Inverse Spectral Problems for Quantum Graphs

Marlena Nowaczyk

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Contents

Preliminaries

1. Historical background

Although the spectral problems for quantum graphs have recently become a rapidly developing field of mathematics and mathematical physics, the first problems of this kind have already been studied many years ago in the eighties. Spectral properties of quantum graphs and different inverse problems have been investigated. These studies include not only conventional "locally" one-dimensional graphs but quantum graphs with inclusions in the form of billiards and even spectral problems for partial differential operators on manifolds.

1.1. Quantum graphs

Since different authors give slightly different definitions of what a quantum graph is we shall define how we will understand the term in this thesis.

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

We will identify each edge Δ_j, $j = 1, 2, \ldots, N$, of the graph with the interval of the real line $\Delta_j = [x_{2j-1}, x_{2j}] \subset \mathbb{R}$, where N is the total number of edges. 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 corresponding valence (degree) of the vertex, i.e. the number of endpoints joined at V_m, will be denoted by v_m.

A metric 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 the every edge rather than only at the vertices as it would be in a discrete model.

In this thesis we will only consider connected graphs with finite number of edges and with finite lengths of edges.

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

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

Differential operators

The first differential operator we would like to consider is the negative second derivative, which we are going to call *the Laplace operator*

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

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

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

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

Finally, even more general magnetic Schrödinger operator, with potentials $q(x)$ and $A(x)$ being real, sufficiently smooth are considered

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

Higher order differential and even pseudo-differential operators arise as well (see, for example, [28; 12] and references therein).

However, in this thesis we will consider only the first case (2). This differential expression does not determine any self-adjoint operator uniquely. Two differential operators in $L^2(\Gamma)$ are naturally associated with that expression: the minimal operator $H_{\min}$ 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:

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

The operator $H_{\max}$ is just the adjoint operator to $H_{\min}$.

Self-adjointness of the Laplace operator

Any self-adjoint operators associated with (2) and the graph Γ can be obtained from $H_{\max}$ by restricting it to some subspace using certain boundary conditions which connect function's boundary values associated with the same vertex.

The self-adjoint restriction exists since the deficiency indices of $H_{\min}$ are equal. Any solution to the differential equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\phi_j - \lambda_j \phi_j = 0 \tag{3}$$

belongs to the deficiency subspace. Note that no boundary condition at the vertices is necessary. Therefore, to determine deficiency indices we need to calculate the dimension of the space of solutions to the system of independent differential equations (3). Every solution to the equation can be written as

$$\phi_j = a_j e^{ik_j x} + b_j e^{-ik_j x}, \quad \text{where } k_j^2 = \lambda_j.$$

Therefore the deficiency subspace has dimension $2N$ for λ with both positive and negative imaginary part. Thus both deficiency indices are equal to $2N$ and to determine a self-adjoint restrictions of $H_{\max}$ we need to impose $2N$ "independent" boundary conditions.

In order to adjust the boundary conditions to the connectivity of a graph we need to impose exactly v_m conditions connecting boundary values at each vertex V_m.

The boundary form of the maximal operator $H_{\max}$ for any two functions f and g from $\mathrm{Dom}(H_{\max})$ is

$$\begin{aligned}\Omega(f,g) &= \, < f, H_{\max} g > - < H_{\max} f, g > \\ &= \sum_{j=1}^{2N} \left(\bar{f}(x_j)\partial_n g(x_j) - \partial_n \bar{f}(x_j) g(x_j) \right),\end{aligned} \tag{4}$$

where ∂_n denotes the normal derivative of a function at the corresponding endpoint. So the boundary conditions may only involve the boundary values of the functions and their derivatives. The most general form of such (homogeneous) condition is

$$A\mathbf{F} + B\mathbf{F}' = 0, \tag{5}$$

where A and B are certain $2N \times 2N$ matrices, $\mathbf{F}$ is the vector of the function's values at the endpoints $(f(x_1), \ldots, f(x_{2N}))^T$ and $\mathbf{F}' = (\partial_n f(x_1), \ldots, \partial_n f(x_{2N}))^T$ is the vector of normal derivatives. To ensure the correct number of independent conditions, matrices A and B must be chosen in such way that the rank of the $4N \times 2N$ matrix (A, B) is maximal, i.e. equal to $2N$.

The necessary and sufficient conditions for matrices A and B that guarantee the self-adjointness of the operator H were presented by V. Kostrykin and R. Schrader [26]. A similar result was obtained by M. Harmer [24] for a graph consisting of n semi-axes connected at a single vertex. He used the discussion of Hermitian symplectic spaces to parametrise all of the self-adjoint boundary conditions at the origin in terms of a unitary matrix U.

Proposition 1. (Kostrykin, Schrader) *All self-adjoint extensions of the minimal operator $H_{\min}$ are described by the boundary conditions (5) where A and B have the following properties:*

1. *the matrix (A, B) has rank $2N$,*
2. *the matrix AB^* is Hermitian.*

PROOF. Let us denote by $[f]$ the vector associated with the values of the function f and its normal derivatives f' namely

$$[f] = (f(x_1), f(x_2), \ldots, f(x_{2N}), f'(x_1), f'(x_2), \ldots, f'(x_{2N}))^T = (\mathbf{F}, \mathbf{F}')^T.$$

Using this notation we can write the boundary form (4) as

$$\Omega(f, g) =< [f], J\,[g] > , \tag{6}$$

where $<\,,\,>$ denotes the scalar product in $\mathbb{C}^{4N}$ and J is the canonical symplectic matrix on $\mathbb{C}^{4N}$:

$$J = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix}$$

Each self-adjoint extension of $H_{\min}$ can be considered as a restriction of $H_{\max}$ to a certain *maximal isotropic subspace* of W_2^2, i.e. a maximal linear subspace on which Ω vanishes identically.

Let Φ^k be the k-th column vector of the matrix $(A, B)^* = (\overline{A}, \overline{B})^T$:

$$\Phi^k = (\bar{a}_{k1}, \ldots, \bar{a}_{k\,2N}, \bar{b}_{k1}, \ldots, \bar{b}_{k\,2N}).$$

The condition (5) can be rewritten as

$$< \Phi^k, [f] >= 0, \quad 1 \leq k \leq 2N \tag{7}$$

because

$$\begin{aligned} &< \Phi^k, [f] > \\ &=<(\bar{a}_{k1}, \ldots, \bar{a}_{k\,2N}, \bar{b}_{k1}, \ldots, \bar{b}_{k\,2N}), (f(x_1), \ldots, f(x_{2N}), f'(x_1), \ldots, f'(x_{2N}))> \\ &= a_{k1} f(x_1) + \ldots + a_{k\,2N} f(x_{2N}) + b_{k1} \partial_n f(x_1) + \ldots + b_{k\,2N} \partial_n f(x_{2N}) = 0 \end{aligned}$$

From the fact that the rank of (A, B) is $2N$ it follows that we have $2N$ linearly independent equations $< \Phi^k, [f] >= 0$.

If we additionally denote the space of all vectors $[f]$ in $\mathbb{C}^{4N}$ such that the condition (5) is fulfilled, by $\mathcal{M} = \mathcal{M}(A, B)$, then our task is to find such matrices A and B that the space $\mathcal{M}$ is maximal isotropic.

First we shall show that $\mathcal{M}$ is maximal isotropic iff the space spanned by Φ^k is maximal isotropic. Since vectors Φ^k are orthogonal to $[f]$ for $1 \leq k \leq 2N$ (7) and all Φ^k are linearly independent, we claim that the space spanned by Φ^k is the subspace orthogonal to $\mathcal{M}$, $span\{\Phi^1, \Phi^2, \dots, \Phi^{2N}\} = \mathcal{M}^\perp$. Furthermore, from relation (6) we can deduce $span\{\Phi^1, \Phi^2, \dots, \Phi^{2N}\} = \mathcal{M}^\perp = J\mathcal{M}$.

Taking into account the properties of symplectic matrix J, namely that $J^2 = -\mathbb{I}$ and $J^* = -J$, we can derive the following equation

$$\begin{aligned}\Omega(f, g) =< [f], J[g] >=< J^*[f], [g] >=< -J[f], [g] >=< J[f], -[g] > \\ =< J[f], J^2[g] >= \Omega(Jf, Jg).\end{aligned}$$

In other words, f and g belong to the maximal isotropic subspace $\mathcal{M}$ if and only if the elements Jf and Jg belong to the maximal isotropic space $\mathcal{M}^\perp$. Thus, $\mathcal{M}$ is maximal isotropic if and only if its orthogonal complement, i.e. the space $span\{\Phi^1, \Phi^2, \dots, \Phi^{2N}\}$, is also maximal isotropic.

In order for $span\{\Phi^1, \Phi^2, \dots, \Phi^{2N}\}$ to be maximal isotropic, the following condition must be fulfilled

$$< \Phi^k, J\Phi^l >= 0, \quad \text{for all} \quad 1 \leq k, l \leq 2N.$$

All these conditions can be written in the matrix form

$$\begin{pmatrix} a_{11} & \dots & a_{1\,2N} & b_{11} & \dots & b_{1\,2N} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ a_{k1} & \dots & a_{k\,2N} & b_{k1} & \dots & b_{k\,2N} \\ \dots & \dots & \dots & \dots & \dots & \dots \\ a_{2N\,1} & \dots & a_{2N\,2N} & b_{2N\,1} & \dots & b_{2N\,2N} \end{pmatrix} J \begin{pmatrix} \bar{a}_{11} & \dots & \bar{a}_{l1} & \dots & \bar{a}_{2N\,1} \\ \dots & \dots & \dots & \dots & \dots \\ \bar{a}_{1\,2N} & \dots & \bar{a}_{l\,2N} & \dots & \bar{a}_{2N\,2N} \\ \dots & \dots & \dots & \dots & \dots \\ \bar{b}_{11} & \dots & \bar{b}_{l1} & \dots & \bar{b}_{2N\,1} \\ \dots & \dots & \dots & \dots & \dots \\ \bar{b}_{1\,2N} & \dots & \bar{b}_{l\,2N} & \dots & \bar{b}_{2N\,2N} \end{pmatrix} = 0$$

or, shorter, as $(A, B)J(A, B)^* = 0$.

