Ark. Mat., **46** (2008), 95–111
DOI: 10.1007/s11512-007-0059-4

Graph Laplacians and topology

Pavel Kurasov

Abstract. Laplace operators on metric graphs are considered. It is proven that for compact graphs the spectrum of the Laplace operator determines the total length, the number of connected components, and the Euler characteristic. For a class of non-compact graphs the same characteristics are determined by the scattering data consisting of the scattering matrix and the discrete eigenvalues.

1. Introduction

A quantum graph is a metric graph Γ together with a differential operator acting in the Hilbert space $L_2(\Gamma)$ of square integrable functions on Γ which are coupled by certain boundary conditions at the vertices. A mathematically rigorous definition of such operators was given first in the 1980s [11], [13], [14] and [16]. These differential operators have attracted the attention of both physicists and mathematicians in recent years due to important applications in physics, e.g. to quantum waveguides and in nano-physics. Another reason for this growing interest is that differential operators on graphs with cycles possess properties of both ordinary and partial differential operators. Therefore, in the study of inverse problems for quantum graphs, methods developed in the 1950s and 1960s for one-dimensional problems have had to be modified substantially – adjusting methods originally developed for partial differential equations.

In the current article we are going to study the inverse spectral problem for compact graphs and the inverse scattering problem for non-compact graphs obtained from compact graphs by attaching several semi-infinite leads. Each of these inverse problems contains in fact three problems:

The author was supported in part by Swedish Research Council Grant #50092501 and the Swedish Royal Academy of Sciences. The author is also a guest researcher at Stockholm University.

(1) reconstruction of the metric graph;

(2) reconstruction of the differential expressions on the edges;

(3) reconstruction of the coupling conditions at the vertices.

From the very beginning it was realized that the inverse problems in general cannot be solved uniquely [15], [3] and [20]. One can even prove that the knowledge of the scattering matrix is not enough to reconstruct any graph with internal symmetries [4]. So far, only the case of star-like graphs is fully understood [14] and [17]. Sophisticated spectral analysis of regular trees (see e.g. [27]) shows the difficulties in solving the inverse problem. It has been proven by different authors that in the case of finite metric trees, the graphs and the potentials can be reconstructed from the corresponding scattering matrix or certain spectral data [1], [2], [7] and [29]. But problems involving graphs with cycles appear to be much more complicated. Therefore it is natural to begin the study of such problems with so-called Laplace operators on graphs (see Definition 3 below), especially if one takes into account that potential in the Sturm–Liouville equation cannot in general be reconstructed from one spectrum. Graph Laplacians are completely determined by the underlying metric graphs and the inverse problem consists of reconstruction of the metric graph itself. The inverse spectral problem in general does not have a unique solution due to the existence of isospectral graphs (the corresponding graph Laplacians have the same spectrum) (see [15] and later [3]). Also the inverse scattering problem in general cannot be solved uniquely if the set of scattering data consists of the scattering matrix alone, since there exists different graphs leading to the same scattering matrix [20] and [4]. An important wide class of graphs uniquely determined by the spectrum of the corresponding Laplacians is formed by the graphs with rationally independent lengths of edges. This class was first suggested by B. Gutkin and U. Smilansky in [15] (see also [19] for a mathematically rigorous treatment of the problem). It was realized later that the condition of rational independence can be weakened [25]. These results are close to the statement proven by L. Friedlander [12]: *generic quantum graphs do not have multiple eigenvalues* and thus generic compact graphs can be reconstructed from the spectrum of the Laplace operator.

On the other hand the connections between the spectral properties of quantum graphs and the topological invariants of the underlying metric graphs have not been studied yet. Such questions have been investigated only for discrete graphs by S. Novikov [23] and Y. Colin de Verdière [9] and [10].

In the current article we establish the following result:

The number of connected components, the total length, and the Euler characteristic of a metric graph are uniquely determined by the spectrum of the Laplacian in the case of compact graphs. The same parameters for non-compact graphs (*with* *the total length substituted by the length of the compact core) are determined by scattering data consisting of the scattering matrix and the discrete spectrum.*

In other words, it is proven that graphs having the same spectrum or scattering data have the same size (total length) and essentially the same complexity (the number of connected components and Euler characteristic). We believe that this result is important for applications, since it shows that it is impossible to replace a certain complicated metric graph by a simpler one and preserve the spectral or scattering data for the corresponding Laplacian. We would like to point out that the set of scattering data needed does not include any normalization constants connected with the bound states, in contrast to the case of the one-dimensional Schrödinger equation.

This result has an important implication: to determine topological characteristics of non-compact metric graphs in the case of Laplacians without discrete spectrum, it is enough to know the scattering matrix. This result is similar to the celebrated Levinson theorem [21] developed in full details by G. Borg [5] and [6] and V. A. Marchenko [22].

