Methods of Functional Analysis and Topology
Vol. 18 (2012), no. 4, pp. 343–359

TRACE FORMULAE FOR GRAPH LAPLACIANS WITH APPLICATIONS TO RECOVERING MATCHING CONDITIONS

YULIA ERSHOVA AND ALEXANDER V. KISELEV

Abstract. Graph Laplacians on finite compact metric graphs are considered under the assumption that the matching conditions at the graph vertices are of either δ or δ' type. In either case, an infinite series of trace formulae which link together two different graph Laplacians provided that their spectra coincide is derived. Applications are given to the problem of reconstructing matching conditions for a graph Laplacian based on its spectrum.

1. Introduction

A graph Laplacian is a particular case of a quantum graph, i.e., a metric graph Γ and an associated second-order differential operator acting on the Hilbert space $L^2(\Gamma)$ of square summable functions on the graph with an additional assumption that the functions belonging to the domain of the operator are coupled by certain matching conditions at the graph vertices. These matching conditions reflect the graph connectivity and usually are assumed to guarantee self-adjointness of the operator. Recently these operators have attracted a considerable interest of both physicists and mathematicians due to a number of important physical applications, e.g., to the study of quantum wavequides. Extensive literature on the subject is surveyed in, e.g., [14].

In the situation of a graph Laplacian the above-mentioned second-order differential operator is simply the operator of negative second derivative.

The present paper is devoted to the study of the inverse spectral problem for graph Laplacians on finite compact metric graphs. One might classify the possible inverse problems for graph Laplacians in the following way.

(i) Given spectral data and the matching conditions (usually one assumes standard matching conditions, see below), to reconstruct the metric graph;
(ii) Given the metric graph and spectral data, to reconstruct the matching conditions.

There exists an extensive literature devoted to the problem (i). To name just a few, we would like to mention the pioneering works [19, 11, 8] and later contributions [15, 16, 1, 9]. These papers utilize an approach to the problem (i) based on the so-called trace formula which relates the spectrum of the quantum graph to the set of closed paths on the underlying metric graph.

On the other hand, the problem (ii) has to the best of our knowledge surprisingly attracted much less interest. After being mentioned in [16], it was treated in [2], but only in the case of star graphs.

2000 *Mathematics Subject Classification.* Primary 47A10; Secondary 47A55.
Key words and phrases. Quantum graphs, graph Laplacians, inverse spectral problem, trace formulae, boundary triples.
The first authors' work was partially supported by the grant DFFD F40.1/008.
The second authors' work was partially supported by the grants RFBR 11-01-90402-Ukr_f_a and RFBR 12-01-00215-a.

The present paper is devoted to the analysis of the same problem (*ii*). Unlike [2], we consider the case of a general connected compact finite metric graph (in particular, this graph is allowed to possess cycles and loops), but only for two classes of matching conditions at the graph vertices, namely, in either the case of δ type matching conditions at the vertices or the case of δ' type matching conditions (see Section 2 for definitions). The methods and mathematical apparatus applied by us in both cases are identical, but the results prove to be somewhat different. The named two classes singled out by us prove to be physically viable [5, 6].

In contrast to [2], where the spectral data used in order to reconstruct the matching conditions it taken to be the Weyl-Titchmarsh M-function (or Dirichlet-to-Neumann map) of the graph boundary, we use the spectrum of graph Laplacian (counting multiplicities) as the data known to us from the outset.

The approach suggested is based on the celebrated theory of boundary triples [7]. Explicit construction a generalized Weyl-Titchmarsh M-function for a properly chosen maximal (adjoint to a symmetric, which we refer to as *minimal*) operator allows us to reduce the study of the spectrum of a graph Laplacian to the study of "zeroes" of the corresponding finite-dimensional analytic matrix function. In order to achieve this goal, we surely have to construct an M-function for the whole graph rather than consider the Dirichlet-to-Neumann map pertaining to the graph boundary. On this path we are then able to derive an infinite series of trace formulae which link together two different graph Laplacians provided that their spectra coincide. These trace formula surprisingly only involve the (diagonal) matrices of coupling constants (i.e., constants appearing in matching conditions) and the diagonal matrix of the vertex valences of the graph Γ.

We would like to point out that the approach suggested seems to be applicable to the analysis of more general differential operators on a given metric graph, most notably, of Schrödinger operators. We leave this question aside for the time being as we plan to make it a subject of a forthcoming publication.

The paper is organized as follows.

Section 2 introduces the notation and contains a brief summary of the material on the boundary triples used by us in the sequel. We continue by providing an explicit "natural" form of the Weyl-Titchmarsh M-function for the case of δ type matching conditions (δ' type, respectively), suitable for our goal. We further pay special attention to the problem of simplicity of our minimal operator, which turns out to be equivalent to the question of whether the M-function together with the matrix of coupling constants accounts for all of the spectrum of graph Laplacian or not.

Section 3 contains our main result, i.e., the trace formulae for graph Laplacians with δ type (δ' type, respectively) matching conditions. In this Section we also draw certain corollaries from the trace formulae obtained pertaining to the inverse spectral problem for graph Laplacians in the setting (*ii*).

2. Boundary triples approach

Definition of the Laplacian on a quantum graph. In order to define the quantum Laplacian, i.e., the Laplace operator on a quantum graph, we begin with the following

Definition 2.1. We call $\Gamma = \Gamma(\mathbf{E_\Gamma}, \sigma)$ a finite compact metric graph, if it is a collection of a finite non-empty set $\mathbf{E_\Gamma}$ of finite closed intervals $\Delta_j = [x_{2j-1}, x_{2j}]$, $j = 1, 2, \dots, n$, called *edges*, and of a partition σ of the set of endpoints $\{x_k\}_{k=1}^{2n}$ into N classes, $\mathbf{V_\Gamma} = \bigcup_{m=1}^N V_m$. The equivalence classes V_m, $m = 1, 2, \dots, N$ will be called *vertices* and the number of elements belonging to the set V_m will be called the *valence* of the vertex V_m.