The last step is to prove that this relation is equivalent to the fact that AB^* is Hermitian. We will show this using the block matrices notation. Namely

$$(A, B) \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix} \begin{pmatrix} \overline{A}^T \\ \overline{B}^T \end{pmatrix} = (A, B) \begin{pmatrix} \overline{B}^T \\ -\overline{A}^T \end{pmatrix} = A\overline{B}^T - B\overline{A}^T = 0$$

Finally, from the last equation we obtain the desired relation

$$AB^* = BA^* \qquad \square$$

Different types of boundary conditions

Suppose that the graph has M vertices $V_1, V_2, \dots, V_M$. Then the boundary conditions, respecting the connectivity of the graph, can be written as:

$$\begin{pmatrix} A_{V_1} & 0 & \dots & 0 \\ 0 & A_{V_2} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & A_{V_M} \end{pmatrix} P\mathbf{F} + \begin{pmatrix} B_{V_1} & 0 & \dots & 0 \\ 0 & B_{V_2} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & B_{V_M} \end{pmatrix} P\mathbf{F}' = 0,$$

where P is a permutation matrix which rearranges the endpoints into sets corresponding to the same vertex. It is then obvious that the matrices

$$A = \begin{pmatrix} A_{V_1} & 0 & \dots & 0 \\ 0 & A_{V_2} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & A_{V_M} \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} B_{V_1} & 0 & \dots & 0 \\ 0 & B_{V_2} & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & B_{V_M} \end{pmatrix}$$

satisfy conditions 1. and 2. from Proposition 1. if and only if for all $m = 1, \dots, M$ A_{V_m} and B_{V_m} satisfy those conditions. Therefore, the boundary conditions corresponding to each vertex, may be treated separately.

In this subsection we will give some basic examples of the boundary conditions for quantum graphs as well as the corresponding matrices A_{V_m} and B_{V_m}.

Boundary conditions of δ-type.

We will begin with conditions defined as follows:

$$\left\{ \begin{array}{l} f(x_j) = f(x_k), \quad x_j, x_k \in V_m, \\ \sum_{x_j \in V_m} \partial_n f(x_j) = \alpha_{V_m} f(V_m), \end{array} \right. \qquad m = 1, 2, \dots, M, \tag{8}$$

where α_{V_m} is a certain fixed number. These conditions can be written in the form (5) using the following matrices:

$$A_{V_m} = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & -1 \\ -\alpha_{V_m} & 0 & 0 & \dots & 0 & 0 \end{pmatrix}$$

and

$$B_{V_m} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 \\ 1 & 1 & \dots & 1 \end{pmatrix}.$$

Therefore we have

$$A_{V_m}B_{V_m}^* = \begin{pmatrix} 0 & \dots & 0 & 0 \\ \vdots & \ddots & \vdots & \vdots \\ 0 & \dots & 0 & -\alpha_{V_m} \end{pmatrix}$$

and, from Proposition 1., the operator H is self-adjoint if and only if α_{V_m} is real.

Standard boundary conditions.

These conditions appear in the literature under many different names, namely: natural, standard, free, Neumann, Kirchhoff. In this thesis we will only use the name standard boundary conditions. These conditions are the most common case of δ-type conditions defined above when $\alpha_{V_m} = 0$, i.e.

$$\begin{cases} f(x_j) = f(x_k), \quad x_j, x_k \in V_m, \\ \sum_{x_j \in V_m} \partial_n f(x_j) = 0, \end{cases} \quad m = 1, 2, \dots, M. \tag{9}$$

Since α_{V_m} is real thus the operator H is immediately self-adjoint. The standard boundary conditions correspond to the quadratic form

$$Q(u,u) = \int |f'(x)|^2 \mathrm{d}x,$$

where f is continuous on the whole graph (see for example [42] for studies on quadratic forms on quantum graphs).

Boundary conditions, example 3.

This kind of conditions is similar to δ-type, just with roles of the function and its derivative exchanged.

$$\begin{cases} \partial_n f(x_j) = \partial_n f(x_k), \quad x_j, x_k \in V_m, \\ \sum_{x_j \in V_m} f(x_j) = \alpha_{V_m} \partial_n f(V_m), \end{cases} \quad m = 1, 2, \dots, M. \tag{10}$$

The corresponding matrices A_{V_m} and B_{V_m} can be chosen equal to

$$B_{V_m} = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ 0 & 1 & -1 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 1 & -1 \\ -\alpha_{V_m} & 0 & 0 & \dots & 0 & 0 \end{pmatrix}$$

and

$$A_{V_m} = \begin{pmatrix} 0 & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & 0 & \dots & 0 \\ 1 & 1 & \dots & 1 \end{pmatrix}.$$

Therefore we have

$$A_{V_m} B^*_{V_m} = \begin{pmatrix} 0 & \dots & 0 \\ \dots & \dots & \dots \\ 0 & \dots & -\alpha_{V_m} \end{pmatrix}.$$

The self-adjointness condition is satisfied again for real α_{V_m} only.

Disconnecting boundary conditions

First we shall consider the vertex Dirichlet boundary conditions, i.e.

$$f(x_j) = 0, \quad \text{for all } \; x_j \in V_m, \;\; m = 1, \dots, M.$$

In this case the operator H decouples into a direct sum of the negative second derivative operators. These boundary conditions describe disconnected edges rather than the connected graph.

The same situation happens when we consider the Neumann boundary conditions at each endpoint of the edges.

$$\frac{\mathrm{d}f}{\mathrm{d}x}(x_j) = 0, \quad \text{for all } \; x_j \in V_m, \;\; m = 1, \dots, M.$$

As one can observe, the boundary conditions are responsible for the connectivity of the graph. By using different boundary conditions one may obtain different graphs (see Fig. 1).

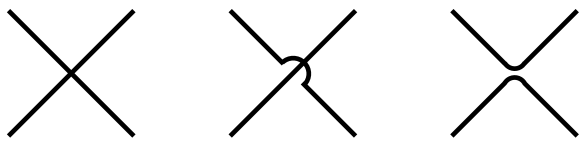


Figure 1: Boundary conditions vs connectivity

We will say that all boundary conditions leading to the same self-adjoint operator are equivalent. Furthermore, let us assume that one of the boundary conditions equivalent to (5) for a vertex V_m can be written in the form

$$\begin{pmatrix} A^1 & 0 \\ 0 & A^2 \end{pmatrix} \mathbf{F}_{V_m} + \begin{pmatrix} B^1 & 0 \\ 0 & B^2 \end{pmatrix} \mathbf{F'}_{V_m} = 0,$$

where A^1, B^1 and A^2, B^2 are square matrices of the same size, F_{V_m} and F'_{V_m} are the vectors of values and derivatives of the function at vertex V_m. In fact, these conditions can be written as (at least) two independent sets of linear equations connecting the boundary values of the function at the endpoints from two disjoint sets. Such boundary conditions correspond to the graph where the vertex V_m is chopped into two.

Definition 2. *The boundary conditions (5) for Schrödinger operator on the graph* Γ *are called non-separable if and only if the graph cannot be cut across the vertices to another graph* Γ' *in such a way that there exists equivalent boundary conditions which connect only the boundary values at vertices of* Γ'.

In the rest of this thesis we are going to consider only graphs with standard boundary conditions, which guarantees that the corresponding operator H is self-adjoint. Moreover, the standard boundary conditions are non-separable. Observe that with these boundary conditions one may remove all vertices of degree two by substituting the two edges joined at such a vertex by one edge, with the length equal to the sum of the lengths of the removed edges. This procedure is called *cleaning* [32] and the graph without vertices of valence 2 is called *clean*.

1.2. Applications of quantum graphs

Applications of quantum graphs arise in many fields of science, such as chemistry (free electron theory of conjugated molecules [21; 22; 40]), superconductivity (thin superconducting networks [1; 39]), nanotechnology (quantum wires circuits [11]), optics (photonic crystals [13; 30; 41]), scattering theory [18], averaging in dynamical systems [14], spectral theory of differential operators in singular domains [9] and others. Quantum graphs are also used as a 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 [35] and to model effects of electron propagation in non-simply-connected media [3].

Free electron theory

The origins of this theory go back to studies of electron trajectories in certain chemical molecules. Consider, for example, the naphthalene molecule, shown in Fig. 2, which contains systems of conjugated (i.e. alternating single and double) bonds (represented as edges). Every atom contributes three electrons to a chemical bonding. Two of those (so called σ-electrons) form bonds that maintain the "skeleton", or the frame of the molecule. The remaining, so-called π-electrons (one per atom), move along the entire structure, confined to the "skeleton" graph by the potential created by this frame.