The main analytic tool is a generalization of the trace formula connecting the spectrum of the Laplace operator with the set of closed paths on the geometric graph. The first version of the trace formula for Laplace operators on graphs was proven by J.-P. Roth [26] using the heat kernel expansion, but we are going to use the trace formula in the form (3.13) first presented by J.-P. Roth as well, but no proof was given. T. Kottos and U. Smilansky used the secular equation ((3.8) below) to derive this version of the trace formula [18], but without paying attention to the fact that the secular equation in general does not determine the correct multiplicity of the eigenvalue zero. Taking this fact into account leads to an extra term in the trace formula related to the Euler characteristic of the underlying graph. This correction allows us to establish the main result of the current article concerning the Euler characteristic of metric graphs. In view of this fact it appears natural to present here a mathematically rigorous proof of the trace formula, using essentially the approach suggested in the pioneering paper [18]. Note that the approach in [18] was developed further in [15] (and later in [19]). These ideas have been extended in a remarkable series of papers on spectral properties of quantum graphs by U. Smilansky and co-authors. Probably it is worth mentioning that a similar approach has been used by R. Carlson to study the inverse problem for directed graphs [8].

2. Definitions

In this section we recall the main definitions and properties of graph Laplacians in order to establish common language and notation.

Definition 1. A *metric graph* $\Gamma = \Gamma(\mathbf{E}, \sigma)$ consists of a finite set $\mathbf{E}$ of finite or semi-infinite closed intervals Δ_j, $j = 1, 2, ..., N$, called *edges*, and a partition σ of the set $\mathbf{V} = \{x_j\}$ of end points x_j of the edges, $\mathbf{V} = \bigcup_{m=1}^{M} V_m$. The equivalence classes V_m, $m = 1, 2, ..., M$, will be called *vertices*, and the number of elements of V_m will be called the *valence* of V_m. The finite and semi-infinite intervals will be called *internal* and *external edges*, respectively.

Let us denote by N_i and N_e the number of internal and external (semi-infinite) edges respectively.

The distance between two points on Γ is the length of the shortest connected path between these two points. This metric introduces a topology on Γ and gives a possibility to study continuous pathes on it. In particular consider the fundamental group for the metric graph assuming that it is connected and compact. Then the number g of generators in this group is related to the Euler characteristic $\chi = M - N$ via the formula

$$g = 1 - \chi. \tag{2.1}$$

In order to preserve the same relation for non-compact graphs, let us use the following

Definition 2. Let Γ be a graph with N_i internal edges and M vertices, then its *Euler characteristic* χ is

$$\chi = M - N_i. \tag{2.2}$$

Note that external edges do not contribute to the Euler characteristic. Another possibility would be to compactify the external edges by introducing extra vertices ∞_j. This recipe would lead to the same value of χ.

The metric induced on Γ determines the Hilbert space $L_2(\Gamma)$ of square integrable functions with the standard scalar product $\langle f, g\rangle = \int_\Gamma \overline{f(x)} g(x)\, dx$. Note that this Hilbert space does not "feel" the connectivity of the graph and can be written as the orthogonal sum

$$L_2(\Gamma) = \bigoplus_{n=1}^{N} L_2(\Delta_n).$$

Definition 3. The *Laplace operator* $L(\Gamma)$ is the operator of negative second derivative in $L_2(\Gamma)$ defined on the domain of functions f from the Sobolev space $\bigoplus_{n=1}^{N} W_2^2(\Delta_n)$ satisfying standard boundary conditions at the vertices

$$\begin{cases} \sum_{x_j \in V_m} \partial_n f(x_j) = 0; \\ f \text{ is continuous at } V_m; \end{cases} \quad m = 1, 2, ..., M, \tag{2.3}$$

where $\partial_n f(x_j)$ denotes the normal derivative of the function f at the end point x_j:

$$\partial_n f(x_j) = \begin{cases} f'(x_j), & \text{if } x_j \text{ is the left end point,} \\ -f'(x_j), & \text{if } x_j \text{ is the right end point.} \end{cases}$$

Note that it is the boundary conditions that reflect the connectivity of the graph. The differentiation in the last definition is just the differentiation along the interval. We would like to point out the following facts.

(1) A metric graph Γ determines the Laplace operator $L(\Gamma)$ completely.

(2) It is not important whether the corresponding graph is planar or not.

(3) Vertices of valence 2 may be removed, since the boundary conditions (2.3) imply that the function and the first derivative are continuous in that case.

Proposition 1. *Let $L(\Gamma)$ be the Laplace operator on the metric graph Γ with N_e external edges. Then its spectrum is a union of the absolutely continuous spectrum $[0,\infty)$ of multiplicity N_e and the non-negative discrete spectrum $\{\lambda_n\}_n$ with only one possible accumulating point ∞.*

Proof. The operator $L(\Gamma)$ is a finite-rank perturbation in the resolvent sense of the orthogonal operator sum $\bigoplus_{j=1}^{N} L(\Delta_j)$. The spectrum of each operator $L(\Delta_j)$ is either purely discrete (internal edges) or purely absolutely continuous $[0,\infty)$ (external edges). Hence the spectrum for compact graphs is purely discrete and accumulates at ∞. For non-compact graphs the continuous spectrum is absolutely continuous and fills in the interval $[0,\infty)$ with the multiplicity N_e. Possible discrete spectrum eigenfunctions are supported by the compact core Γ_c of the graph Γ – the metric graph obtained from Γ by deleting all external edges (see formula (5.1) below), since only the zero function is a square integrable solution to the equation $-\psi''=k^2\psi$ on semi-infinite edges. Thus the discrete spectrum of $L(\Gamma)$ is a subset of the spectrum of $L(\Gamma_c)$. $\square$

It is natural to study the inverse spectral and inverse scattering problems for compact and non-compact graphs respectively.