With a finite compact metric graph Γ we associate the Hilbert space

$$L_2(\Gamma) = \bigoplus_{j=1}^{n} L_2(\Delta_j).$$

This Hilbert space obviously doesn't feel the connectivity of the graph, being the same for each graph with the same number of edges of the same lengths.

In what follows, we single out two natural [5] classes of so-called *matching conditions* which lead to a properly defined self-adjoint operator on the graph Γ, namely, the matching conditions of δ and δ' types. In order to describe these, we will introduce the following notation. For a smooth enough function $f \in L_2(\Gamma)$, we will use throughout the following definition of the normal derivative on a finite compact metric graph:

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

Definition 2.2. If $f \in \oplus_{j=1}^{n} W_2^2(\Delta_j)$ and α_m is a complex number (referred to below as a coupling constant),

(δ) the condition of continuity of the function f through the vertex V_m (i.e., $f(x_j) = f(x_k)$ if $x_j, x_k \in V_m$) together with the condition

$$\sum_{x_j \in V_m} \partial_n f(x_j) = \alpha_m f(V_m)$$

is called δ-type matching at the vertex V_m;

(δ') the condition of continuity of the normal derivative $\partial_n f$ through the vertex V_m (i.e., $\partial_n f(x_j) = \partial_n f(x_k)$ if $x_j, x_k \in V_m$) together with the condition

$$\sum_{x_j \in V_m} f(x_j) = \alpha_m \partial_n f(V_m)$$

is called δ'-type matching at the vertex V_m.

Remark 2.3. Note that the δ-type matching condition in a particular case when $\alpha_m = 0$ reduces to the so-called standard, or Kirchhoff, matching condition at the vertex V_m. Note also that at the graph boundary (i.e., at the set of vertices of valence equal to 1) the δ- and δ'-type conditions reduce to the usual 3rd type one, whereas the standard matching conditions lead to the Neumann condition at the graph boundary.

We are all set now to define the graph Laplacian (i.e., the Laplace operator on a graph) on the graph Γ with δ- or δ'-type matching conditions.

Definition 2.4. The graph Laplacian A on a graph Γ with δ-type (δ'-type, respectively) matching conditions is the operator of negative second derivative in the Hilbert space $L_2(\Gamma)$ on the domain of functions belonging to the Sobolev space $\oplus_{j=1}^{n} W_2^2(\Delta_j)$ and satisfying δ-type (δ'-type, respectively) matching conditions at every vertex V_m, $m = 1, 2, \dots, N$.

Remark 2.5. Note that the matching conditions reflect the graph connectivity: if two graphs with the same edges have different topology, the resulting operators are different.

Provided that all coupling constants α_m, $m = 1, \dots, N$, are real, it is easy to verify that the Laplacian A is a self-adjoint operator in the Hilbert space $L_2(\Gamma)$ [5, 10]. Throughout the present paper, we are going to consider this self-adjoint situation only, although it has to be noted that the approach developed can be used for the purpose of analysis of the general non-self-adjoint situation as well.

Clearly, the self-adjoint operator thus defined on a finite compact metric graph has purely discrete spectrum that might accumulate to $+\infty$ only. In order to ascertain this, one only has to note that the operator considered is a finite-dimensional perturbation in the resolvent sense of the direct sum of Sturm-Liouville operators on the individual edges.

Remark 2.6. Note that w.l.o.g. each edge Δ_j of the graph Γ can be considered to be an interval $[0, l_j]$, where $l_j = x_{2j} - x_{2j-1}$, $j = 1 \dots n$ is the length of the corresponding edge. Indeed, performing the corresponding linear change of variable one reduces the general situation to the one where all the operator properties depend on the lengths of the edges rather than on the actual edge endpoints.

We now pass over to the main subject of the present paper, i.e., to the derivation of an infinite series of trace formulae for the graph Laplacian with δ- or δ' matching conditions at the vertices. In order to do so, we will first need to establish an explicit formula for the generalized Weyl-Titchmarsh M-function of the operator considered. The most elegant and straightforward way to do so is in our view by utilizing the apparatus of boundary triples developed in [7, 12, 13, 4]. We briefly recall the results essential for our work.

Boundary triplets and the Weyl-Titchmarsh matrix M-function. Suppose that $A_{\min}$ is a symmetric densely defined closed linear operator acting in the Hilbert space H ($D(A_{\min}) \equiv D_{A_{\min}}$ and $R(A_{\min}) \equiv R_{A_{\min}}$ denoting its domain and range respectively; $D(A_{\max}) \equiv D_{A_{\max}}$, $R(A_{\max}) \equiv R_{A_{\max}}$ denoting the domain and range of operator $A_{\max}$ adjoint to $A_{\min}$). Assume that $A_{\min}$ is completely nonselfadjoint (simple), i.e., there exists no reducing subspace H_0 in H such that the restriction $A_{\min}|H_0$ is a selfadjoint operator in H_0. Further assume that the deficiency indices of $A_{\min}$ (probably being infinite) are equal: $n_+(A_{\min}) = n_-(A_{\min}) \leq \infty$.

Definition 2.7. ([7, 12, 4]). Let Γ_0, Γ_1 be linear mappings of $D_{A_{\max}}$ to $\mathcal{H}$ – a separable Hilbert space. The triple $(\mathcal{H}, \Gamma_0, \Gamma_1)$ is called *a boundary triple* for the operator $A_{\max}$ if:

(1) for all $f, g \in D_{A_{\max}}$
$$(A_{\max} f, g)_H - (f, A_{\max} g)_H = (\Gamma_1 f, \Gamma_0 g)_{\mathcal{H}} - (\Gamma_0 f, \Gamma_1 g)_{\mathcal{H}}.$$
(2) the mapping γ defined as $f \longmapsto (\Gamma_0 f; \Gamma_1 f)$, $f \in D_{A_{\max}}$ is surjective, i.e., for all $Y_0, Y_1 \in \mathcal{H}$ there exists such $y \in D_{A_{\max}}$ that $\Gamma_0 y = Y_0$, $\Gamma_1 y = Y_1$.