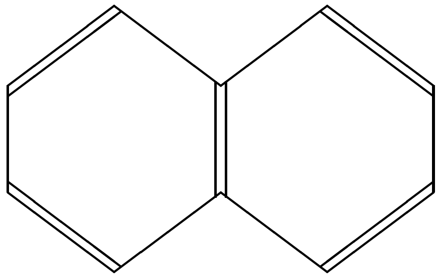


Figure 2: Naphthalene molecule

Ruedenberg and Scherr in [40] suggested to use a second order differential operator on the skeleton as a Hamiltonian for π-electrons. First, they assumed that the single particle Hamiltonian for π-electron is the Laplace operator in a narrow tube around the frame, with zero Dirichlet boundary condition on the tube boundary. Afterwards they considered the limit as the width of the tube tends to zero.

Quantum wires circuits

Quantum wires are quasi-one-dimensional objects, semi-conductor or metallic, whose other two dimensions are limited to a few nanometers. So we can consider a fatten graph Γ^f, where all its edges have thickness $d \ll 1$. Wave propagation in Γ^f can be described by the Laplace operator with Dirichlet or Neumann boundary conditions on the boundary of Γ^f. Quantum wires are useful models for studying electromagnetic and acoustic waveguides and thin superconducting structures. In such models it is interesting to determine how the spectra of Laplace operator (with different boundary conditions) behave as we shrink the thickness $d \to 0$.

2. Spectral problems for quantum graphs

The inverse spectral problems for the Schrödinger operator on the halfline have been studied by many authors. The issue is to recover the potential in the Schrödinger operator, or even the Sturm-Liouville operator, given their spectrum. One of the first people to study this problem was V. A. Ambarzumian [2] in 1929. Twenty years later G. Borg [5] proved that the inverse scattering problem on the halfline has a unique solution. V. A. Marčenko [33] investigated the uniqueness of solutions of the Sturm-Liouville equation, with slightly different boundary conditions. The question of solvability of the inverse problem was also taken up by M. G. Kreĭn [27]. Later on I. M. Gel'fand and B. M. Levitan [16] gave an explicit method for calculating the potential $q(x)$, known as Gelfand-Levitan-Marchenko equation.

A corresponding problem for two-dimensional manifolds was formulated by M. Kac as "Can one hear the shape of a drum?" In this thesis we are going to show that methods developed for studying the inverse spectrum problem, both in one and in several dimensions, can be applied to quantum graphs.

The first mathematically rigorous study of the scattering problem on graphs is the article by B. S. Pavlov and N. I. Gerasimenko from 1988 [18]. They considered the Schrödinger equation with real potentials $q_i(x)$ (where index i goes through all edges) and with standard boundary conditions at vertices, both for compact graphs and for graphs with several infinite branches. The following theorem was proven

Theorem 3. (Gerasimenko, Pavlov) *The spectrum of the Schrödinger operator $H = -d^2/dx_i^2 + q_i(x)$, where real potentials $q_i(x)$ are bounded below, with standard boundary conditions is discrete if the graph is compact.*

PROOF. The resolvent of the Schrödinger operator with standard boundary conditions, can be treated as a rank $2N$ perturbation of the resolvent of the same differential operator, but with Dirichlet boundary conditions at the vertices. As we mentioned before, the case of vertex Dirichlet boundary conditions corresponds to the graph consisting of disconnected edges. The corresponding operator is equal to the orthogonal sum of Schrödinger operators in the spaces $L^2(\Delta_j)$, with Dirichlet boundary conditions at the endpoints. The spectrum of each of those operators is discrete. Therefore, the spectrum of the operator H, on the whole graph Γ, with Dirichlet boundary conditions at vertices, is also discrete. Thus for any finite interval, the number of eigenvalues inside it — for the operator with standard and Dirichlet boundary conditions — differ by at most $2N$ ([4], Chapter 9, Theorem 3). Hence, the spectrum of the Schrödinger operator with standard boundary conditions is discrete. $\square$

Various other interesting models, involving quantum graphs, were considered by P. Exner and P. Šeba in [11; 12]. Besides one dimensional case, they also studied more complicated structures: graphs with higher dimensional inclusions, such as a wire attached to a plane and graph superlattices [10].

The inverse scattering problems for quantum graphs were also discussed in [32] by P. Kurasov and F. Stenberg and in [24] by M. Harmer. In the first one the authors showed that, in general, the scattering matrix does not determine the topology of the graph, the potentials on the edges nor the boundary conditions.

Recently, an analog of the Borg-Levison theorem for Sturm-Louville operator on trees was proven by B. M. Brown and R. Weikard in [6] and by V. Yurko in [44].

Spectral problems for quantum graphs (with cycles), in general, are much more sophisticated than those for trees. The main reason is that the Cauchy problem, on a graph with cycles, cannot be, for arbitrary Cauchy data, solved at all or cannot be solved uniquely. This is the main reason why differential equations on graphs possess properties of both ordinary and partial differential equations.

It turns out that methods developed for certain partial differential operators can be applied to quantum graphs. Thus let us now discuss the solution of the inverse spectral problem for Laplace operator in planar domains.

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

Mark Kac, in 1966, posed the question "Can one hear the shape of a drum?" [25]. Namely, if D_1 and D_2 are two isospectral domains in the Euclidean plane, must D_1 and D_2 be actually isometric? In the same paper Kac has shown that the eigenvalues *do* determine certain properties of domain D, for example the area, the circumference and the number of connected components. Two years earlier, in 1964, Milnor found two 16-dimensional tori that are not congruent but are nevertheless isospectral [34]. Afterwards, it was proven that there exist non-isometric pairs of Riemannian manifolds that are, nevertheless, isospectral.

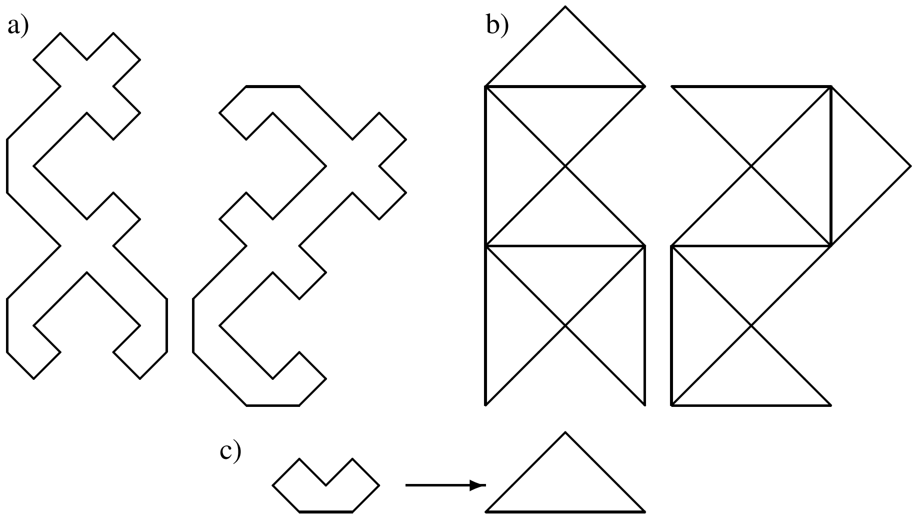


Figure 3: Two isospectral planar domains

Finally, in 1992, the Kac's question was finally answered, and this answer was negative (see [19] and [20]). Gordon, Webb and Wolpert, using the method by Sunada (see [43]), gave an explicit example of two non-isometric, simply-connected domains in the Euclidean plane which are both Dirichlet and Neumann isospectral. The Fig. 3a shows these two isospectral domains. Moreover, the authors of that paper pointed out that one can make a simple geometric substitution (Fig. 3c) to get another two isospectral domains shown in Fig. 3b.

Using the same method by Sunada, Buser et al. [7] found 17 families of isospectral pairs of non-congruent planar domains (shown in Fig. 4).

