conditions in the literature).

7. Trace formula for non-resonant boundary conditions

The trace formula connects together the spectrum of a quantum graph and the set of periodic orbits for the underlying metric graph. It was first suggested independently

by J.-P. Roth and B. Gutkin and U. Smilansky [15; 5]. In 2005 the authors provided a rigorous proof of this formula [13] discovering important relations with the Euler characteristic of the graph [11]. For considered there standard boundary conditions it was used that the vertex scattering matrix S_v is independent of the energy. Thus one can easily generalize the proof of the trace formula for any Laplace operator on a metric graph with any properly connecting non-resonant boundary conditions. The only difficulty appears when one tries to calculate the spectral and algebraic multiplicities of the zero eigenvalue.

Let L be the Laplace operator on a metric graph Γ formed by N edges connected at M vertices V_m of valence v_m and having C connected components. The set of all edges will be denoted by $E = \{\Delta_1, \dots, \Delta_N\}$, $\Delta_j = [x_{2j-1,x_{2j}}]$ and the set of vertices $V = \{V_1, \dots V_M\}$ is a partition of the set of endpoints $\{x_j\}_{j=1}^{2N}$. The maximal Laplace operator $L_{\max}$ is defined on the Sobolev space $W_2^2(\Gamma \setminus V)$. Consider the vectors of boundary values and normal partial derivatives associated with each vertex V_m, i. e. v_m-dimensional vectors $\boldsymbol{\psi}(V_m)$ and $\partial_n\boldsymbol{\psi}(V_m)$ with components $\psi(x_j)$ and $\partial_n\psi(x_j)$ respectively for $x_j \in V_m$. Then the boundary form of the maximal Laplace operator operator is given by

$$\langle L_{\max}\psi, \psi\rangle - \langle \psi, L_{\max}\psi\rangle = \sum_{V_m} (\langle \boldsymbol{\psi}(V_m), \partial_n\boldsymbol{\psi}(V_m)\rangle - \langle \partial_n\boldsymbol{\psi}(V_m), \boldsymbol{\psi}(V_m)\rangle)$$

The theorems for a star graph can now be easily generalized for any arbitrary graph Γ.

Theorem 11. *The family of self-adjoint restrictions of $L_{\max}$ can be described by boundary conditions connecting the boundary values $\boldsymbol{\psi} = (\boldsymbol{\psi}(V_1), \dots, \boldsymbol{\psi}(V_M))$ and $\partial_n\boldsymbol{\psi} = (\partial_n\boldsymbol{\psi}(V_1), \dots, \partial_n\boldsymbol{\psi}(V_M))$*

$$i(S - I)\boldsymbol{\psi} = (S + I)\partial_n\boldsymbol{\psi}. \tag{20}$$

This boundary conditions are properly connecting iff they have the form

$$i(S^m - I)\boldsymbol{\psi}(V_m) = (S^m + I)\partial_n\boldsymbol{\psi}(V_m), \tag{21}$$

where S^m is a unitary $v_m \times v_m$ matrix with $N_{-1}(S^m)$ not perpendicular to any coordinate subspace in $\mathbb{C}^{v_m}$.

The non-resonant boundary conditions are given by:

$$P_{N_1^m}\partial_n\boldsymbol{\psi}(V_m) = 0, \quad P_{N_{-1}^m}\boldsymbol{\psi}(V_m) = 0, \tag{22}$$

where $N_1^m \oplus N_{-1}^m = \mathbb{C}^{v_m}$.