3. Trace formula

In this section we are going to study the spectral problem for compact graphs, i.e. where the graph Γ is built up from finite edges $\Delta_j=[x_{2j-1},x_{2j}]$. We shall essentially follow the program suggested in [18] and [15] but making it mathematically rigorous. In order to establish the secular equation (see (3.8) below) for the spectrum of the Laplace operator $L(\Gamma)$ let us note that every eigenfunction $\psi(x,k)$, corresponding to the energy $\lambda = k^2$ is a solution to the differential equation

$$-\frac{d^2}{dx^2}\psi(x,k) = k^2\psi(x,k), \tag{3.1}$$

on the edges, satisfying the boundary conditions (2.3) at the vertices. For $k \neq 0$ every solution to (3.1) can be written using either a basis of incoming or one of outgoing waves

$$\begin{aligned} \psi(x,k) &= a_{2j-1}e^{ik|x-x_{2j-1}|} + a_{2j}e^{ik|x-x_{2j}|} \\ &= b_{2j-1}e^{-ik|x-x_{2j-1}|} + b_{2j}e^{-ik|x-x_{2j}|}, \quad x \in \Delta_j = [x_{2j-1}, x_{2j}]. \end{aligned} \tag{3.2}$$

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

$$\vec{b} = \mathbf{S}_e\vec{a}, \quad \text{where } \mathbf{S}_e(k) = \begin{pmatrix} S_e^1 & 0 & \cdots \\ 0 & S_e^2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}, \quad \text{and } S_e^j = \begin{pmatrix} 0 & e^{ikd_j} \\ e^{ikd_j} & 0 \end{pmatrix}, \tag{3.3}$$

where d_j is the length of Δ_j. The second relation between the amplitudes is obtained by considering the boundary conditions at the vertices V_m one by one. For that purpose it is convenient to use the following representation for the solution to (3.1), using only amplitudes related to every end point x_j from V_m,

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

Then the boundary conditions are fulfilled if and only if

$$\begin{cases} a_j + b_j = a_l + b_l, & x_j, x_l \in V_m \\ \sum_{x_j \in V_m}(a_j - b_j) = 0. \end{cases} \tag{3.4}$$

Let the vectors $\vec{a}^m$ and $\vec{b}^m$ denote the amplitudes of all incoming and outgoing waves for the vertex V_m, $m = 1, 2, \dots, M$, respectively. Then (3.4) imply that $\vec{a}^m$ and $\vec{b}^m$ are connected through the unitary vertex scattering matrix

$$(S_v^m)_{ij} = \begin{cases} \dfrac{2}{v_m}, & i \neq j, \\ \dfrac{2-v_m}{v_m}, & i = j, \end{cases}, \quad \text{where } v_m \text{ is the valence of } V_m, \tag{3.5}$$

as follows

$$\vec{a}^m = S_v^m \vec{b}^m, \quad m = 1, 2, \dots, M. \tag{3.6}$$

The last equation implies that

$$\begin{pmatrix} \vec{a}^1 \\ \vec{a}^2 \\ \vdots \\ \vec{a}^M \end{pmatrix} = \mathbf{S}_v \begin{pmatrix} \vec{b}^1 \\ \vec{b}^2 \\ \vdots \\ \vec{b}^M \end{pmatrix}, \quad \text{with } \mathbf{S}_v = \begin{pmatrix} S_v^1 & 0 & \cdots \\ 0 & S_v^2 & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix}. \tag{3.7}$$

Note that the matrices $\mathbf{S}_e$ and $\mathbf{S}_v$ possess the block representations (3.3) and (3.7) in different bases. Clearly a vector $\vec{a}$ determines an eigenfunction of the Laplace operator if and only if the following equation holds

$$\det(\mathbf{S}(k)-I)=0, \quad \text{where } \mathbf{S}(k)=\mathbf{S}_v\mathbf{S}_e(k). \tag{3.8}$$

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

$$\|\mathbf{S}(k)\|<1 \text{ for } \operatorname{Im} k>0 \quad \text{and} \quad \|\mathbf{S}^{-1}(k)\|<1 \text{ for } \operatorname{Im} k<0, \tag{3.9}$$

since the matrix $\mathbf{S}_v$ is unitary (independent of k) and the matrix $\mathbf{S}_e(k)$ satisfy (3.9).

Equation (3.8) determines the spectrum of $L(\Gamma)$ with correct multiplicities for all non-zero values of the energy, but the multiplicity $m_a(0)$ of the zero eigenvalue given by this equation, i.e. the dimension of $\operatorname{Ker}(\mathbf{S}(k)-I)$, to be called *algebraic multiplicity*, may be different from the dimension $m_s(0)$ of the zero eigensubspace of $L(\Gamma)$, to be called *spectral multiplicity*. The following theorem connects these multiplicities with the Euler characteristics of Γ.