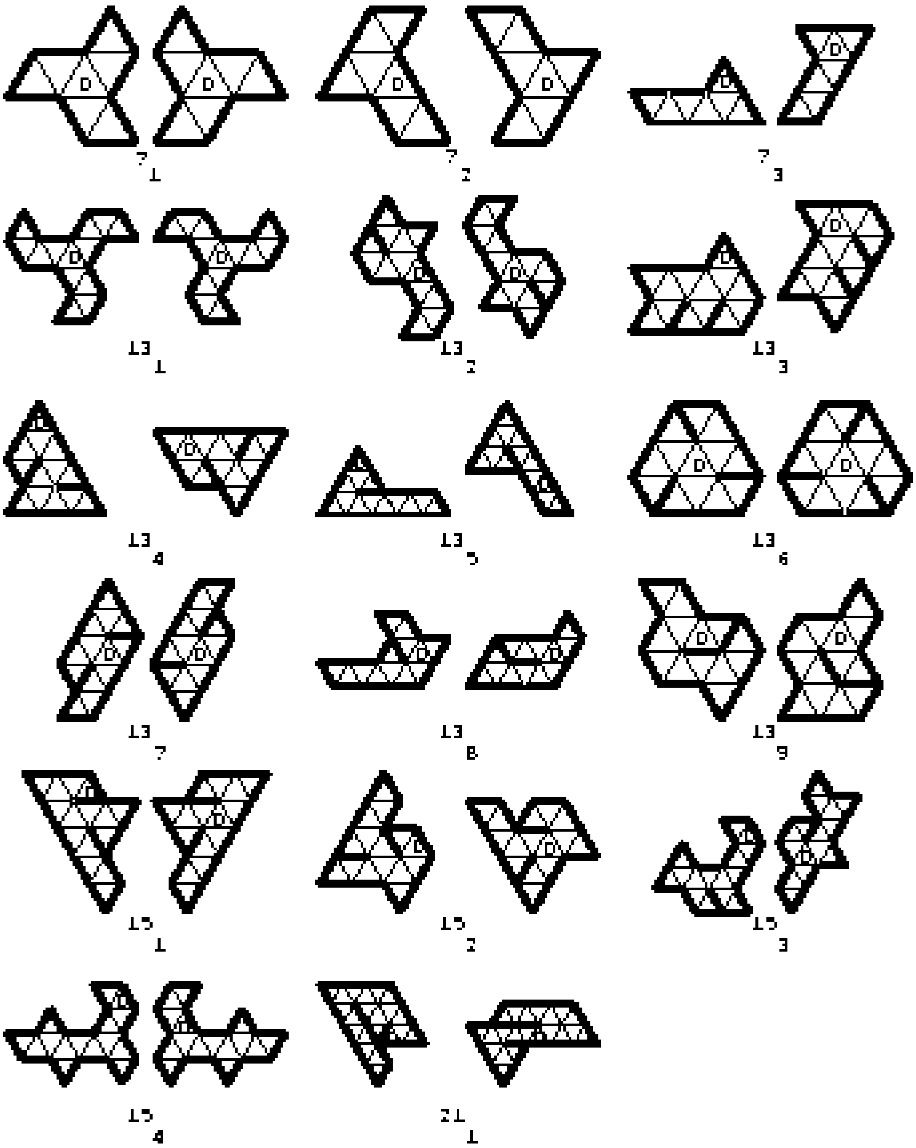


Figure 4: Families of isospectral planar domains

In 1995, Chapman [8] proposed the method called ”paper folding and connecting” to prove that the two domains presented at Fig. 4 are isospectral. Furthermore, he has shown that more exotic shapes can also be created, by cutting out the same part of each triangle (Fig. 5). The cutout will be in one piece if and only if there is a segment left uncut on each edge of the triangle.

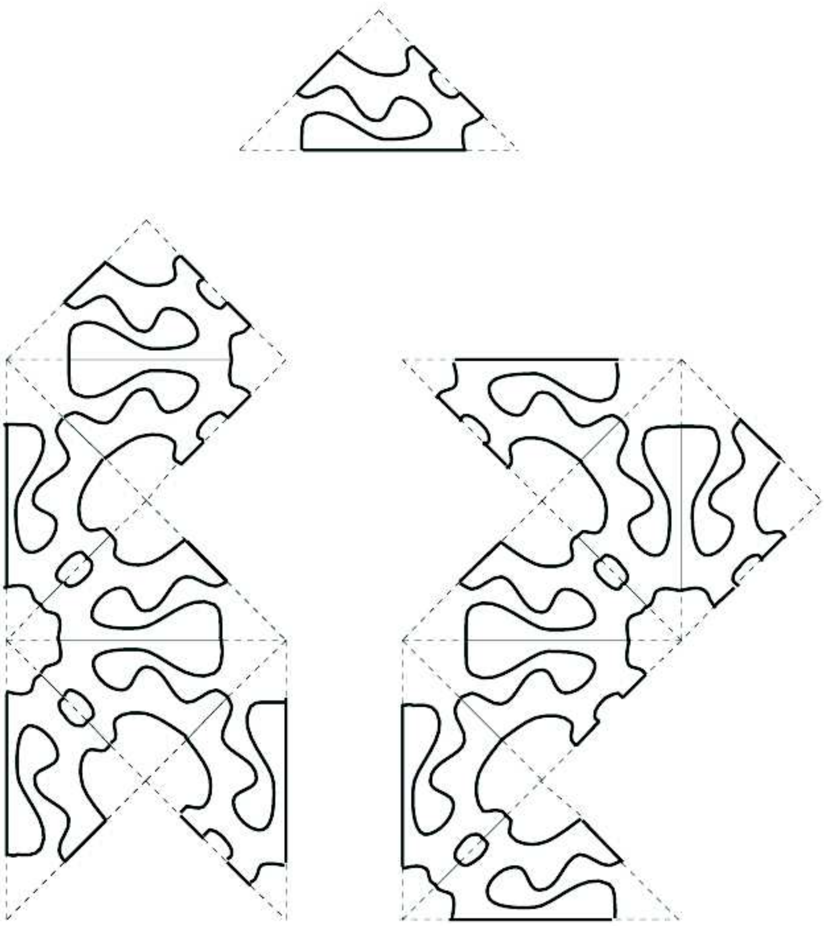


Figure 5: Two ”exotic” isospectral planar domains

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

We can follow M. Kac question and ask "Can one hear the shape of the graph?" B. Gutkin and U. Smilansky in the paper [23] gave a negative answer, based on the two-dimensional case. The idea was to use the example of Gordon and Webb of two isospectral planar domains [19] and then to apply the result of Chapman [8] to construct the isospectral graphs.

First we take two isospectral domains shown in Fig. 3b. Then we choose the subset of V-shape of each triangle as suggested on Fig. 3c in order to obtain the domains like those in Fig. 3a. 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. This way, we obtain graphs shown in Fig. 6.

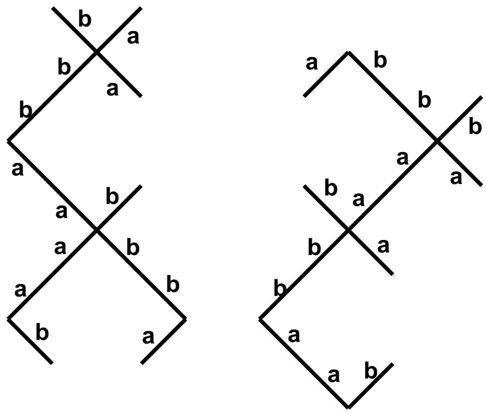


Figure 6: Two isospectral graphs

Afterwards, we straighten the bend edges, keeping the lengths. We get graphs presented at Fig. 7. From this construction, it should be more or less 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 at all vertices.

It is possible to directly calculate the spectra of corresponding Laplace operators and to compare them. Some calculations (without comparisons) were presented in [23], while we explicitly show here, for the first time, the equality of those spectra.

We shall label the functions on the edges with numbers from 1 to 7. Moreover, the loose endpoint at each edge has coordinate 0. Similarly, the "centre" edge has, in both graphs, coordinate 0 at vertex V_1.

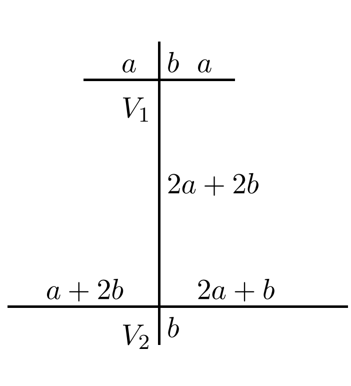


Figure 7: Two isospectral but non-isometric graphs. The edge lengths are expressed in terms of the two arbitrary lengths a and b.

Consider the first graph (shown on the left side). The functions at external edges have the form $\varphi_i(x) = A_i \sin(kx)$ and the boundary conditions at the vertex V_1 are as follows:

$$\varphi_1(b) = \varphi_2(a) = \varphi_3(a) = \varphi_4(0), \tag{11}$$

$$-\frac{\mathrm{d}\varphi_1}{\mathrm{d}x}(b) - \frac{\mathrm{d}\varphi_2}{\mathrm{d}x}(a) - \frac{\mathrm{d}\varphi_3}{\mathrm{d}x}(a) + \frac{\mathrm{d}\varphi_4}{\mathrm{d}x}(0) = 0. \tag{12}$$

The boundary conditions at the vertex V_2 are as follows:

$$\varphi_4(2a+2b) = \varphi_5(a+2b) = \varphi_6(2a+b) = \varphi_7(b), \tag{13}$$

$$\frac{\mathrm{d}\varphi_4}{\mathrm{d}x}(2a+2b) + \frac{\mathrm{d}\varphi_5}{\mathrm{d}x}(a+2b) + \frac{\mathrm{d}\varphi_6}{\mathrm{d}x}(2a+b) + \frac{\mathrm{d}\varphi_7}{\mathrm{d}x}(b) = 0. \tag{14}$$

For the second graph the functions have the form $\psi_i(x) = B_i \sin(kx)$ and the boundary conditions are:

$$\psi_1(a) = \psi_2(2a+3b) = \psi_3(b) = \psi_4(0), \tag{15}$$

$$-\frac{\mathrm{d}\psi_1}{\mathrm{d}x}(a) - \frac{\mathrm{d}\psi_2}{\mathrm{d}x}(2a+3b) - \frac{\mathrm{d}\psi_3}{\mathrm{d}x}(b) + \frac{\mathrm{d}\psi_4}{\mathrm{d}x}(0) = 0, \tag{16}$$

$$\psi_4(2a) = \psi_5(a) = \psi_6(b) = \psi_7(a+2b), \tag{17}$$

$$\frac{\mathrm{d}\psi_4}{\mathrm{d}x}(2a) + \frac{\mathrm{d}\psi_5}{\mathrm{d}x}(a) + \frac{\mathrm{d}\psi_6}{\mathrm{d}x}(b) + \frac{\mathrm{d}\psi_7}{\mathrm{d}x}(a+2b) = 0. \tag{18}$$

In the first graph one can assume that $\varphi_2(x) = \varphi_3(x)$ — otherwise there is an obvious solution equal to $\sin(ka) = 0$ on the edges Δ_2 and Δ_3 and 0 on all other edges.