Assume that the boundary conditions at the vertices are non-resonant. Then every eigenfunction $\psi(x, k)$, corresponding to the energy $\lambda = k^2$ is a solution to the differential equation

$$-\frac{d^2}{dx^2}\psi(x, k) = k^2\psi(x, k), \tag{23}$$

on the edges, satisfying the boundary conditions (20) at the vertices. For $k \neq 0$ every solution to (23) can be written using either a basis of incoming or one of outgoing

waves

$$\begin{aligned}\psi(x,k) &= a_{2j-1}e^{ik|x-x_{2j-1}|} + a_{2j}e^{ik|x-x_{2j}|} \qquad x \in \Delta_j = [x_{2j-1}, x_{2j}].\\ &= b_{2j-1}e^{-ik|x-x_{2j-1}|} + b_{2j}e^{-ik|x-x_{2j}|}\end{aligned} \tag{24}$$

The amplitudes $\boldsymbol{a} = \{a_j\}_{j=1}^{2N}$ and $\boldsymbol{b} = \{b_j\}_{j=1}^{2N}$ are related by the edge scattering matrix

$$\boldsymbol{b} = \mathbf{S}_e\boldsymbol{a}, \text{ where } \mathbf{S}_e(k) = \left(\begin{array}{c|c|c} S_e^1 & 0 & \dots \\ \hline 0 & S_e^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array}\right), \; S_e^j(k) = \begin{pmatrix} 0 & e^{ikd_j} \\ e^{ikd_j} & 0 \end{pmatrix}, \tag{25}$$

where d_j are the lengths of the edge Δ_j. The amplitudes are also related by the vertex scattering matrices, which are obtained from the requirement that $\psi(x,k)$ satisfies (3). For that purpose it is convenient to use the following representation for the solution to (23), using only amplitudes related to every end point x_i from V_m

$$\psi(x,k) = a_j e^{ik|x-x_j|} + b_j e^{-ik|x-x_j|}$$

and corresponding vectors $\boldsymbol{a}^m, \boldsymbol{b}^m \in \mathbb{C}^{v_m}$ of amplitudes. Then for all $k \neq 0$ the boundary conditions (22) are equivalent to

$$\begin{cases} P_{N_{-1}^m}(\boldsymbol{a}^m + \boldsymbol{b}^m) = 0, \\ P_{N_1^m}(\boldsymbol{a}^m - \boldsymbol{b}^m) = 0. \end{cases} \tag{26}$$

It follows that $\boldsymbol{a}^m$ and $\boldsymbol{b}^m$ are related by the corresponding vertex scattering matrix S_v^m as follows

$$\boldsymbol{a}^m = S_v^m \boldsymbol{b}_m, \; m = 1, 2, ..., M. \tag{27}$$

The last equation implies that

$$\begin{pmatrix} \boldsymbol{a}^1 \\ \boldsymbol{a}^2 \\ \vdots \\ \boldsymbol{a}^M \end{pmatrix} = \mathbf{S}_v \begin{pmatrix} \boldsymbol{b}^1 \\ \boldsymbol{b}^2 \\ \vdots \\ \boldsymbol{b}^M \end{pmatrix}, \text{ with } \mathbf{S}_v = \left(\begin{array}{c|c|c} S_v^1 & 0 & \dots \\ \hline 0 & S_v^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array}\right). \tag{28}$$

Note that the matrices $\mathbf{S}_e$ and $\mathbf{S}_v$ possess the block representations (25) and (28) in different bases. Clearly a vector $\boldsymbol{a}$ determines an eigenfunction of the Laplace operator if and only if the following equation holds

$$\det\left(\mathbf{S}(k) - I\right) = 0, \text{ where } \mathbf{S}(k) = \mathbf{S}_v\mathbf{S}_e(k). \tag{29}$$

The matrix $\mathbf{S}(k)$ is unitary for real k since it is a product of two unitary matrices. It is easy to see that

$$\| \mathbf{S}(k) \| < 1 \text{ for } \mathrm{Im}k > 0, \text{ and } \| \mathbf{S}^{-1}(k) \| < 1 \text{ for } \mathrm{Im}k < 0, \tag{30}$$

since the (independent of k) matrix $\mathbf{S}_v$ is unitary and the matrix $\mathbf{S}_e(k)$ satisfy (30).

Equation (29) determines the spectrum of $L(\Gamma)$ with correct multiplicities for all nonzero values of the energy, but the multiplicity $m_a(0)$ of the zero eigenvalue given by this equation, i.e. the dimension of $\ker\left(\mathbf{S}(k) - I\right)$, to be called *algebraic multiplicity*, may be different from the dimension $m_s(0)$ of the zero eigensubspace of $L(\Gamma)$, to be called *spectral multiplicity*.