Theorem 1. *Let Γ be a compact metric graph with C connected components and Euler characteristic χ, and let $L(\Gamma)$ be the corresponding Laplace operator. Then $\lambda=0$ is an eigenvalue with spectral multiplicity $m_s(0)=C$ and algebraic multiplicity $m_a(0)=2C-\chi$.*

Proof. Spectral multiplicity. Every eigenfunction for eigenvalue zero is a solution to the differential equation $-d^2/dx^2\psi(x,0)=0$ on every edge and satisfies boundary conditions (2.3) at every vertex. Every such function is continuous on Γ and therefore attains its maximum on Γ. It is a linear function of x on every edge and therefore the maximum is attained at (at least) one of the vertices. Consider the normal derivatives at such a vertex. All these derivatives are less than or equal to zero (a maximum point), but their sum is equal to zero. We conclude that the function is equal to its maximum on all neighboring intervals and at all directly connected vertices. Repeating the same arguments we conclude that the function is constant on every connected component of Γ. Hence the dimension of the zero eigensubspace, $m_s(0)$, is equal to the number C of connected components.

Algebraic multiplicity. The calculation of the dimension of the kernel of the matrix Ker $(\mathbf{S}_v\mathbf{S}_b(0)-I)$ can be carried out by using standard methods of linear algebra [19] and [24], but we shall calculate this dimension directly from the original equations (3.3) and (3.4) in order to clarify the relation between the algebraic multiplicity and the number g of generators of the fundamental group for Γ. Therefore we assume first that the graph is connected.

In the case $k=0$ the system (3.3) takes the form $a_{2j-1}=b_{2j}$ and $a_{2j}=b_{2j-1}$, and the coefficients b_j can be excluded from (3.4). Thus we get the following linear system with $2N$ unknowns

$$\begin{cases} a_{2j-1}+a_{2j}=a_{2l-1}+a_{2l}, & j,l=1,2,...,N; \\ \sum_{j:x_j\in V_m}(a_j-a_{j-(-1)^j})=0, & m=1,2,...,M. \end{cases} \tag{3.10}$$

The first series of equations implies that the function $\psi(x,0)$ is constant on the whole graph Γ,

$$\psi(x,0)=a_{2j-1}+a_{2j}\equiv c, \quad j=1,2,...,N$$

(as is expected for simply connected graphs). The reason that the spectral and algebraic multiplicities may be different is that the constant function $\psi(x,0)=c$ may be represented by different vectors $\vec{a}$.

With every edge Δ_j we associate the *flux* $f(\Delta_j)$(1) defined as follows

$$f(\Delta_j)=a_{2j-1}-a_{2j}. \tag{3.11}$$

Then the second set of equations (3.10) implies that the total flux through every vertex is zero,

$$\sum_{\Delta_j \text{ starts at } v_m} f(\Delta_j)=\sum_{\Delta_j \text{ ends at } v_m} f(\Delta_j), \quad m=1,2,...,M. \tag{3.12}$$

Let us prove that the dimension of the space of solutions to this system of equations is equal to the number g of generators for the fundamental group.

(1) The interpretation of $f(\Delta_j)$ as a flux can be justified by the following reasoning. The probability flux into the interval $\Delta_j=[x_{2j-1},x_{2j}]$ from the left and right end points is given by $|a_{2j-1}|^2-|b_{2j-1}|^2$ and $|a_{2j}|^2-|b_{2j}|^2$, respectively. Then the unitarity of the edge scattering matrix S_e expresses the fact that the total probability flux for each edge is zero. In the case $\lambda=0$ the coefficients a_j and b_j may be chosen real and the probability flux through the edge from the left to the right end point is given by

$$|a_{2j-1}|^2-|b_{2j-1}|^2=a_{2j-1}^2-a_{2j}^2=(a_{2j-1}-a_{2j})(a_{2j-1}+a_{2j})=f(\Delta_j)c.$$

Hence $f(\Delta_j)$ coincides with the flux up to multiplication by the constant c.

Assume that Γ is a tree ($N=M-1$), then the only possible flux is zero. First we note that the flux on all loose edges is zero. Then it is clear that the flux is zero on all edges connected by at least one of the end points to loose edges. Continuing in this way we conclude that the flux is zero on the whole tree.

Assume now, that Γ is an arbitrary connected graph. Then by removing certain $N-(M-1)$ edges it may be transformed to a certain tree T. Let us denote the removed edges by $\Delta_1, \Delta_2, ..., \Delta_{N-M+1}$ so that

$$T=\Gamma\setminus \bigcup_{j=1}^{N-M+1} \Delta_j.$$

Every edge Δ_j determines one non-trivial class of closed pathes on $T\cup\Delta_j$. Let us denote by l_j the shortest pass from this class. To each path l_j we associate the *basic flux* f_j supported by l_j,

$$f_j(\Delta_k)=\begin{cases} \pm 1, & \text{if } \Delta_k\in l_j, \\ 0, & \text{if } \Delta_k\notin l_j, \end{cases}$$

where the sign in the last formula depends on whether the path l_j runs along Δ_k in the positive $(+)$ or negative $(-)$ direction. Without loss of generality we assume that $f_j(\Delta_j)=1$. Every such flux satisfies the system of equations (3.12).

Consider any flux f on Γ satisfying the conservation law (3.12). We claim that it can be written as a linear combination of the basic fluxes f_j. Really the flux

$$f-\sum_{j=1}^{N-M+1} f(\Delta_j) f_j$$

is supported on the tree T, it satisfies (3.12) and therefore it is equal to zero.