Assume now that $\varphi_2(x) = \varphi_3(x)$. The eigenfunctions for both graphs are:

$$\begin{aligned}
\varphi_1(x) &= A_1 \sin(kx) & \psi_1(x) &= B_1 \sin(kx)\\
\varphi_2(x) &= A_2 \sin(kx) & \psi_2(x) &= B_2 \sin(kx)\\
\varphi_3(x) &= A_2 \sin(kx) & \psi_3(x) &= B_3 \sin(kx)\\
\varphi_4(x) &= A_4 \sin(kx) + A_4' \cos(kx) & \psi_4(x) &= B_4 \sin(kx) + B_4' \cos(kx)\\
\varphi_5(x) &= A_5 \sin(kx) & \psi_5(x) &= B_5 \sin(kx)\\
\varphi_6(x) &= A_6 \sin(kx) & \psi_6(x) &= B_6 \sin(kx)\\
\varphi_7(x) &= A_7 \sin(kx) & \psi_7(x) &= B_7 \sin(kx)
\end{aligned}$$

For the sake of brevity we shall always write α and β, instead of ka and kb, respectively.

Let us calculate the spectrum of the first graph. The system of homogeneous relations (11) – (14), with seven variables and seven equations, can be written using the matrix:

$$\begin{pmatrix}
-\sin(\beta) & \sin(\alpha) & 0 & 0 & 0 & 0 & 0\\
0 & \sin(\alpha) & 0 & 0 & 0 & 0 & -1\\
-\cos(\beta) & -2\cos(\alpha) & 0 & 0 & 0 & 1 & 0\\
0 & 0 & -\sin(\alpha+2\beta) & 0 & 0 & \sin(2\alpha+2\beta) & \cos(2\alpha+2\beta)\\
0 & 0 & \sin(\alpha+2\beta) & -\sin(2\alpha+\beta) & 0 & 0 & 0\\
0 & 0 & \sin(\alpha+2\beta) & 0 & -\sin(\beta) & 0 & 0\\
0 & 0 & \cos(\alpha+2\beta) & \cos(2\alpha+\beta) & \cos(\beta) & \cos(2\alpha+2\beta) & -\sin(2\alpha+2\beta)
\end{pmatrix}$$

A nonzero solution to this system exists only if the determinant of the matrix is equal to 0. Thus, in order to compare the spectra of the two graphs, we will calculate the determinant, compare it to zero and check whether two solutions (in variable k) are equal for both graphs.

The determinant for the first graph is equal to:

$$\begin{aligned}
\mathcal{D}_I = \; & -\sin(3\alpha+3\beta)\sin(\beta)(\alpha_1+\beta_1+\gamma_1)\\
& -\sin(2\alpha+3\beta)\sin(\alpha+\beta)\sin(\alpha+2\beta)\sin(2\alpha+\beta),
\end{aligned} \tag{19}$$

where

$$\alpha_1 = \sin(\beta)\sin(3\alpha+2\beta),$$

$$\begin{aligned}
\beta_1 = \; & \sin(\alpha+2\beta)\sin(2\alpha+\beta) = \sin(\alpha+\beta)\sin(\alpha+\beta)(2\cos(\alpha)\cos(\beta)\\
& -\sin(\alpha)\sin(\beta)) + \cos(\alpha+\beta)\cos(\alpha+\beta)\sin(\alpha)\sin(\beta),
\end{aligned}$$

$$\gamma_1 = \sin(\alpha+\beta)\sin(2\alpha+2\beta) = 2\sin(\alpha+\beta)\sin(\alpha+\beta)\cos(\alpha+\beta).$$

The spectrum of the second graph can be obtained in the same way using the following matrix

$$\begin{pmatrix}
\sin(\alpha) & -\sin(2\alpha+3\beta) & 0 & 0 & 0 & 0 & 0 & 0 \\
\sin(\alpha) & 0 & -\sin(\beta) & 0 & 0 & 0 & 0 & 0 \\
\sin(\alpha) & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\
\cos(\alpha) & \cos(2\alpha+3\beta) & \cos(\beta) & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \sin(2\alpha) & \cos(2\alpha) & -\sin(\alpha) & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \sin(\alpha) & -\sin(\beta) & 0 \\
0 & 0 & 0 & 0 & 0 & \sin(\alpha) & 0 & -\sin(\alpha+2\beta) \\
0 & 0 & 0 & \cos(2\alpha) & -\sin(2\alpha) & \cos(\alpha) & \cos(\beta) & \cos(\alpha+2\beta)
\end{pmatrix}$$

The determinant for the second graph is equal to

$$\begin{aligned}
\mathcal{D}_{II} &= -\sin(\alpha)\sin(\beta)\sin(3\alpha+3\beta)[\alpha_2+\beta_2+\gamma_2] \\
&\quad -\sin(\alpha)\sin(2\alpha+3\beta)\sin(\alpha+\beta)\sin(\alpha+2\beta)\sin(2\alpha+\beta),
\end{aligned}$$

where

$$\begin{aligned}
\alpha_2 &= 2\cos(\alpha)\sin(\alpha+\beta)\sin(\alpha+2\beta) \\
&= 2\sin(\alpha+\beta)\sin(\alpha+\beta)\cos(\alpha)\cos(\beta)+2\sin(\alpha+\beta)\cos(\alpha+\beta)\cos(\alpha)\sin(\beta) \\
\beta_2 &= \sin(\beta)\sin(3\alpha+2\beta) \ = \ \alpha_1 \\
\gamma_2 &= \sin(\alpha)\sin(2\alpha+3\beta) \\
&= -\sin(\alpha+\beta)\sin(\alpha+\beta)\sin(\alpha)\sin(\beta) \\
&\quad +\cos(\alpha+\beta)\cos(\alpha+\beta)\sin(\alpha)\sin(\beta)+2\sin(\alpha+\beta)\cos(\alpha+\beta)\sin(\alpha)\cos(\beta)
\end{aligned}$$

We can see that:

$$\alpha_1+\beta_1+\gamma_1 = \alpha_2+\beta_2+\gamma_2,$$

and therefore

$$\mathcal{D}_I\sin(\alpha) = \mathcal{D}_{II}. \tag{20}$$

Let us remind that calculating the spectrum of the first operator we have assumed $\varphi_2(x) = \varphi_3(x)$ — otherwise there exists explicit solution $\sin(ka) = 0$. Thus, the spectra of the Laplace operator on the two graphs coincide and can be written as a set of solutions to the equation $\mathcal{D}_{II} = 0$. Obviously, those graphs are non-isometric, since they have edges of different lengths.

The determinant $\mathcal{D}_{II}$ is a finite combination of exponentials, so it is an analytic function of k. Therefore, the zeroes of this function form a discrete set. This directly proves that the spectra of the Laplace operators on those graphs are discrete.

5. Trace formula

The following sections are based on two papers: [31] and [36].

At the beginning let us remind the assumptions. We consider a graph Γ, consisting of N edges $\Delta_j = [x_{2j-1}, x_{2j}] \subset \mathbb{R}$, $1 \leq j \leq N$ with respective lengths $d_j = |x_{2j} - x_{2j-1}|$ and M vertices $V_m, m = 1, 2, \ldots, M$. We also assume that the graph Γ is clean, finite and connected, but we allow it to have loops and multiple edges.

The Laplace operator H on the metric graph Γ is the operator

$$H = \oplus \sum_{j=1}^{N} \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} \right) , \tag{21}$$

defined on the set of those functions from $W_2^2(\Gamma \setminus \{V_m\})$ that satisfy the standard boundary conditions

$$\begin{cases} f(x_j) = f(x_k), \quad x_j, x_k \in V_m, \\ \sum_{x_j \in V_m} \partial_n f(x_j) = 0, \end{cases} \qquad m = 1, 2, \ldots, M, \tag{22}$$

where $\partial_n f(x_j)$ denotes the normal derivative of the function f at the endpoint x_j. This operator is self-adjoint in $L_2(\Gamma)$ and is uniquely determined by the graph Γ. Therefore, we are going to denote it by $H(\Gamma)$. The inverse spectral problem for $H(\Gamma)$ amounts to reconstructing the graph Γ from the set of eigenvalues of the operator $H(\Gamma)$. We have already proven that the spectrum of $H(\Gamma)$ is discrete. The Laplace operator $H(\Gamma)$ is in addition nonnegative, since its quadratic form is given by

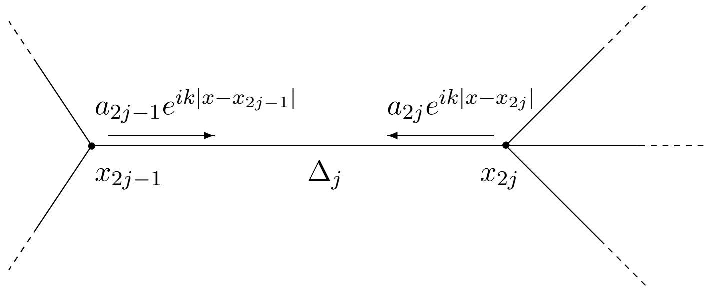
$$Q_H(f, f) = \int_\Gamma |f'|^2 \mathrm{d}x$$

and its domain consists of all continuous functions from $W_2^1(\Gamma \setminus \{V_m\})$. It is clear that $Q(f, f) \geq 0$ and, therefore, the spectrum of $H(\Gamma)$ is nonnegative.