Theorem 12. *(Trace formula) Let Γ be a compact finite metric graph with the total length $\mathcal{L}$ and let L be the Laplace operator in $L_2(\Gamma)$ determined by properly connecting non-resonant boundary conditions at the vertices. Then the following two trace formulae establish the relation between the spectrum $\{k_n^2\}$ of $L(\Gamma)$ and the set $\mathcal{P}$ of closed paths on the metric graph Γ*

$$u(k) \equiv 2m_s(0)\delta(k) + \sum_{k_n \neq 0} (\delta(k-k_n) + \delta(k+k_n)) \tag{31}$$

$$= (2m_s(0) - m_a(0))\delta(k) + \frac{\mathcal{L}}{\pi} + \frac{1}{2\pi}\sum_{p\in\mathcal{P}} l(\mathrm{prim}\,(p))\big(S(p)e^{ikl(p)} + S^*(p)e^{-ikl(p)}\big),$$

and

$$\sqrt{2\pi}\hat{u}(l) = 2m_s(0) + \sum_{k_n\neq 0} 2\cos k_n l \tag{32}$$

$$= 2m_s(0) - m_a(0) + 2\mathcal{L}\delta(l) + \sum_{p\in\mathcal{P}} l(\mathrm{prim}\,(p))\Big(S(p)\delta(l-l(p)) + S^*(p)\delta(l+l(p))\Big),$$

where

- $m_s(0)$ *and* $m_a(0)$ *are spectral and algebraic multiplicities of the eigenvalue zero;*
- p *is a closed path on* Γ*;*
- $l(p)$ *is the length of the closed path* p*;*
- $\mathrm{prim}\,(p)$ *is one of the primitive paths for* p*;*
- $S(p)$ *is the product of all vertex scattering coefficients along the path* p*.*

Proof. The proof follow step by step the proof of Theorem 2 from [11]. □

This theorem shows, that both spectral and algebraic multiplicities of the eigenvalue zero may be calculated from the spectrum of the Laplace operator: the spectral multiplicity is trivially equal to the multiplicity of $\lambda = 0$, the algebraic multiplicity is determined by the spectral asymptotics. Therefore in the following section we are going to study spectral and algebraic multiplicites for different types of boundary conditions.

8. Spectral and algebraic multiplicities of the ground state for hyperplanar Neumann and Dirichlet conditions

8.1. On the ground state eigenfunction

We show first, that every eigenfunction corresponding to the zero eigenvalue is piecewise constant.

Lemma 13. *Let L be the Laplace operator on a metric graph defined on the functions satisfying non-resonant boundary conditions. Then every eigenfunction corresponding to $\lambda = 0$ is a piecewise constant function.*

Proof. Every such function is a solution to the equation $-\psi''(x) = 0$ and therefore is a piecewise linear function on every edge

$$\psi(x) = \alpha_j x + \beta_j, \quad x \in \Delta_j.$$

Consider the corresponding Dirichlet integral

$$\int_\Gamma |\psi'(x)|^2 dx = \sum_{j=1}^{N} |\alpha_j|^2 d_j \geq 0,$$

where d_j denotes the length of the edge Δ_j. On the other hand integrating by parts we get

$$\begin{aligned}\int_\Gamma \psi'(x)\overline{\psi'(x)}dx &= -\int_\Gamma \psi''(x)\overline{\psi(x)}dx - \sum_{x_j} \partial_n\psi(x_j)\overline{\psi(x_j)} \\ &= -\sum_{m=1}^{M}\sum_{x_j\in V_m} \partial_n\psi(x_j)\overline{\psi(x_j)} \\ &= -\sum_{m=1}^{M} \langle \partial_n \boldsymbol{\psi}^m, \boldsymbol{\psi}^m\rangle_{\mathbb{C}^{v_m}} = 0,\end{aligned}$$

since for every V_m the vectors $\boldsymbol{\psi}^m$ and $\partial_n\boldsymbol{\psi}^m$ belong to two mutually orthogonal subspaces. Hence $\alpha_j = 0$ and every such function is piecewise constant. □

8.2. Hyperplanar Neumann boundary conditions

In this subsection we will investigate in more details the hyperplanar Neumann boundary conditions defined as (18). We shall calculate the spectral and algebraic multiplicities of the eigenvalue 0. Moreover we will need to consider two cases of hyperplanar boundary conditions: consistent and inconsistent.