Summing up we conclude that for connected graphs the algebraic multiplicity of the zero eigenvalue is given by

$$m_a(0)=1+N-(M-1)=2-\chi.$$

Since the Euler characteristic χ is additive for non-connected graphs, it is straightforward to see that the formula $m_a(0)=2C-\chi$ holds in the general case. $\square$

This theorem implies that two graph Laplacians can be isospectral only if the underlying graphs have the same number of connected components. It can clearly be seen from the proof that the spectral and algebraic multiplicities for connected graphs are equal only if the fundamental group is trivial, i.e. if the graph is a tree.

We now prove the trace formula relating the spectrum of the Laplace operator with the set of closed continuous paths on the graph Γ. We consider only closed paths p on Γ which do not turn back in the interior of any edge, but which may turn back at any vertex. If the graph has no loops (compact edges attached by both end points to one and the same vertex), then every closed continuous path is uniquely determined by the sequence of edges which this path goes along. Cyclic permutations of the sequences lead to the same closed path. It might be helpful to view such paths as periodic orbits of a point particle moving on the metric graph. This particle is moving freely along the edges, but may be reflected by the vertices. By a primitive path of p, $\mathrm{prim}(p)$, we denote any closed continuous path, such that the path p can be obtained by repeating the path $\mathrm{prim}(p)$.

Theorem 2. (Trace formula) *Let Γ be a compact metric graph with Euler characteristic χ and total length $\mathcal{L}$, and let $L(\Gamma)$ be the corresponding Laplace operator. Then the following two trace formulae establish the relation between the spectrum $\{k_n^2\}_n$ of $L(\Gamma)$ and the set $\mathcal{P}$ of closed paths on the metric graph Γ*

$$\begin{aligned} u(k) &\equiv 2m_s(0)\delta(k)+\sum_{k_n\neq 0}(\delta(k-k_n)+\delta(k+k_n)) \\ &= \chi\delta(k)+\frac{\mathcal{L}}{\pi}+\frac{1}{\pi}\sum_{p\in\mathcal{P}} l(\mathrm{prim}(p))S(p)\cos kl(p), \end{aligned} \tag{3.13}$$

and

$$\begin{aligned} \sqrt{2\pi}\hat{u}(l) &= 2m_s(0)+\sum_{k_n\neq 0} 2\cos k_n l \\ &= \chi+2\mathcal{L}\delta(l)+\sum_{p\in\mathcal{P}} l(\mathrm{prim}(p))S(p)(\delta(l-l(p))+\delta(l+l(p))), \end{aligned} \tag{3.14}$$

where

(1) $m_s(0)$ *is the multiplicity of the eigenvalue zero*([2]);

(2) p *is a closed path on* Γ;

(3) $l(p)$ *is the length of the closed path* p;

(4) $\mathrm{prim}(p)$ *is one of the primitive paths for* p;

(5) $S(p)$ *is the product of all vertex scattering coefficients along the path* p.

Proof. Consider the following distribution determined entirely by the spectrum of the Laplace operator

$$u(k) = 2m_s(0)\delta(k)+\sum_{k_n\neq 0}(\delta(k-k_n)+\delta(k+k_n)), \tag{3.15}$$

where the sum is taken over all non-zero eigenvalues respecting their multiplicity. The sum is converging in the distributional sense, since the eigenvalues accumu-

([2]) It is equal to the number C of connected components in accordance with Theorem 1.

late towards ∞. (One may prove that Weyl asymptotics is valid.) All non-zero points (including correct multiplicity) can be obtained as zeros of the analytic (just a combination of exponentials) function

$$f(k) = \det(\mathbf{S}(k) - I). \tag{3.16}$$

It follows that the distribution (3.15) can be obtained by integrating the logarithmic derivative of $f(k)$ around the zeroes. We here present formal calculations which are valid in the distributional sense (for details see [19])

$$\begin{aligned}
u(k) &= (2m_s(0) - m_a(0))\delta(k) \\
&\quad + \frac{1}{2\pi i}\left(\frac{d}{dk}\log\det(\mathbf{S}(k-i0)-I) - \frac{d}{dk}\log\det(\mathbf{S}(k+i0)-I)\right) \\
&= \chi\delta(k) + \frac{1}{2\pi i}\left(\operatorname{Tr}\frac{d}{dk}\log(\mathbf{S}(k-i0)-I) - \operatorname{Tr}\frac{d}{dk}\log(\mathbf{S}(k+i0)-I)\right) \\
&= \chi\delta(k) + \frac{1}{2\pi i}\operatorname{Tr}\frac{d}{dk}\left(-\sum_{n=1}^{\infty}\frac{1}{n}\mathbf{S}^{-n}(k-i0) + \log S(k-i0) + \sum_{n=1}^{\infty}\frac{1}{n}\mathbf{S}^{n}(k+i0)\right) \\
&= \chi\delta(k) + \frac{1}{2\pi i}\operatorname{Tr}\sum_{n=-\infty}^{+\infty}\mathbf{S}^n(k)\mathbf{S}'(k),
\end{aligned}$$

where we have taken into account that under Tr the matrices may be permutated cyclically. We have also used that $\|\mathbf{S}^{\pm 1}(k \pm i0)\| < 1$ so that the expansions are in fact converging. Taking into account that $\mathbf{S}'(k) = \mathbf{S}_v\mathbf{S}'_e(k) = \mathbf{S}_v\mathbf{S}_e(k)i\mathbf{D} = \mathbf{S}(k)i\mathbf{D}$, where $\mathbf{D}$ is the following diagonal matrix

$$\mathbf{D} = \operatorname{diag}\{d_1, d_1, d_2, d_2, \ldots, d_N, d_N\},$$

we see that the distribution u can be calculated as a trace of the infinite sum of matrices:

$$u(k) = \chi\delta(k) + \frac{1}{2\pi}\left(\operatorname{Tr}\sum_{n=-\infty}^{\infty}\mathbf{S}^n(k)\mathbf{D}\right).$$