A boundary triple can be constructed for any operator $A_{\min}$ of the class considered. Moreover, the space $\mathcal{H}$ can be chosen in a way such that $\dim \mathcal{H} = n_+ = n_-$.

Definition 2.8. ([7, 4]). A nontrivial extension A_B of the operator $A_{\min}$ such that $A_{\min} \subset A_B \subset A_{\max}$ is called *almost solvable* if there exists a boundary triple $(\mathcal{H}, \Gamma_0, \Gamma_1)$ for $A_{\max}$ and a bounded linear operator B defined everywhere on $\mathcal{H}$ such that for every $f \in D_{A_{\max}}$
$$f \in D_{A_B} \quad \text{if and only if} \quad \Gamma_1 f = B \Gamma_0 f.$$

It can be shown that if an extension A_B of $A_{\min}$, $A_{\min} \subset A_B \subset A_{\max}$, has regular points (i.e., the points belonging to the resolvent set) in both upper and lower half-planes of the complex plane, then this extension is almost solvable.

The following theorem holds:

Theorem 2.9. ([7, 4]). *Let $A_{\min}$ be a closed densely defined symmetric operator with $n_+(A_{\min}) = n_-(A_{\min})$, let $(\mathcal{H}, \Gamma_0, \Gamma_1)$ be a boundary triple of $A_{\max}$. Consider the almost solvable extension A_B of $A_{\min}$ corresponding to the bounded operator B in $\mathcal{H}$. Then*

(1) $y \in D_{A_{\min}}$ *if and only if* $\Gamma_0 y = \Gamma_1 y = 0$,
(2) A_B *is maximal, i.e.,* $\rho(A_B) \neq \emptyset$,
(3) $(A_B)^* \subset A_{\max}$, $(A_B)^* = A_{B^*}$,
(4) *operator* A_B *is dissipative if and only if* B *is dissipative,*
(5) $(A_B)^* = A_B$ *if and only if* $B^* = B$.

The generalized Weyl-Titchmarsh M-function is then defined as follows.

Definition 2.10. ([4, 7, 13]). Let $A_{\min}$ be a closed densely defined symmetric operator, $n_+(A_{\min}) = n_-(A_{\min})$, $(\mathcal{H}, \Gamma_0, \Gamma_1)$ is its space of boundary values. The operator-function $M(\lambda)$, defined by

$$M(\lambda)\Gamma_0 f_\lambda = \Gamma_1 f_\lambda, \quad f_\lambda \in \ker(A_{\max} - \lambda), \quad \lambda \in \mathbb{C}_\pm, \tag{1}$$

is called the Weyl-Titchmarsh M-function of a symmetric operator $A_{\min}$.

The following Theorem describing the properties of the M-function clarifies its meaning.

Theorem 2.11. ([7, 4]*, in the form adopted in* [20]). *Let $M(\lambda)$ be the M-function of a symmetric operator $A_{\min}$ with equal deficiency indices ($n_+(A_{\min}) = n_-(A_{\min}) < \infty$). Let A_B be an almost solvable extension of $A_{\min}$ corresponding to a bounded operator B. Then for every $\lambda \in \mathbb{C}$:*

1. *$M(\lambda)$ is analytic operator-function when $\operatorname{Im}\lambda \neq 0$, its values being bounded linear operators in $\mathcal{H}$.*
2. $(\operatorname{Im}\ M(\lambda))\operatorname{Im}\lambda > 0$ *when* $\operatorname{Im}\lambda \neq 0$.
3. $M(\lambda)^* = M(\overline{\lambda})$ *when* $\operatorname{Im}\lambda \neq 0$.
4. *$\lambda_0 \in \rho(A_B)$ if and only if $(B - M(\lambda))^{-1}$ admits bounded analytic continuation into the point λ_0.*

In view of the last Theorem, one is tempted to reduce the study of the spectral properties of the Laplacian on a quantum graph to the study of the corresponding Weyl-Titchmarsh M-function. Indeed, if one considers the operator under investigation as an extension of a properly chosen symmetric operator defined on the same graph and constructs a boundary triple for the latter, one might utilize all the might of the complex analysis and the theory of analytic matrix R-functions, since in this new setting the (pure point) spectrum of the quantum Laplacian is located exactly at the points into which the matrix-function $(B - M(\lambda))^{-1}$ cannot be extended analytically (vaguely speaking, these are "zeroes" of the named matrix-function).

It might appear as if the non-uniqueness of the space of boundary values and the resulting non-uniqueness of the Weyl-Titchmarsh M-function leads to some problems on this path; but on the contrary, this flexibility of the apparatus is an advantage of the theory rather than its weakness. Indeed, as we are going to show below, this allows us to "separate" the data describing the metric graph (this information will be carried by the M-function) from the data describing the matching conditions at the vertices (this bit of information will be taken care of by the matrix B parameterizing the extension). In turn, this "separation" proves to be quite fruitful in view of applications that we have in mind.

There is yet another question to be taken care of along the way. As mentioned above, in order to make the approach suggested work one must ensure that the symmetric operator $A_{\min}$ is simple, i.e., does not have self-adjoint "parts". If it so happens that this operator looses simplicity (as we will show below, this certainly happens if the graph contains loops and might happen if it contains cycles), one then ends up with the matrix-function $B - M(\lambda)$ which no longer carries all the information about the spectrum of the corresponding quantum Laplacian. Namely, all the (point) spectrum of the self-adjoint "part" of the symmetric operator $A_{\min}$ will be invisible for this matrix-function.