Consider a closed path p of discrete length $n(p)$. Every such path can be uniquely defined by a sequence of endpoints $(x_{l_1}, x_{l_2}, \ldots, x_{l_{2n(p)}})$ that the path comes across, where $x_{l_{2k}}$ and $x_{l_{2k+1}}$ as well as $x_{l_{2n(p)}}$ and x_{l_1} belong to the same vertex while $x_{l_{2k-1}}$ and $x_{l_{2k}}$ are endpoints of the same edge.

Definition 14. *We say that hyperplanar Neumann boundary conditions are consistent iff for every closed path $p = (x_{l_1}, x_{l_2}, \ldots, x_{l_{2n(p)}})$ it holds*

$$\prod_{k=1}^{n(p)} w(x_{l_{2k}}) = \prod_{k=0}^{n(p)-1} w(x_{l_{2k+1}}). \tag{33}$$

Lemma 15. *The spectral multiplicity of the eigenvalue $\lambda = 0$ of the Laplace operator with consistent hyperplanar Neumann boundary conditions is equal to the number C of connected components of Γ.*

Proof. Consider any connected graph Γ and assume that (33) holds. Let ψ be any zero energy eigenfunction. Lemma 13 implies that ψ is piecewise constant and therefore the second condition in (18) for every vector $\boldsymbol{w}$ is trivially satisfied.

Choose any edge Δ_j and let $\psi(x)|_{x\in\Delta_j} = 1$. Let V_l be one of the two vertices that Δ_j connects. Then the values of ψ on all the edges connected at V_l can be calculated since the vector $\boldsymbol{\psi}(V_l)$ is proportional to $\boldsymbol{w}^l$ and one of the coordinates is known. In this way the values of the function ψ on all neighboring edges may be calculated and hence on the whole graph, since it is connected.Condition (33) guarantees that no contradiction occurs. Constructed in this way ψ is unique for any connected Γ. It is clear that such ψ cannot vanish on any edge, since all components of vectors $\boldsymbol{w}^m$ are different from zero.

For any not necessarily connected Γ the number of linearly independent vectors is then equal to the number of connected components C. □

Lemma 16. *The algebraic multiplicity of the eigenvalue $\lambda = 0$ of the Laplace operator with consistent hyperplanar Neumann boundary conditions is equal to $2C + N - M$*

Proof. The algebraic multiplicity of $\lambda = 0$ is equal to the dimension of the space of solutions to the system of equations (26) and (25) with

$$S_e^j(0) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad j = 1, 2, \ldots, N.$$

First of all the vector $\boldsymbol{b}$ can be excluded leading to the following system on $\boldsymbol{a}$:

$$\begin{cases} a_j + a_{j-(-1)^j} = \alpha_m w^m(x_j), \quad x_j \in V_m \\ \sum_{x_j\in V_m}(a_j - a_{j-(-1)^j})\overline{w^m(x_j)} = 0 \end{cases} \qquad m = 1, \ldots, M. \tag{34}$$

The equations can be separated by introducing new N-dimensional vectors $\boldsymbol{f}$ and $\boldsymbol{s}$ where $f_j = a_{2j} - a_{2j-1}$ and $s_j = a_{2j} + a_{2j-1}$. The values f_j and s_j can be interpreted as flows and values of the eigenfunction on the edge Δ_j.

The equations on s_j are just the same as the equations determining the function ψ in Lemma 15. Therefore the dimension of corresponding set of solutions is just C as before, since the conditions are consistent.