Let us establish the secular equation determining all positive eigenvalues of the operator $H(\Gamma)$ (the eigenvalue $E = 0$ needs special attention and will be later discussed in more details). 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 equation on each edge $-\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = k^2\psi$. The general solution to the differential equation on the edge Δ_j can be expressed in the basis of incoming waves as follows

$$\psi(x) = a_{2j-1} e^{ik|x - x_{2j-1}|} + a_{2j} e^{ik|x - x_{2j}|}, \tag{23}$$

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



This solution, in the basis of outgoing waves, has a similar representation

$$\psi(x) = b_{2j}e^{-ik|x-x_{2j}|} + b_{2j-1}e^{-ik|x-x_{2j-1}|}. \tag{24}$$

By comparing these two representations, we can write the relation between the vectors of amplitudes of incoming and outgoing waves

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

as

$$\mathbf{b} = \mathcal{E}\mathbf{a}, \quad \text{where } \mathcal{E} = \left(\begin{array}{c|c|c} e^1 & 0 & \cdots \\ \hline 0 & e^2 & \cdots \\ \hline \vdots & \vdots & \ddots \end{array} \right) \quad \text{and } e^j = \begin{pmatrix} 0 & e^{ikd_j} \\ e^{ikd_j} & 0 \end{pmatrix}. \tag{25}$$

Let us now introduce, for any vertex $V_m = \{x_{l_1}, x_{l_2}, ..., x_{l_{v_m}}\}$ of valence $v_m = \mathrm{val}\,(V_m)$ (i.e. connecting exactly v_m edges, counting multiplicities), the notations

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

The relation between the vectors $\mathbf{a^m}$ and $\mathbf{b^m}$ can then be described by the vertex scattering matrix σ^m, which can be calculated from the boundary conditions at the chosen vertex V_m

$$\mathbf{a^m} = \sigma^{\mathbf{m}}\mathbf{b^m}. \tag{26}$$

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

$$\sigma^m_{jk} = \begin{cases} \frac{2}{v_m}, & j \neq k, \\ \frac{2-v_m}{v_m}, & j = k, \end{cases} \qquad v_m \geq 1. \tag{27}$$

The connection between the amplitudes $\mathbf{b}$ and $\mathbf{a}$ given by the vertex scattering matrices can be expressed in a simple way if we consider the basis associated with the vertices

$$\begin{pmatrix} \mathbf{a}^1 \\ \mathbf{a}^2 \\ \vdots \\ \mathbf{a}^M \end{pmatrix} = \Sigma \begin{pmatrix} \mathbf{b}^1 \\ \mathbf{b}^2 \\ \vdots \\ \mathbf{b}^M \end{pmatrix}, \quad \text{where } \Sigma = \left(\begin{array}{c|c|c} \sigma^1 & 0 & \dots \\ \hline 0 & \sigma^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array} \right). \tag{28}$$

Formulae (25) and (28) imply then, 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

$$U(k) = \Sigma\mathcal{E}(k) \tag{29}$$

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 $H(\Gamma)$ is equal to zeroes of the following function:

$$f(k) = \det(U(k) - I) = 0. \tag{30}$$

Let us call by *spectral multiplicity* the multiplicity of the eigenvalue E of the operator $H(\Gamma)$ and by *algebraic multiplicity* the dimension of the linear space of solutions to the equation (30).

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 $\psi(x)$, as given by (23).

Let us consider now the eigenvalue $E = 0$. It turns out that in this case spectral and algebraic multiplicities differ.

Lemma 4. *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 $H(\Gamma)$ with the spectral multiplicity 1 and algebraic multiplicity $N - M + 2$.*

PROOF. The proof of the fact that the spectral multiplicity is equal to 1 can be found in Paper I, Lemma 1. It is also proven there that the eigenfunction is a constant function.

To calculate the algebraic multiplicity of $E = 0$ we need to calculate the dimension of the kernel of the matrix $U(0) - I$, i.e. the number of linearly independent solutions $\mathbf{a} = (a_1, a_2, \dots, a_{2N})$ of the linear system $U(0)\mathbf{a} = \mathbf{a}$. Instead of solving this system of equations directly, it is easier to go back and consider the boundary conditions in their original form (22). The first condition, continuity of the eigenfunctions, implies that the amplitudes a_j have to fulfill the relations $a_{2j-1} + a_{2j} = a_{2k-1} + a_{2k}$, where j, k are indices such that the edges Δ_j and Δ_k have a common vertex. Since the graph Γ is connected, those relations are equivalent to a system of $N-1$ linearly independent equations: $a_1 + a_2 = a_{2j-1} + a_{2j}$, where $j = 2, \ldots, N$.

The second condition implies that the sum of incoming waves to a vertex is equal to the sum of outgoing waves from that vertex, i.e. that for every vertex V_m in Γ

$$\sum_{j, x_j \in V_m} b_j = \sum_{j, x_j \in V_m} a_j, \tag{31}$$

where $\mathbf{a}$ and $\mathbf{b}$ are bases for incoming and outgoing waves, respectively (see equations 23 and 24).

We shall now prove that equations (31) correspond to $M-1$ linearly independent relations on the elements of vector $\mathbf{a}$. First, observe that elements from both bases fulfill the following relations

$$a_{2j-1} = b_{2j} \ \text{ and } \ a_{2j} = b_{2j-1} \quad j = 1, \ldots, N, \tag{32}$$

which can be written in a matrix form as

$$P\mathbf{a} = \begin{pmatrix} J & \ldots & 0 \\ & \ddots & \\ 0 & \ldots & J \end{pmatrix} \mathbf{a} = \mathbf{b}, \qquad \text{where } J = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{33}$$

Moreover, the equations (31) for all vertices, can be written using the $M \times 2N$ matrix C, defined in such a way that $C\mathbf{b} = C\mathbf{a}$. This matrix can be chosen in such a way that it has elements 0 and 1 only, and each row m corresponds to a vertex V_m and columns $2j-1$ and $2j$ correspond to an edge Δ_j. Moreover, we can see that, in matrix C, there is exactly one non-zero element in each column and there are exactly v_m ones in each row m.

The matrix C reflects the connectivity of the graph Γ, namely if Δ_j connects vertices V_i and V_k then either

$$c_{i,2j-1} = 1, \quad c_{k,2j-1} = 0, \quad c_{i,2j} = 0, \quad c_{k,2j} = 1$$

or

$$c_{k,2j-1} = 1, \quad c_{i,2j-1} = 0, \quad c_{k,2j} = 0, \quad c_{i,2j} = 1.$$

In addition, since $P\mathbf{a} = \mathbf{b}$, see (33), the equation $C\mathbf{a} = C\mathbf{b}$ can be written as $(C - CP)\mathbf{a} = D\mathbf{a} = 0$

$$D\mathbf{a} = \begin{pmatrix} c_{11} - c_{12} & c_{12} - c_{11} & \dots & c_{1,2N} - c_{1,2N-1} \\ c_{22} - c_{21} & c_{24} - c_{23} & \dots & \dots \\ \vdots & \vdots & \ddots & \vdots \\ c_{M,2} - c_{M,1} & c_{M,4} - c_{M,3} & \dots & c_{M,2N} - c_{M,2N-1} \end{pmatrix} \mathbf{a} = 0$$

or, with the help of column vectors,

$$D\mathbf{a} = (C_1, -C_1, C_3, -C_3, \dots, C_{2N-1}, -C_{2N-1})\mathbf{a} = 0. \tag{34}$$

EXAMPLE. Consider the graph in Fig. 8 below.

For this graph, the condition that the sum of outgoing waves are equal, is given by the following four equations:

$$\begin{aligned} b_1 &= a_1 \\ b_3 &= a_3 \\ b_5 &= a_5 \\ b_2 + b_4 + b_6 &= a_2 + a_4 + a_6 \end{aligned}$$

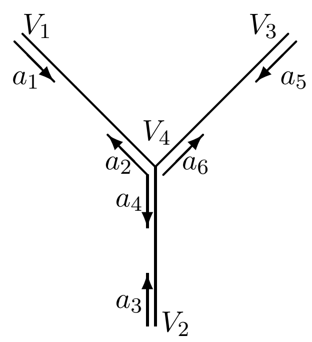


Figure 8: Y-shaped graph

Therefore, the relation $C\mathbf{b} = C\mathbf{a}$ can be written as follows

$$\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{pmatrix}$$

and the equation $D\mathbf{a} = (C - CP)\mathbf{a} = 0$ becomes

$$\begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \\ -1 & 1 & -1 & 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \\ a_6 \end{pmatrix} = 0.$$

CONTINUATION OF THE PROOF of Lemma 4.

Consider now the equation (34). As mentioned before, every two columns D_{2j-1} and D_{2j} correspond to Δ_j, an edge between vertices V_i and V_k. Observe that in each of those columns there are exactly two non-zero elements, 1 and -1, placed exactly at i-th and k-th row.

In addition, the sum of all rows in the matrix D is equal to the zero vector. Thus, not all M equations (31) are linearly independent. On the other hand, we will now show that the rank of matrix D is $M-1$.

Consider a linear combination of row vectors from D

$$\alpha_1 D_1^T + \alpha_2 D_2^T + \ldots + \alpha_M D_M^T = 0.$$

Due to the properties of matrix D, for every i, k such that V_i and V_k are neighbour vertices, $\alpha_i = \alpha_k$. Since the graph Γ is connected, we can rewrite those equations as $\alpha_1 = \alpha_j$, where $j = 2, \ldots, M$.