Although as it is easily seen this is hardly a problem from the point of view of the present paper, it might complicate the issue when investigating other kinds of direct and inverse spectral problems. It is due to this reason that we have elected to cover the question of simplicity in some details in the present paper (see Theorems 2.22 and 2.26 towards the end of this Section).

We proceed with an explicit construction of the "natural" boundary triple and M-function in the case of graph Laplacians.

Construction of a boundary triple and calculation of the M-function in the case of a quantum Laplacian. Let Γ be a fixed finite compact metric graph. Let us denote by $\partial\Gamma$ the graph boundary, i.e., all the vertices of the graph which have valence 1. W.l.o.g. we further assume that at all the vertices the matching conditions are of δ type (the case when they are of δ' type is treated along the same lines and we provide the corresponding results without a proof; the mixed case can be looked at in more or less the same fashion; we omit any discussion of the latter in order to improve readability of the paper).

As the operator $A_{\max}$ rather then $A_{\min}$ is crucial from the point of view of construction of a boundary triple, we start with this maximal operator and explicitly describe its action and domain: $A_{\max} = -\frac{d^2}{dx^2}$,

$$D(A_{\max}) = \left\{ f \in \bigoplus_{j=1}^{n} W_2^2(\Delta_j) \mid \forall\ V_m \in V_{\Gamma\setminus\partial\Gamma}\ f \text{ is continuous at } V_m \right\}. \tag{2}$$

Remark 2.12. Note that the operator chosen is not the "most maximal" maximal one: one could of course skip the condition of continuity through internal vertices; nevertheless, the choice made proves to be the most natural from the point of view expressed above. This is exactly due to the fact that the graph connectivity is thus reflected in the domain of the maximal operator and therefore propels itself into the expression for the M-matrix. Moreover, it should be noted that this choice is also natural since the dimension of the M-matrix will be exactly equal to the number of graph vertices.

The choice of the operators Γ_0 and Γ_1, acting onto $\mathbb{C}_N$, $N = |V_\Gamma|$ is made as follows (cf., e.g., [17] where a similar choice is suggested, but only for the graph boundary):

$$\Gamma_0 f = \begin{pmatrix} f(V_1) \\ f(V_2) \\ \dots \\ f(V_N) \end{pmatrix}, \quad \Gamma_1 f = \begin{pmatrix} \sum\limits_{x_j : x_j \in V_1} \partial_n f(x_j) \\ \sum\limits_{x_j : x_j \in V_2} \partial_n f(x_j) \\ \dots \\ \sum\limits_{x_j : x_j \in V_N} \partial_n f(x_j) \end{pmatrix}. \tag{3}$$

Here the symbol $f(V_j)$ denotes the value of the function $f(x)$ at the vertex V_j. The latter is meaningful because of the choice of the domain of the maximal operator.

Remark 2.13. If one ascertains that the triple $(\mathbb{C}_N, \Gamma_0, \Gamma_1)$ satisfies Definition 2.7, the corresponding minimal operator $A_{\min}$ will therefore be the following one: $A_{\min} = -\frac{d^2}{dx^2}$,

$$\begin{aligned} D(A_{\min}) = \Bigg\{ f \in \bigoplus_{j=1}^{n} W_2^2(\Delta_j) \mid \forall\ V_m,\ m = 1, \dots, N,\ f(V_m) = 0, \\ \forall\ V_m,\ m = 1, \dots, N, \sum_{x_j \in V_m} \partial_n f(x_j) = 0 \Bigg\}. \end{aligned} \tag{4}$$

This operator will be symmetric with deficiency indices (N, N). This follows from the fact that the domain of the minimal operator admits the following characterization in terms of boundary triples: $D(A_{\min}) = \{f \in D(A_{\max}) | \Gamma_0 f = \Gamma_1 f = 0\}$ (see Theorem 2.9).

Lemma 2.14. *The triple $(\mathbb{C}_N; \Gamma_0, \Gamma_1)$, $N = |V_\Gamma|$ is a boundary triple for the operator $A_{\max}$ in the sense of Definition 2.7.*

Proof. First, we verify the abstract Green formula. Indeed, performing double integration by parts,

$$\langle A_{\max} f, g\rangle - \langle f, A_{\max} g\rangle \\ = \sum_{j=1}^{n} [-f(x_{2j})\bar{g}'(x_{2j}) + f(x_{2j-1})\bar{g}'(x_{2j-1}) + f'(x_{2j})\bar{g}(x_{2j}) \\ -f'(x_{2j-1})\bar{g}(x_{2j-1})] = \sum_{k=1}^{2n} [\partial_n f(x_k)\bar{g}(x_k) - f(x_k)\partial_n \bar{g}(x_k)],$$

where the definition of the normal derivative on the graph has been taken into account. Splitting the last sum into parts corresponding the graph vertices, one arrives at:

$$\langle A_{\max} f, g\rangle - \langle f, A_{\max} g\rangle \\ = \sum_{i=1}^{N} \sum_{k:x_k\in V_i} \partial_n f(x_k)\bar{g}(x_k) - \sum_{i=1}^{N} \sum_{k:x_k\in V_i} f(x_k)\partial_n \bar{g}(x_k) \\ = \langle \Gamma_1 f, \Gamma_0 g\rangle_{\mathbb{C}_n} - \langle \Gamma_0 f, \Gamma_1 g\rangle_{\mathbb{C}_n},$$

as required.

It remains to be shown that the mapping $f \mapsto \Gamma_0 f \oplus \Gamma_1 f$, $f \in D(A_{\max})$ is surjective as a mapping onto $\mathbb{C}_n \oplus \mathbb{C}_n$.