The equations on f_j can be written as a "balance of flows"(see footnote 1 in [11]):

$$\sum_{j, x_{2j}\in V_m} f_j\, \overline{w}^m(x_{2j}) = \sum_{j, x_{2j-1}\in V_m} f_j\, \overline{w}^m(x_{2j-1}). \tag{35}$$

Consider the case when Γ is a tree. Then on all loose edges $f_j = 0$, since hyperplanar Neumann boundary conditions at loose endpoints are nothing else than usual Neumann conditions. Considering the balance equation at any vertex V_m connecting together $v_m - 1$ loose edges, we conclude that f_j is equal to zero on every edge connected only to the loose edges (remember that all $w^m(x_j)$ are different from zero). Continuing in this way we conclude that all f_j are zero.

Consider now an arbitrary graph Γ. It can be turned into a forest (a sum of several trees) T with the same number of connected components by deleting exactly

$g = N - M + C$ edges. Let us denote those edges by $\Delta_1, \Delta_2, \ldots, \Delta_g$. For every such edge denote by p_j the shortest closed path on $T \cup \Delta_j$. Let us prove that there exists a solution $\boldsymbol{f}^j$ supported just by p_j. Assume for the sake of simplicity that $p_j = (x_1, x_2, \ldots, x_{2n(p)})$. and it runs through the vertices $V_1, V_2, \ldots, V_{n(p)}$. Then boundary conditions at these vertices build a system of equations:

$$\left\{ \begin{array}{rcl} f_1\overline{w}^1(x_2) & = & f_2\overline{w}^1(x_3) \\ f_2\overline{w}^2(x_4) & = & f_3\overline{w}^2(x_5) \\ & \ldots & \\ f_{n(p)}\overline{w}^{n(p)}(x_{2n(p)}) & = & f_1\overline{w}^{n(p)}(x_1) \end{array} \right. .$$

Multiplying both sides we get the following relation

$$\frac{w^1(x_2)w^2(x_4)\ldots w^{n(p)-1}(x_{2n(p)-2})w^{n(p)}(x_{2n(p)})}{w^1(x_3)w^2(x_5)\ldots w^{n(p)-1}(x_{2n(p)-1})w^{n(p)}(x_1)} = 1,$$

which is exactly the consistency relation (33) for the hyperplanar Neumann boundary conditions. Therefore there exists a unique (up to multiplication by a constant) solution $\boldsymbol{f}^j$ of (35) for each basic cycle p_j in the graph Γ. Consider now

$$\boldsymbol{f} - \sum_{j=1}^{g} s_j \, \boldsymbol{f}^j. \tag{36}$$

Obviously this function is supported by T and satisfies equation (26). Therefore it is zero and it follows that every $\boldsymbol{f}$ can be written as a combination of $\boldsymbol{f}^j$ which are of course linearly independent.

Thus the algebraic multiplicity of $\lambda = 0$ is equal to the number of basic cycles in Γ plus the number of connected components C. Hence the algebraic multiplicity is equal to $(N - M + C) + C = 2C + N - M$. □

The algebraic multiplicity can be characterized by the Euler characteristic $\chi = M - N$, $m_a^N(0) = 2C - \chi$.

8.3. Hyperplanar Dirichlet boundary conditions

Consider now N_{-1} spanned by one vector $\boldsymbol{u}^m = (u_1, u_2, \ldots, u_{v_m})$ with all components different from zero. Then we obtain the hyperplanar Dirichlet boundary conditions described before by (19). To calculate the spectral and algebraic multiplicities one has to perform the same steps as for hyperplanar Neumann boundary conditions arriving at the following system (instead of (34)) :

$$\left\{ \begin{array}{l} \tilde{a}_j - \tilde{a}_{j-(-1)^j} = \beta_m u^m(x_j), \quad x_j \in V_m \\ \sum_{x_j \in V_m} (\tilde{a}_j + \tilde{a}_{j-(-1)^j})\overline{u^m(x_j)} = 0 \end{array} \right. \qquad m = 1, \ldots, M, \tag{37}$$

where $\tilde{a}_j$ denote the corresponding amplitudes in representation (24).