The space orthogonal to the space spanned by row vectors of matrix D is equal to $t(1, 1, \ldots, 1)$. Therefore, it has dimension 1, from which immediately follows that the rank of matrix D is $M-1$ and so the rank of matrix C is also $M-1$.

Hence, we have found a set of $M-1$ independent conditions on $\mathbf{a}$. From the continuity of the eigenfunctions condition we have earlier obtained another $N-1$ linearly independent equations $a_1 + a_2 = a_{2j-1} + a_{2j}$, where $j = 2, \ldots, N$. It now suffices to show that all these conditions are independent and, therefore, there are, in total, $N-1+M-1$ linearly independent equations on the $2N$ dimensional vector $\mathbf{a}$.

Let us now introduce $f_j = a_{2j-1} + a_{2j}$ and $g_j = a_{2j-1} - a_{2j}$, for every $j = 1, \ldots, M$. It is clear that the first condition can be written using only f_j, while the second condition can be written using only g_j. Therefore, the set of first $N-1$ equations is linearly independent from the set of second $M-1$ equations.

Concluding, the number of linearly independent solutions $(a_1, a_2, \ldots, a_{2N})$ is equal to $2N - (N-1) - (M-1) = N - M + 2$. Hence $E = 0$ is an eigenvalue for the Laplace operator $H(\Gamma)$ with the algebraic multiplicity $N - M + 2$. $\square$

Having proven that, we now 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, with help of function f, as follows

$$u[\varphi] = \lim_{\varepsilon \to 0} \frac{1}{2\pi i} \int_{-\infty}^{\infty} \left(\frac{f'(k-i\varepsilon)}{f(k-i\varepsilon)} - \frac{f'(k+i\varepsilon)}{f(k+i\varepsilon)} \right) \varphi(k) \mathrm{d}k - (N - M + 1)\varphi(0). \quad (35)$$

Moreover we have the following relation

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

Taking into account that the matrix Σ is independent of the energy we obtain

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

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. This allows us to substitute $iU\mathcal{D}$ into the previous formula, arriving at

$$
\begin{aligned}
u[\varphi] + (N-M+1)\varphi(0) = \frac{1}{2\pi i}\lim_{\varepsilon\to 0}\int_{-\infty}^{\infty}&[\mathrm{Tr}((I+U(k+i\varepsilon)+\ldots)U(k+i\varepsilon)i\mathcal{D}) \\
+\mathrm{Tr}((U^{-1}(k-i\varepsilon)+U^{-2}(k-i\varepsilon)+\ldots)&U(k-i\varepsilon)i\mathcal{D})]\varphi(k)\mathrm{d}k \qquad (36)
\end{aligned}
$$

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), obtaining the following formula

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

i.e.

$$u = \frac{1}{2\pi i}\mathrm{Tr}\left[(\ldots+U^{-1}(k)+I+U(k)+\ldots)i\mathcal{D}\right] - (N-M+1)\delta(k). \quad (37)$$

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. To any We can associate with every such (continuous) periodic orbit p, a *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 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, of course). When the orbit goes from one edge to another, passing through a vertex, we 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 (37) can be divided into three parts: identity, all positive powers of U and all negative powers of U. 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 U) is equal to

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

And the third part (all negative powers of U) is equal to

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

For the sake of simplicity we introduce:

$$\mathcal{A}_p = l(\mathrm{prim}(p))\Big(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \sigma_{ij}^m\Big), \qquad \mathcal{A}_p^* = l(\mathrm{prim}(p))\Big(\prod_{\sigma_{ij}^m \in \mathcal{T}(p)} \overline{\sigma_{ij}^m}\Big). \quad (38)$$

Theorem 5. (Trace formula) *Let $H(\Gamma)$ be the Laplace operator on a finite connected metric graph Γ. The following two trace formulae establish the relation between the spectrum $\{k_j^2\}$ of $H(\Gamma)$ and the set of periodic orbits $\mathcal{P}$, the number of edges N, the number of vertices M and the total length $\mathcal{L}$:*

$$u(k) \equiv \delta(k) + \sum_{n=1}^{\infty} (\delta(k-k_n) + \delta(k+k_n)) = \quad (39)$$

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

and

$$\hat{u}(l) \equiv 1 + \sum_{n=1}^{\infty}\Big(e^{-ik_n l} + e^{ik_n l}\Big) \quad (40)$$

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

where $\mathcal{A}_p$, $\mathcal{A}_p^*$ are complex numbers given by (38), which are independent of the energy.

6. Uniqueness theorems

In this section we will discuss under what conditions it is possible to reconstruct the graph Γ from the spectrum of $H(\Gamma)$, i.e. whether the spectrum of $H(\Gamma)$ determine Γ uniquely.

The set of lengths of all periodic orbits L is usually called the *length spectrum*. In some cases, formula (40) allows us to recover the length spectrum (of periodic orbits) from the energy spectrum (of the Laplace operator $H(\Gamma)$). 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* $L' \subset L$ defined as

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

The following example shows that sets L and L' can differ.
EXAMPLE. In this example we will show a case of vanishing coefficient $\mathcal{A}_p$. Consider the graph presented at Fig. 9 below. There exist exactly three periodic orbits with length equal to $2d_1 + d_2 + d_3 + d_4 + d_5$.

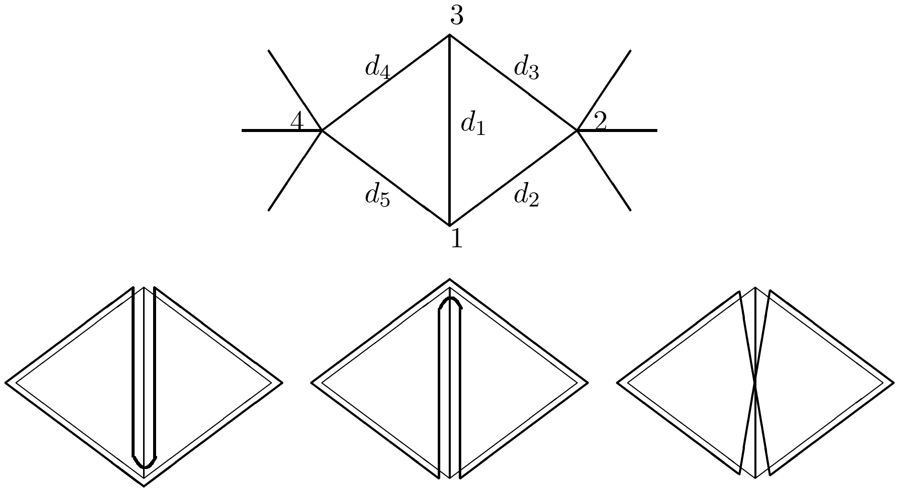


Figure 9: Periodic orbits of length $2d_1 + d_2 + d_3 + d_4 + d_5$

Assume that the degrees of vertices 2 and 4 are arbitrary and $v_1 = v_3 = 3$. If $l = 2d_1 + d_2 + d_3 + d_4 + d_5$, then

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

6.1. Graphs with rationally independent edges

In this section we are going to describe the main results from Paper I, which studied graphs with rationally independent lengths of edges. We shall skip the proofs of the theorems, as they can be found there.

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 this spectrum.

Lemma 6. *Let Γ be a finite, clean and connected 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 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 is to recover the lengths of the edges from the total length of the graph and the set of reduced length spectrum L'.

Lemma 7. *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 L' (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 6. 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 8. *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 L' — the subset of all periodic orbits defined by (41), provided that d_j are rationally independent.*

A graph is called *simple* if it contains no loops and no multiple edges. Any graph Γ can be reduced to a simple subgraph Γ^* by deleting all loops and removing all but one 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 9. *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.*