All we need to do is to show that for a pair of arbitrary vectors $y = (y_1, \dots, y_N)$, $z = (z_1, \dots, z_N)$ there exists a function $f \in D(A_{\max})$ such that $\Gamma_0 f = y$, $\Gamma_1 f = z$.

Consider the vertex V_1 of valence v_1. Fix some edge containing V_1 and denote it γ_1. The rest of the edges containing V_1 will be numbered in some arbitrary order and denoted $\gamma_2, \dots, \gamma_{v_1}$. Put $\partial_n f_{\gamma_1}(V_1) = z_1$, $\partial_n f_{\gamma_j}(V_1) = 0$, $j = 2, \dots, v_1$ and $f_{\gamma_j}(V_1) = y_1$, $j = 1, \dots, v_1$. Then both required conditions are satisfied: the function to be constructed is continuous through the vertex V_1, whereas $\sum_{x_j\in V_1} \partial_n f(x_j) = z_1$. Now pick the remaining vertices one by one. We end up with the trivial task of finding a function belonging to $\oplus_{j=1}^{n} W_2^2(\Delta_j)$ such that on each individual interval Δ_j the values of the function itself and of its derivative at both endpoints are fixed to some predetermined values. □

Remark 2.15. If one considers a graph Laplacian with matching conditions of δ' type, the choice of the maximal operator and the corresponding boundary triple (an analogue of Lemma 2.14 can be obtained along the same lines) has to change accordingly: $A_{\max} = -\frac{d^2}{dx^2}$,

$$D(A_{\max}) = \left\{ f \in \bigoplus_{j=1}^{n} W_2^2(\Delta_j) | \forall\ V_m \in V_{\Gamma\setminus\partial\Gamma}\ \partial_n f \text{ is continuous at } V_m \right\}, \tag{5}$$

$$\Gamma_0 f = \begin{pmatrix} \partial_n f(V_1) \\ \partial_n f(V_2) \\ \dots \\ \partial_n f(V_N) \end{pmatrix}, \quad \Gamma_1 f = \begin{pmatrix} \sum_{x_j:x_j\in V_1} f(x_j) \\ \sum_{x_j:x_j\in V_2} f(x_j) \\ \dots \\ \sum_{x_j:x_j\in V_N} f(x_j) \end{pmatrix}. \tag{6}$$

Then the minimal operator $A_{\min} = -\frac{d^2}{dx^2}$ on the domain

$$(7)\quad D(A_{\min}) = \Bigg\{ f \in \bigoplus_{j=1}^{n} W_2^2(\Delta_j) \mid \forall\, V_m,\, m=1,\dots,N\ \partial_n f(V_m) = 0, \\ \forall\, V_m, m=1,\dots,N,\ \sum_{x_j \in V_m} f(x_j) = 0 \Bigg\}$$

is again a symmetric operator with deficiency indices equal to (N, N).

We are now ready to formulate our main result of the present section, namely, the formula for the Weyl-Titchmarsh M-function associated with the boundary triple (3).

Theorem 2.16. *Let Γ be a finite compact metric graph. Let the operator $A_{\max}$ be the negative second derivative on the domain* (2)*. Let the boundary triple for $A_{\max}$ be chosen as $(\mathbb{C}^N, \Gamma_0, \Gamma_1)$, where N is the number of vertices of Γ and the operators Γ_0 and Γ_1 are defined by* (3)*. Then the generalized Weyl-Titchmarsh M-function is an $N \times N$ matrix with matrix elements given by the following formula.*

$$(8)\qquad m_{jp} = \begin{cases} -k \sum\limits_{\Delta_t \in E_j} \cot kl_t + 2k \sum\limits_{\Delta_t \in L_j} \tan \frac{kl_t}{2}, & j=p, \\ k \sum\limits_{\Delta_t \in C_{j,p}} \frac{1}{\sin kl_t}, & j \neq p, \textit{vertices } V_j \textit{ and } V_p \\ & \textit{are connected by an edge}, \\ 0, & j \neq p, \textit{vertices } V_j \textit{ and } V_p \\ & \textit{are not connected by an edge}. \end{cases}$$

Here $k = \sqrt{\lambda}$ (the branch of the square root is fixed so that $\operatorname{Im} k \geq 0$), E_j is the set of the graph edges such that they are not loops and one of their endpoints belongs to the vertex V_j, L_j is the set of the loops attached to the vertex V_j, and finally, $C_{j,p}$ is the set of all graph edges which have both V_j and V_p as endpoints (i.e., graph edges connecting vertices V_j and V_p).

Proof. The proof is an explicit calculation.

Consider the set of functions $f^\lambda \in \operatorname{Ker}(A_{\max} - \lambda I)$. Clearly, on each edge Δ_t of the graph Γ the function $f^\lambda|_{\Delta_t}$ is of the form $a_t^+ e^{ikx} + a_t^- e^{-ikx}$, where a_t^+ and a_t^- are some constants. These constants are chosen in a way such that the function f^λ is continuous through every internal vertex of the graph.

By definition of the Weyl-Titchmarsh M-matrix (see Definition 2.10), the identity $M(\lambda)\Gamma_0 f^\lambda = \Gamma_1 f^\lambda$ has to hold for all f^λ such that $f^\lambda \in \operatorname{Ker}(A_{\max} - \lambda I)$.