Consider the following mapping:

$$\left\{ \begin{array}{l} a_k = (-1)^k \tilde{a}_k \\ w(x_k) = (-1)^{k+1} u(x_k), \end{array} \right. \tag{38}$$

which establishes a one-to-one correspondence between solutions to (34) and (37). In the case of hyperplanar Neumann boundary conditions the spectral and algebraic multiplicities satisfy

$$m_s^N(0) = C, \qquad m_a^N(0) - m_s^N(0) = C + N - M. \tag{39}$$

As a result of mapping (38) we get the following relations between spectral $m_s^D(0)$ and algebraic $m_a^D(0)$ multiplicities of the zero eigenvalue for hyperplanar Dirichlet boundary conditions:

$$\begin{array}{l} m_s^D(0) = m_a^N(0) - m_s^N(0) = C + N - M, \\ m_a^D(0) - m_s^D(0) = m_s^N(0) = C. \end{array} \tag{40}$$

Therefore $m_s^D(0) = C + N - M$ and $m_a^D(0) = 2C + N - M$.

We have proven the following theorem.

Theorem 17. *The spectral and algebraic multiplicities of the ground state eigenvalue $\lambda = 0$ for the Laplace operator with consistent hyperplanar Neumann and Dirichlet boundary conditions are equal to:*

$$\begin{array}{ll} m_s^N(0) = C, & m_a^N(0) = m_a^D(0) = 2C - \chi, \\ m_s^D(0) = C - \chi, & \end{array} \tag{41}$$

where C is the number of connected components and $\chi = M - N$.

Formulas (31) and (32) show that the knowledge of the spectrum allows one to calculate $m_s(0)$ and $2m_s(0) - m_a(0)$ following ideas of [11] and [12]. This means that the algebraic multiplicity $m_a(0)$ is determined by the spectrum of the Laplacian. Observe that $m_a(0)$ for both hyperplanar Neumann and Dirichlet conditions is equal to $2C - \chi$. In particular for connected graphs the Euler characteristics is determined by the spectrum for both hyperplanar Neumann and Dirichlet boundary conditions without knowing a priori which class of conditions occurs.

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Paper IV

On the Reconstruction of the Boundary Conditions for Star Graphs *

Sergei Avdonin, Pavel Kurasov and Marlena Nowaczyk

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

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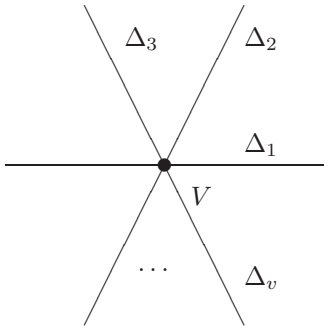

been discussed in [10], but the whole family of boundary conditions has not been investigated yet.

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 $\Gamma_{\rm star}$ 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 $L_2(\Gamma_{\rm star})$ defined on the set of functions from $W_2^2(\Gamma_{\rm star} \setminus V)$ satisfying the following matching conditions at the vertex

$$i(S-I)\boldsymbol{\psi}(V) = (S+I)\partial_n\boldsymbol{\psi}(V), \tag{1}$$

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 (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 $\Gamma_{\rm star}$. 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 (1) determines connection between the amplitudes of incoming and outgoing waves

$$\boldsymbol{a} = S_v(k)\boldsymbol{b}, \tag{2}$$

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

$$S_v(k) = \frac{(k+1)S + k - 1}{(k-1)S + k + 1}, \; k \neq 0. \tag{3}$$

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

$$S_v(k) = \frac{(k+k_0)S_v(k_0) + k - k_0}{(k-k_0)S_v(k_0) + k + k_0}, \; k, k_0 \neq 0. \tag{4}$$

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]

$$N_{-1}^\infty = N_{-1} \;\text{ and }\; N_1^\infty = \mathbb{C}^v \ominus N_{-1} = N_{-1}^\perp. \tag{5}$$

Then it is not hard to prove the following

Proposition 2 (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, but doesn't 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 $L_2(\Gamma_{\rm star})$

$$(T_\theta f)(x)=\begin{cases} f(x), & x\in\Delta_j, j=1,2,...,v-1;\\ e^{i\theta}f(x), & x\in\Delta_v.\end{cases} \tag{6}$$