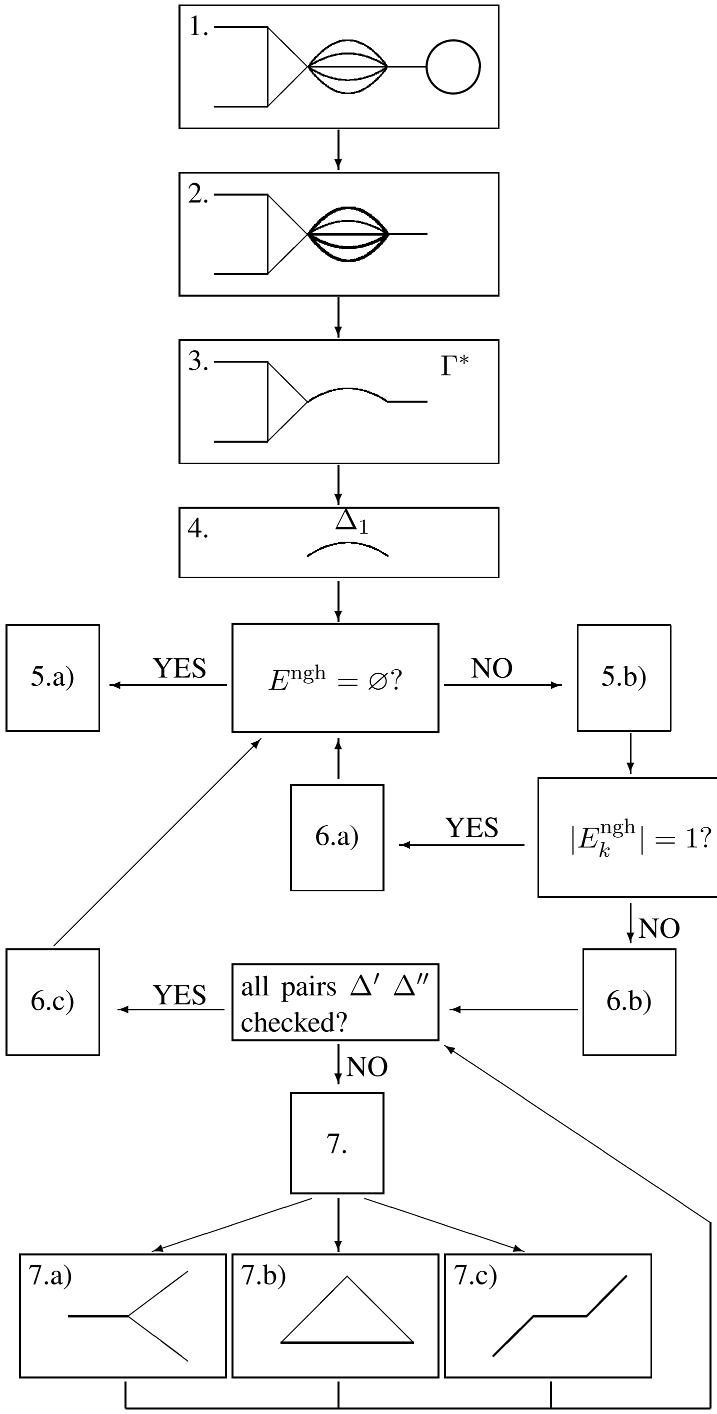
In the proof we introduce the set of edges $\mathbf{E} = \{\Delta_j\}_{j=1}^N$, which is uniquely determined by $\mathbf{D} = \{d_j\}$. We do the reconstruction iteratively, by constructing an increasing finite sequence of graphs such that $\Gamma_1 \subset \Gamma_2 \subset \dots \Gamma_{N^*} = \Gamma^*$. We denote by $\mathbf{E}_k$ the subsets of edges corresponding to k-th graph. Moreover, we denote by $\mathbf{E}^{\mathrm{ngh}}$ the set of all edges from $E \setminus E_k$ which are neighbours of Γ_k.

The rigorous proof of this theorem can be found in the Paper I, but in this section we will provide the sketch of reconstruction algorithm.

1. Remove from E all Δ_k which are loops and from L' all l which contain d_k.
2. If Δ_k, Δ_j connect the same two vertices.
   Remove one of them (say Δ_j) and all periodic orbits containing d_j.
3. The above steps give us Γ^*, a maximal simple subgraph of Γ.
4. Consider an arbitrary edge, say Δ_1, as the graph Γ_1 (first step, $k = 1$).
5. (a) If $E^{\mathrm{ngh}} = \varnothing$ then Γ^* is reconstructed.
   Add multiple edges and loops. Stop here.
   (b) Else choose Δ_{k+1}, which is a neighbour to one of the edges in Γ_k.
   Let E_k^{ngh} be a set of all neighbours of Δ_{k+1} in Γ_k.
6. (a) If E_k^{ngh} consists of exactly one element Δ then attach Δ_{k+1} to Γ_k, at a loose end of Δ. Set the resulting graph as Γ_{k+1} and go to 5.a)
   (b) Else consider any (new) pair Δ', Δ'' from E_k^{ngh}.
   (c) If all pairs of neighbours are checked then attach Δ_{k+1} at the endpoints V_1 and V_2. Set the resulting graph as Γ_{k+1} and go to 5.a)
7. Check if Δ' and Δ'' are neighbours to each other
   (a) If they are and if $d' + d'' + d_{k+1} \notin L'$ then Δ', Δ'' belong to the same class of endpoints. Go to 6.b)
   (b) If they are and if $d' + d'' + d_{k+1} \in L'$ then Δ', Δ'' belong to different classes of endpoints. Go to 6.b)
   (c) If they are not then Δ', Δ'' belong to different classes of endpoints. Go to 6.b)

In point 7. the idea is to separate E_k^{ngh} into two classes V_1 and V_2, which determine two endpoints of the edge Δ_{k+1}.

The theorem implies, in particular, that almost all graphs can be reconstructed from the spectrum of $H(\Gamma)$. This result has been proven independently in [15] by L. Friedlander, but our approach provides an effective algorithm to reconstruct the graph.


1.
2.
3.
Γ^*
4.
Δ_1
5.a)
YES
$E^{\mathrm{ngh}} = \varnothing$?
NO
5.b)
6.a)
YES
$|E_k^{\mathrm{ngh}}| = 1$?
NO
6.c)
YES
all pairs Δ' Δ'' checked?
6.b)
NO
7.
7.a)
7.b)
7.c)

6.2. Graphs with rationally dependent edges

In this section we are going to describe the main results from Paper II, which studied graphs with rationally dependent lengths of edges. We shall skip the proofs of the theorems, as they can be found there.

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, while 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 enough edges having rationally independent lengths. We restrict our considerations to graphs that are not only finite, clean and connected, but simple as well (i.e. without loops or multiple edges).

We shall begin by generalising Lemma 6. to the case of graphs with trivially rationally dependent edges.

Lemma 10. *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 L' contains at least the following lengths:*

- $4d_j$, *for all* $j = 1, \dots, N$;
- $2d_j$ *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, existing in the graph Γ.

Lemma 11. *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 $\beta_2, \dots,$ number of edges of length d_n by β_n (where $\beta_i \geq 1$ for $i = 1 \dots n$).*

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).

Lemma 12. *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 L'.

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

Theorem 13. *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 14. *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*

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

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 15. *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 L' determine the lengths of all edges.*

Lemma 16. *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 L'.*

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

Theorem 17. *The spectrum of the Laplace operator $H(\Gamma)$ on a metric graph Γ determines the graph uniquely, provided that:*

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

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Paper I

Inverse Spectral Problem for Quantum Graphs*

Pavel Kurasov[1,2] **Marlena Nowaczyk**[1]
[1] Department of Mathematics, Lund Institute of Technology, Box 118,210 00 Lund, Sweden
[2]Dept. of Physics, S:t Petersburg Univ., 198504 S:t Petersburg, Russia

E-mail: kurasov@maths.lth.se and marlena@maths.lth.se

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

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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 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

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

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.).

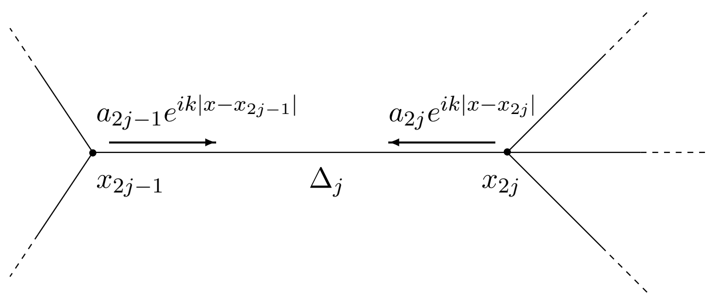
3. Trace formula

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

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

the relation (5) can be written as

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

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 $\sigma = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^\dagger$ 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.

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

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

† Obseve 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.

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 nondecreasing order as follows

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

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 $N - M + 2$. $\square$

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

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

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

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

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

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

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

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

$$+\mathrm{Tr}((U^{-1}(k-i\varepsilon) + U^{-2}(k-i\varepsilon) + \ldots)U(k-i\varepsilon)i\mathcal{D})]\varphi(k)\mathrm{d}k \tag{17}$$

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.

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

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:

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

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. $\square$

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

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

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 $1/2$

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

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. $\square$

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^{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^{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^{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^{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 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^{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**

Marlena Nowaczyk

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].

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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 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 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

$$\left\{ \begin{array}{l} f(x_j) = f(x_k), \quad x_j, x_k \in V_m, \\ \sum_{x_j \in V_m} \partial_n f(x_j) = 0, \end{array} \right. \qquad m = 1, 2, \dots, M, \tag{3}$$

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:*

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

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

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* $j = 1, \dots, N$;
- $2d_j$ *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* $\beta_2, \ldots,$ *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* 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 $\Gamma^{(1)}, \Gamma^{(2)}, \dots, \Gamma^{(s)}$. The reconstruction will be done iteratively and we will construct an increasing finite sequence of subgraphs such that $\Gamma_1 \subset \Gamma_2 \subset \dots \subset \Gamma_{N^*} = \Gamma^*$. The corresponding subsets of edges will be denoted by E_k for $k = 1, \dots, N^*$.

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 $\Gamma_{k+1}^{(j)}$.

When there are no more edges left which are neighbours of $\Gamma_k^{(j)}$, 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 $\mathbb{E}_n^1, \mathbb{E}_n^2, \dots, \mathbb{E}_n^{\alpha_n}$ which correspond to vertices $v_1, v_2, \dots, v_{\alpha_n}$ where $\alpha_n \le 2\beta_n$.

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 $d' \in \mathbb{E}_n^i$ and $d'' \in \mathbb{E}_n^j$ 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 $d' \in \mathbb{E}_n^i$ and $d'' \in \mathbb{E}_n^j$ 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. $\square$

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. $\square$

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*

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

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 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 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

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

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. $\square$

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^*. $\square$

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. $\square$

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Department of Mathematics, Lund Institute of Technology, Box 118, 210 00 Lund, Sweden
E-mail adress: marlena@maths.lth.se