Consider a vertex V_j having valence v_j and check that

$$M^j(k)\Gamma_0 f^\lambda = (\Gamma_1 f^\lambda)_j,$$

where $M^j(k)$ is the j-th row of the matrix $M(k)$ given by the formula (8). Since $\Gamma_0 f_\lambda = (f^\lambda(V_1),\, f^\lambda(V_2),\, \dots,\, f^\lambda(V_N))$, we immediately obtain

$$(9)\quad M^j(k)\Gamma_0 f_\lambda = \left[-k \sum_{\Delta_t \in E_j} \cot kl_t + 2k \sum_{\Delta_t \in L_j} \tan \frac{kl_t}{2} \right] f^\lambda(V_j) \\ + k \sum_{p: C_{j,p} \neq \varnothing} \sum_{\Delta_t \in C_{j,p}} \frac{1}{\sin kl_t} f^\lambda_{\Delta_t}(V_p),$$

where $f^\lambda_{\Delta_t} := f^\lambda|_{\Delta_t}$.

Note that in our notation $\cup_{p: C_{j,p} \neq \varnothing} C_{j,p} = E_j$. Moreover, due to continuity of the function f^λ through the vertex V_j one has: $f^\lambda(V_j) = f^\lambda_{\Delta_t}(V_j)$ for all $t : \Delta_t \in E_j$. This gives ground to the separate consideration of terms in the last sum, related to each particular edge Δ_t and connecting the vertex V_j with a vertex V_p for any admissible p (for the moment we shift our attention away from the loops attached to V_j, thus $p \neq j$). If the vertex V_j is the left endpoint of the edge $\Delta_t = [0, l_t]$ and the vertex V_p is the right one, we obtain

$$\begin{aligned}
&\frac{1}{\sin(kl_t)} f^\lambda_{\Delta_t}(V_p) - \cot(kl_t) f^\lambda_{\Delta_t}(V_j) \\
&\quad = \frac{1}{\sin(kl_t)} \left(a^+_{\Delta_t}[\exp(ikl_t) - \cos(kl_t)] + a^-_{\Delta_t}[\exp(-ikl_t) - \cos(kl_t)] \right) \\
&\qquad\qquad = i\left(a^+_{\Delta_t} - a^-_{\Delta_t}\right) = i {f^\lambda_{\Delta_t}}'(0) = i\partial_n f^\lambda_{\Delta_t}(V_j).
\end{aligned}$$

If on the other hand V_j is the right endpoint of the edge $\Delta_t = [0, l_t]$, V_p being the left one, then

$$\begin{aligned}
&\frac{1}{\sin(kl_t)} f^\lambda_{\Delta_t}(V_p) - \cot(kl_t) f^\lambda_{\Delta_t}(V_j) = \frac{1}{\sin(kl_t)} f^\lambda_{\Delta_t}(0) - \cot(kl_t) f^\lambda_{\Delta_t}(l_t) \\
&\quad = \frac{1}{\sin(kl_t)} \left(a^+_{\Delta_t}[1 - \exp(ikl_t)\cos(kl_t)] + a^-_{\Delta_t}[1 - \exp(-ikl_t)\cos(kl_t)] \right) \\
&\qquad\qquad = -ia^+_{\Delta_t}\exp(ikl_t) + a^-_{\Delta_t}\exp(-ikl_t) = -i{f^\lambda_{\Delta_t}}'(l_t) = i\partial_n f^\lambda_{\Delta_t}(V_j).
\end{aligned}$$

If, finally, a loop $\Delta = [0, l]$ is attached to the vertex V_j, the set L_j is non-empty and the sum over L_j in (9) gives us the corresponding term of the form $2k \tan \frac{kl}{2}$. Then

$$\begin{aligned}
2k \tan\frac{kl}{2} f^\lambda_\Delta(V_j) &= k\tan\frac{kl}{2}\left[f^\lambda_\Delta(0) + f^\lambda_\Delta(l)\right] \\
&= k\tan\frac{kl}{2}\left[\alpha^+_\delta(1+\exp(ikl)) + \alpha^-_\delta(1+\exp(-ikl))\right] \\
&= -ik\frac{\exp(i\frac{kl)}{2}) - \exp(i\frac{-kl_t}{2})}{\exp(i\frac{kl}{2}) + \exp(-i\frac{kl}{2})}\left[\alpha^+_\delta(1+\exp(ikl)) + \alpha^-_\delta(1+\exp(-ikl))\right] \\
&= -ik\left[\alpha^+_\delta\,(1+\exp(ikl))\,\frac{\exp(ikl)-1}{\exp(ikl)+1}\right. \\
&\left. + \alpha^-_\delta\,(1+\exp(-ikl_t))\,\frac{1-\exp(-ikl)}{1+\exp(-ikl)}\right] \\
&= ik\left[\alpha^+_\delta(1-\exp(ikl)) - \alpha^-_\delta(1-\exp(-ikl))\right] = i\left({f^\lambda_\Delta}'(0) - {f^\lambda_\Delta}'(l)\right).
\end{aligned}$$

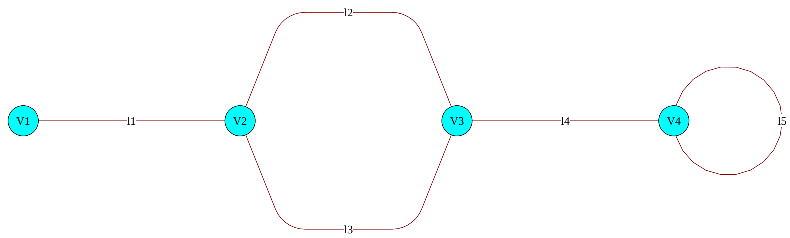
Thus we have ascertained that

$$M^j(k)\Gamma_0 f^\lambda = ik \sum \partial_n f^\lambda_{\Delta_t}(V_j) = (\Gamma_1 f^\lambda)_j,$$

where the sum in the last formula is taken over all edges coming into or out of the vertex V_j.