The contribution from the zero term in the sum is just $\operatorname{Tr}\mathbf{D} = 2\mathcal{L}$. A term with number n gives a non-zero contribution only if there is a path p on Γ with the discrete length (= the number of vertices the path comes across) n. Every such path contributes twice as many times as the discrete length of the primitive path $\operatorname{prim} p$. (This will be exactly the number of different pathes if we would distinguish between the pathes with different initial points and having different orientations.) Each contribution is then equal to $l(p)S(p)e^{ikl(p)} + l(p)S(p)e^{-ikl(p)}$. Summing up we obtain the result. □

This statement was used to prove that graphs with rationally independent lengths of edges are uniquely determined by the spectra of the corresponding Laplace operators. But the trace formula has another important implication described in the following section.

4. Uniqueness results for inverse spectral problem

In this section we again consider only compact graphs. Then the Euler characteristic of the underlying metric graph can be calculated as follows.

Theorem 3. *Let Γ be a compact metric graph and $L(\Gamma)$ be the corresponding Laplace operator. Then the Euler characteristics $\chi(\Gamma)$ is uniquely determined by the spectrum $\{\lambda_n\}_n$ of the Laplace operator $L(\Gamma)$,*

$$\chi = 2m_s(0) + \lim_{t\to\infty} \sum_{k_n\neq 0} \frac{2t}{k_n} \sin\frac{k_n}{t}\Big(2\cos\frac{k_n}{t} - 1\Big), \quad k_n^2 = \lambda_n. \tag{4.1}$$

Proof. Let φ be any $C_0^\infty(\mathbb{R})$ function with the following properties

$$0 \notin \operatorname{supp}\varphi \quad \text{and} \quad \int_{-\infty}^{\infty} \varphi(x)\,dx = 1.$$

Consider the scaled sequence $\varphi_t(x)=t\varphi(tx)$ having the same properties. Then formula (3.14) implies the limit

$$\chi(\Gamma) = \sqrt{2\pi}\lim_{t\to\infty} \hat{u}[\varphi_t]. \tag{4.2}$$

The function φ in the proof can be chosen equal to a step function, for example

$$\varphi(l) = \begin{cases} 1, & 1\le l\le 2,\\ 0, & \text{otherwise},\end{cases}$$

since for sufficiently large t the support of φ_t belongs to the regular support of the distribution $\hat{u}$. The Fourier transform of φ_t is

$$\widehat{\varphi}_t(k) = \frac{e^{ik/t}}{\sqrt{2\pi}} \frac{e^{ik/t}-1}{ik/t}.$$

Formula (3.13) can now be used in order to get (4.1) for the Euler characteristic of Γ. $\square$

This theorem implies that Laplacians on two metric graphs having different Euler characteristics are not isospectral. Taking in addition into account that the eigenvalues satisfy Weyl's asymptotic law [28] and that the spectral multiplicity of the eigenvalue zero is equal to the number of connected components (Theorem 1) we can formulate the following result.

Uniqueness theorem 1. *If two Laplace operators on compact graphs have the same spectrum* $\{\lambda_n\}_n$ *then the underlying metric graphs have the same*

(1) *number of connected components*;
(2) *total length*;
(3) *Euler characteristic.*

The result concerning Euler characteristic appears substantial, while the remaining two points are recalled here for the sake of completeness.

5. Uniqueness results for inverse scattering problems

The uniqueness result proven for compact graphs are generalized in this section to include non-compact graphs. Let Γ be a non-compact graph with N_i internal (finite) edges $\Delta_j=[x_{2j-1},x_{2j}]$, $j=1,2,...,N_i$, and N_e external (semi-infinite) edges $\Delta_{N_i+j}=[x_{2N_i+j},\infty)$, $j=1,2,...,N_e$. Let us denote by Γ_c the *compact core* of the graph Γ obtained by cutting off the external edges

$$\Gamma_c=\Gamma\setminus\Gamma_\infty, \quad \text{where } \Gamma_\infty=\bigcup_{j=1}^{N_e}\Delta_{N_i+j}. \tag{5.1}$$

Note that it may happen that the chopped vertices have valence 2. In this case the two neighboring intervals must be substituted by one edge, but we do not want to dwell at this point.