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 (1) has to be substituted with

$$S^\theta=R_\theta S^0 R_{-\theta},\quad S^0=S, \tag{7}$$

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

$$R_\theta=\mathrm{diag}\,\{1,1,...,1,e^{i\theta}\}=\begin{pmatrix} 1 & 0 & \dots & 0 & 0\\ 0 & 1 & \dots & 0 & 0\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & \dots & 1 & 0\\ 0 & 0 & \dots & 0 & e^{i\theta}\end{pmatrix}. \tag{8}$$

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 (3) implies that

$$S_v^\theta(k)=R_\theta S_v^0(k)R_{-\theta}, \tag{9}$$

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 3. *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*

$$S_v^\theta(k)=R_\theta S_v^0(k)R_{-\theta}, \tag{10}$$

where R_θ is given by (8) *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:

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

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.**

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

$$S_v^{\alpha,\beta}(k_0)=R_\alpha S_v^0(k_0)R_\beta, \tag{11}$$

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 (10). 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 (10) for $k=k_0$. Then formula (4) implies that (10) 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 (9) (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.

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

**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.

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 (7) and (8).

Theorem 4. *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*

$$S_v^\theta(k)=R_\theta S_v^0(k)R_{-\theta}, \tag{12}$$

where R_θ is given by (8) 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 (11). 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 (11). Then the scattering matrix for all values of the energy parameter k can be calculated using (4)

$$S_v^{\alpha,\beta}(k)=\frac{(k+k_0)S_v^{\alpha,\beta}(k_0)+k-k_0}{(k-k_0)S_v^{\alpha,\beta}(k_0)+k+k_0}. \tag{13}$$

In particular, its element with the index 11 is

$$\begin{aligned}\left(S_v^{\alpha,\beta}(k)\right)_{11} &= \frac{k+k_0}{k-k_0}-\frac{4kk_0}{k^2-k_0^2}\left(S_v^{\alpha,\beta}(k_0)+\frac{k+k_0}{k-k_0}\right)^{-1}_{11}\\ &= \frac{k+k_0}{k-k_0}-\frac{4kk_0}{k^2-k_0^2}\left(S_v^{0}(k_0)+\frac{k+k_0}{k-k_0}R_{-\alpha-\beta}\right)^{-1}_{11},\end{aligned} \tag{14}$$

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

$$\left(S_v^{\alpha,\beta}(k)\right)_{11}=\sigma-\left(\sigma-\frac{1}{\sigma}\right)\frac{\det(S_v^0(k_0)+\sigma)_{1;1}+\sigma(e^{-i\gamma}-1)\det(S_v^0(k_0)+\sigma)_{1,v;1,v}}{\det(S_v^0(k_0)+\sigma)+\sigma(e^{-i\gamma}-1)\det(S_v^0(k_0)+\sigma)_{v;v}}, \tag{15}$$

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

$$\det(S_v^0(k_0)+\sigma)\det(S_v^0(k_0)+\sigma)_{1,v;1,v}-\det(S_v^0(k_0)+\sigma)_{1;1}\det(S_v^0(k_0)+\sigma)_{v;v}=0 \tag{16}$$

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 (16) holds for all $\sigma > 0$ (remember that $\sigma = \frac{k+k_0}{k-k_0}$). Using Jacobi identity (Section 3.6.1 from [20])

$$\det(S_v^0(k_0)+\sigma)\det(S_v^0(k_0)+\sigma)_{1,v;1,v}$$
$$= \det(S_v^0(k_0)+\sigma)_{1;1}\det(S_v^0(k_0)+\sigma)_{v;v} - \det(S_v^0(k_0)+\sigma)_{1;v}\det(S_v^0(k_0)+\sigma)_{v;1} \tag{17}$$

condition (16) can be written as

$$\det(S_v^0(k_0)+\sigma)_{1;v}\det(S_v^0(k_0)+\sigma)_{v;1} = 0, \tag{18}$$

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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