Since $j = 1, \ldots, N$ is arbitrary, this completes the proof. $\square$

Example 2.17. Suppose the graph Γ is



Then the Weyl-Titchmarsh M-function of Theorem 2.16 for this graph has the following form:

$$\begin{pmatrix} -k\cot(kl_1) & \frac{k}{\sin(kl_1)} & 0 & 0 \\ \frac{k}{\sin(kl_1)} & -k\sum\limits_{t=1}^{3}\cot(kl_t) & k\sum\limits_{t=2}^{3}\frac{1}{\sin(kl_t)} & 0 \\ 0 & k\sum\limits_{t=2}^{3}\frac{1}{\sin(kl_t)} & -k\sum\limits_{t=2}^{4}\cot(kl_t) & \frac{k}{\sin(kl_4)} \\ 0 & 0 & \frac{k}{\sin(kl_4)} & -k\cot(kl_4)+2k\tan(\frac{kl_5}{2}) \end{pmatrix}.$$

A few remarks are in order.

Remark 2.18. As follows from the proof given, the Weyl-Titchmarsh M-function in our setting does not depend on the directions of graph edges, i.e., the M-function stays the same if on any of the graph edges the left endpoint and the right endpoint swap places. This effect is of course well in line with what is well-known about spectra of quantum graphs, see e.g., [16, 14].

Remark 2.19. Provided that the graph has no loops, the value of M-function at zero, $M(0) := \lim_{\lambda\to 0} M(\lambda)$, turns out to be equal to the adjacency matrix C_Γ of the metric graph defined in the following way:

$$\{C_\Gamma\}_{jp} := \begin{cases} \sum_{\Delta_t\in E_j}\frac{1}{l_t}, & j=p, \\ \sum_{\Delta_t\in C_{j,p}}\frac{1}{l_t}, & j\neq p. \end{cases}$$

This adjacency matrix in the special case when all the edges have unit lengths is exactly the sum of the classical adjacency matrix A_Γ and the diagonal matrix of vertex valences, where A_Γ is defined as follows:

$$\{A_\Gamma\}_{jp} := \begin{cases} 0, & j=p, \\ \sum_{\Delta_t\in C_{j,p}} 1, & j\neq p. \end{cases}$$

Thus one might convince oneself that the information on the connectivity of the graph is actually represented in the M-function (w.r.t. the boundary triple used by us) in a very transparent way.

In the situation when matching conditions at all the graph vertices are of δ' type (and the maximal operator $A_{\max}$ and the boundary triple for is are chosen accordingly) the following result can be easily obtained along the same lines.

Theorem 2.20. *Let Γ be a finite compact metric graph. Let the operator $A_{\max}$ be the negative second derivative on the domain* (5)*. Let the boundary triple for $A_{\max}$ be chosen as $(\mathbb{C}^N,\Gamma_0,\Gamma_1)$, where N is the number of vertices of Γ and the operators Γ_0 and Γ_1 are defined by* (6)*. Then the generalized Weyl-Titchmarsh M-function is an $N\times N$ matrix* *with matrix elements given by the following formula:*

$$m_{jp} = \begin{cases} \frac{1}{k} \sum\limits_{\Delta_t \in E_j} \cot(kl_t) + 2\frac{1}{k} \sum\limits_{\Delta_t \in L_j} \cot \frac{kl_t}{2}, & j=p, \\ k \sum\limits_{\Delta_t \in C_{j,p}} \frac{1}{\sin kl_t}, & j \neq p, \text{vertices } V_j \text{ and } V_p \\ & \text{are connected by an edge}, \\ 0, & j \neq p, \text{ vertices } V_j \text{ and } V_p \\ & \text{are not connected by an edge}. \end{cases}$$

Here $k = \sqrt{\lambda}$ (the branch of the square root is fixed so that $\operatorname{Im} k \geq 0$), E_j is the set of the graph edges such that they are not loops and one of their endpoints belongs to the vertex V_j, L_j is the set of the loops attached to the vertex V_j, and finally, $C_{j,p}$ is the set of all graph edges which have both V_j and V_p as endpoints (i.e., graph edges connecting vertices V_j and V_p).

Now the following obvious statement demonstrates that the choice of maximal operators made in (2) ((5), respectively) and of boundary triples made in (3) ((6), respectively) is indeed natural for the study of spectral properties of quantum Laplacians with matching conditions of δ type (δ' type, respectively).

Lemma 2.21. *(i) A quantum Laplacian with δ-type matching conditions in the sense of Definition 2.4 is an almost solvable extension of the symmetric operator $A_{\min} = A^*_{\max}$, where $A_{\max}$ is defined by (2), w.r.t. the boundary triple $(\mathbb{C}^N, \Gamma_0, \Gamma_1)$ with Γ_0 and Γ_1 defined by (3). Its parameterizing matrix B w.r.t. this boundary triple is diagonal, $B = \operatorname{diag}(\alpha_1, \dots, \alpha_N)$, where $\{\alpha_k\}_{k=1}^N$ are the coupling constants of Definition 2.2.*
(ii) A quantum Laplacian with δ'-type matching conditions in the sense of Definition 2.4 is an almost solvable extension of the symmetric operator $A_{\min} = A^*_{\max}$, where $A_{\max}$ is defined by (5), w.r.t. the boundary triple $(\mathbb{C}^N, \Gamma_0, \Gamma_1)$ with Γ_0 and Γ_1 defined by (6). Its parameterizing matrix B w.r.t. this boundary triple is diagonal, $B = \operatorname{diag}(\alpha_1, \dots, \alpha_N)$, where $\{\alpha_k\}_{k=1}^N$ are the coupling constants of Definition 2.2.

It follows now from Theorem 2.11 out that at least *a part* of the spectrum of a quantum Laplacian with δ or δ' matching conditions can be characterized in terms of the $N \times N$ analytic matrix R-function $B - M(\lambda)$, where B is the diagonal matrix of coupling constants and $M(\lambda)$ is the corresponding Weyl-Titchmarsh M-function. Moreover, provided that the corresponding minimal operator $A_{\min}$ is simple, i.e., has no reducing self-adjoint parts, *all* of the spectrum of the quantum Laplacian can be characterized this way. It turns out that in our situation we are able to give a criterion of when this happens.