In order to study the absolutely continuous spectrum one introduces the scattering matrix $\mathbb{S}(k)$ which is the $N_e\times N_e$ unitary matrix connecting the amplitudes of the scattered waves on the semi-infinite edges. Let $\psi(x,k)$ be a solution to the differential equation (3.1) on the edges satisfying the boundary conditions (2.3) at the vertices. Then on the semi-infinite edges this function is equal to a combination of incoming and outgoing plane waves:

$$\psi(x,k)|_{x\in[x_{2N_i+j},\infty)}=\alpha_j e^{ik|x-x_{2N+j}|}+\beta_j e^{-ik|x-x_{2N+j}|}. \tag{5.2}$$

Then the scattering matrix connects the amplitudes of the incoming $e^{-ik|x-x_{2N+j}|}$ and outgoing $e^{ik|x-x_{2N+j}|}$ waves

$$\mathbb{S}(k)\colon \vec{\beta}\longmapsto\vec{\alpha}. \tag{5.3}$$

In [20] and [4] it was shown that the knowledge of the scattering matrix is not sufficient to reconstruct the Euler characteristic of the graphs, but it appears that the knowledge of the scattering matrix *and* the discrete spectrum is enough to calculate χ.

Theorem 4. *Let Γ be a non-compact metric graph with the compact core Γ_c and N_e semi-infinite edges attached to it. Then the spectrum of the Laplace operator $L(\Gamma_c)$ is uniquely determined by the scattering data $(\mathbb{S}(k), \{\lambda_n\}_n)$ for $L(\Gamma)$.*

Proof. Consider any eigenfunction $\psi(\,\cdot\,, k_n)$ of $L(\Gamma_c)$ corresponding to a certain eigenvalue $\mu_n = k_n^2$. Let us continue this function to the rest of Γ by taking into account its values at the chopped vertices as follows:

$$\psi(x, k_n) = \psi(x_{2N_i+j}, k_n) \cos k_n |x - x_{2N_i+j}|, \quad x \in [x_{2N_i+j}, \infty). \tag{5.4}$$

If all $\psi(x_{2N_i+j}, k_n), j = 1, 2, ..., N_1$, are zero, then the corresponding function is a (discrete spectrum) eigenfunction for the operator $L(\Gamma)$ and therefore k_n^2 coincides with one of the λ_m.

If at least one of the values at the chopped vertices is not zero, then the extended function is a generalized eigenfunction corresponding to the absolutely continuous spectrum. Considering the asymptotics of this function we conclude that the corresponding scattering matrix should have eigenvalue 1, i.e.

$$\det(\mathbb{S}(k) - I) = 0. \tag{5.5}$$

On the other hand every solution to this equation determines an eigenfunction of $L(\Gamma_c)$.

Hence we conclude that the spectrum of $L(\Gamma_c)$ is given by the eigenvalues λ_m of $L(\Gamma)$ and the solutions to (5.5). $\square$

This theorem allows us to generalize the uniqueness theorem proven for compact graphs.

Uniqueness theorem 2. *If two Laplace operators on non-compact graphs have the same scattering data $(\mathbb{S}(k), \{\lambda_n\}_n)$ then the underlying metric graphs have the same*

(1) *number of connected components*;
(2) *total length of the compact core*;
(3) *Euler characteristic.*

The number of connected components can be calculated directly summing up

(1) the number of compact connected components equal to the multiplicity of the eigenvalue $E = 0$;

(2) the number of non-compact components equal to the maximal number of unitary blocks in the scattering matrix $\mathbb{S}(k)$.

The total length of the compact core depends of course on the way we cut off the semi-infinite edges. It is possible to cut off the semi-infinite edges without chopping the vertices, but at certain points $O_j \in (x_{2N+j}, \infty)$. This corresponds in some sense to a new parametrization of the scattering waves and leads to a slightly different scattering matrix.

The counterexamples constructed in [20] show two graphs with the same scattering matrix but different Euler characteristics. These examples do not contradict our result, since the discrete spectra of the corresponding Laplacians are different. The result we have proven states that additional knowledge of the discrete spectrum allows one to calculate the Euler characteristic. A formula similar to (4.1) can be derived. At the same time the theorem implies that if a graph Laplacian has no discrete spectrum, then the Euler characteristic of the underlying graph is determined by the scattering matrix only.

Acknowledgements. The author is grateful to all mathematicians who discussed parts of this work, in particular to J.-E. Björk, J. Boman, A. Holst, A. Luger, M. Nowaczyk, and participants of the conference "Semiclassical Analysis and Mathematical Quantum Mechanics" (Bologna, 2006). Special thanks to the referees for careful reading of the manuscript and comments helping to improve the presentation.

References

1. Belishev, M. I., Boundary spectral inverse problem on a class of graphs (trees) by the BC method, *Inverse Problems* **20** (2004), 647–672.
2. Belishev, M. I., On the boundary controllability of a dynamical system described by the wave equation on a class of graphs (on trees), *Zap. Nauchn. Sem. S.-Peterburg. Otdel. Mat. Inst. Steklov.* (*POMI*) **308** (2004), 23–47, 252 (Russian). English transl.: *J. Math. Sci.* (*N.Y.*) **132** (2006), 11–25.
3. von Below, J., Can one hear the shape of a network?, in *Partial Differential Equations on Multistructures* (*Luminy, 1999*), Lect. Notes Pure Appl. Math. **219**, pp. 19–36, Marcel Dekker, New York, 2001.
4. Boman, J. and Kurasov, P., Symmetries of quantum graphs and the inverse scattering problem, *Adv. Appl. Math.* **35** (2005), 58–70.
5. Borg, G., Eine Umkehrung der Sturm–Liouvilleschen Eigenwertaufgabe. Bestimmung der Differentialgleichung durch die Eigenwerte, *Acta Math.* **78** (1946), 1–96.
6. Borg, G., Uniqueness theorems in the spectral theory of $y''+(\lambda-q(x))y=0$, in *Den* 11*te Skandinaviske Matematikerkongress* (*Trondheim, 1949*), pp. 276–287, Johan Grundt Tanums Forlag, Oslo, 1952.
7. Brown, B. M. and Weikard, R., A Borg–Levinson theorem for trees, *Proc. R. Soc. Lond. Ser. A Math. Phys. Eng. Sci.* **461** (2005), 3231–3243.

8. Carlson, R., Inverse eigenvalue problems on directed graphs, *Trans. Amer. Math. Soc.* **351** (1999), 4069–4088.
9. Colin de Verdière, Y., Spectres de variétés Riemanniennes et spectres de graphes, in *Proceedings of the International Congress of Mathematicians, Vol.* 1, 2 (*Berkeley, Calif., 1986*), pp. 522–530, Am. Math. Soc., Providence, RI, 1987.
10. Colin de Verdière, Y., *Spectres de Graphes*, Cours Spécialisés **4**, Société Mathématique de France, Paris, 1998.
11. Exner, P. and Sheba, P., Free quantum motion on a branching graph, *Rep. Math. Phys.* **28** (1989), 7–26.
12. Friedlander, L., Genericity of simple eigenvalues for a metric graph, *Israel J. Math.* **146** (2005), 149–156.
13. Gerasimenko, N. I., The inverse scattering problem on a noncompact graph, *Teoret. Mat. Fiz.* **75** (1988), 187–200 (Russian). English transl.: *Theoret. and Math. Phys.* **75** (1988), 460–470.
14. Gerasimenko, N. I. and Pavlov, B. S., A scattering problem on noncompact graphs, *Teoret. Mat. Fiz.* **74** (1988), 345–359 (Russian). English transl.: *Theoret. and Math. Phys.* **74** (1988), 230–240.
15. Gutkin, B. and Smilansky, U., Can one hear the shape of a graph?, *J. Phys. A* **34** (2001), 6061–6068.
16. Kostrykin, V. and Schrader, R., Kirchhoff's rule for quantum wires, *J. Phys. A* **32** (1999), 595–630.
17. Kostrykin, V. and Schrader, R., Kirchhoff's rule for quantum wires. II. The inverse problem with possible applications to quantum computers, *Fortschr. Phys.* **48** (2000), 703–716.
18. Kottos, T. and Smilansky, U., Periodic orbit theory and spectral statistics for quantum graphs, *Ann. Physics* **274** (1999), 76–124.
19. Kurasov, P. and Nowaczyk, M., Inverse spectral problem for quantum graphs, *J. Phys. A* **38** (2005), 4901–4915.
20. Kurasov, P. and Stenberg, F., On the inverse scattering problem on branching graphs, *J. Phys. A* **35** (2002), 101–121.
21. Levinson, N., On the uniqueness of the potential in a Schrödinger equation for a given asymptotic phase, *Danske Vid. Selsk. Mat.-Fys. Medd.* **25** (1949), 29pp.
22. Marchenko, V. A., Some questions of the theory of one-dimensional linear differential operators of the second order. I, *Tr. Mosk. Mat. Obs.* **1** (1952), 327–420 (Russian).
23. Novikov, S., Discrete Schrödinger operators and topology, *Asian J. Math.* **2** (1998), 921–933.
24. Nowaczyk, M., *Inverse Spectral Problems for Quantum Graphs*, Licentiate Thesis, Lund University, Lund, 2005.
25. Nowaczyk, M., Inverse spectral problems for quantum graphs with rationally dependent edges, in *Proceedings of Operator Theory, Analysis and Mathematical Physics* (*Będlewo, Poland, 2004*), Oper. Theory Adv. Appl. **174**, pp. 105–116, Birkhäuser, Basel, 2007
26. Roth, J. P., Le spectre du Laplacien sur un graphe, in *Théorie du Potentiel* (*Orsay, 1983*), Lect. Notes in Math. **1096**, pp. 521–539, Springer, Berlin–Heidelberg, 1984.

27. Sobolev, A. V. and Solomyak, M., Schrödinger operators on homogeneous metric trees: spectrum in gaps, *Rev. Math. Phys.* **14** (2002), 421–467.
28. Solomyak, M., On eigenvalue estimates for the weighted Laplacian on metric graphs, in *Nonlinear Problems in Mathematical Physics and Related Topics*, I, Int. Math. Ser. (N.Y.) **1**, pp. 327–347, Kluwer/Plenum, New York, 2002.
29. Yurko, V., Inverse spectral problems for Sturm–Liouville operators on graphs, *Inverse Problems* **21** (2005), 1075–1086.

Pavel Kurasov
Department of Mathematics LTH
Lund University
P. O. Box 118
SE-221 00 Lund
Sweden
kurasov@maths.lth.se

Received June 28, 2006
in revised form May 7, 2007
published online October 24, 2007