Theorem 2.22. *Suppose that Γ is a finite compact metric graph. Let the operator $A_{\max}$ be the negative second derivative on the domain (2). Let $A_{\min} = A^*_{\max}$ (the domain of $A_{\min}$ is then described by (4)). Then the symmetric operator $A_{\min}$ is simple if and only if (i) the graph Γ has no loops* and *(ii) every cycle belonging to the graph Γ has rationally independent edge lengths.*

In order to carry out the proof of this Theorem, we start with the following almost obvious Lemma.

Lemma 2.23. *In the setting of the preceding Theorem, the operator $A_{\min}$ is simple if and only if it has no real eigenvalues.*

Proof of Lemma. Suppose first that the operator $A_{\min}$ has an eigenvalue λ_0 with an associated eigenfunction ϕ_0. Then the subspace generated by ϕ_0 is invariant for $A_{\min}$ and hence reducing [3]. It follows immediately that the operator $A_{\min}$ is not simple.

On the other hand, let $A_{\min}$ have no eigenvalues and suppose that it has a reducing subspace H_0, the restriction of the operator onto which is self-adjoint. Then this subspace will be necessarily reducing for every extension of the operator $A_{\min}$, in particular, for the self-adjoint operator of Dirichlet decoupling A_D defined as the negative second derivative on the following domain:

$$D(A_D) = \Big\{ f \in \bigoplus_{j=1}^{n} W_2^2(\Delta_j) | \forall x_k,\ k = 1, \dots, 2n,\ f(x_k) = 0 \Big\}.$$

Moreover, since $A_{\min}|H_0$ is already self-adjoint by assumption, the following equality holds: $A_{\min}|H_0 = A_D|H_0$. The operator A_D is equal to the orthogonal sum over all the graph edges of regular Sturm-Liouville operators with Dirichlet boundary conditions,

$$\begin{aligned} A_D = \oplus_{j=1}^{n} A_D(\Delta_j), \quad \text{where} \quad A_D(\Delta_j) = -\frac{d^2}{dx^2} \quad \text{on} \\ D(A_D(\Delta_j)) = \{ f \in W_2^2(\Delta_j) | f(x_{2j-1}) = f(x_{2j}) = 0 \}. \end{aligned} \tag{10}$$

It follows that A_D (and thus $A_D|H_0$) has purely discrete spectrum. Therefore we arrive at the conclusion that the operator $A_{\min}|H_0$ ought to have at least one real eigenvalue, and thus the same applies to $A_{\min}$. The contradiction we have arrived to completes the proof. □

We are now all set to continue with the proof of Theorem 2.22.

Proof of Theorem. We first prove that if the graph Γ has no cycles and if every cycle belonging to it has rationally independent edge lengths, then the operator $A_{\min}$ has no real eigenvalues. Assume the opposite. Let λ_0 be its eigenvalue and ϕ_0 be the associated eigenfunction.

First, we will show that ϕ_0 cannot be supported by a tree (in the case when Γ is a tree graph, this will complete the proof). Indeed, let $\Gamma_0 \subset \Gamma$ be a tree and suppose that ϕ_0 is supported by Γ_0. Since on every edge $\Delta_j = [x_{2j-1}, x_{2j}]$ of Γ not belonging to Γ_0 the eigenfunction ϕ_0 is identically equal to zero and thus satisfies boundary conditions $\phi_0(x_{2j-1}) = \phi_0(x_{2j}) = \phi_0'(x_{2j-1}) = \phi_0'(x_{2j}) = 0$, on Γ_0 the function ϕ_0 ought to satisfy the boundary conditions (4) as long as it satisfies them on the larger graph Γ. Now pick any boundary vertex $V_k \in \partial\Gamma_0$ (i.e., a vertex having valence 1). At this vertex the function ϕ_0 together with its first derivative must therefore be zero, from where it follows immediately that the edge leading to the vertex V_k does not support ϕ_0.

The same applies to all vertices forming the graph boundary and to all the edges leading to them. As these do not support the function ϕ_0, one may then drop them altogether, which leads to a smaller graph $\tilde{\Gamma}_0 \subset \Gamma_0$, which is still a tree. The procedure of trimming the tree graph Γ_0 can be repeated as many times, as required. Since Γ_0 is a tree by assumption, after some finite number of iterations we are left with a graph with no edges.

Having established the fact that ϕ_0 cannot be supported by a tree subgraph of Γ, we immediately obtain that it must be supported by at least one cycle belonging to Γ. Indeed, if this is not so, ϕ_0 must be supported by a tree or a collection of trees leading to an immediate contradiction.

Now pick a cycle $\Gamma_1 \subset \Gamma$ which belongs to the support of ϕ_0. The function ϕ_0 has to be equal to $\sin(\sqrt{\lambda_0}x)$ on each edge $\Delta_j = [0, l_j]$ (shifting as before w.l.o.g. the edge Δ_j so that its left endpoint is at zero) forming this cycle as the solution of the differential equation $-\phi_0'' = \lambda_0\phi_0$ with zero boundary condition at the left endpoint. It is clear now that in order for the non-trivial (i.e., supported by all edges of Γ_1) function ϕ_0 to be equal to zero at all the right endpoints of the edges forming Γ_1 it is necessary for the lengths of these edges to be rationally dependent.

Repeating this argument for every cycle of Γ we arrive at the contradiction sought.

The proof of the inverse implication is by explicit construction. Indeed, in order to show that $A_{\min}$ on a graph Γ containing a cycle with rationally dependent edge lengths has an eigenvalue, one simply constructs an eigenfunction supported solely by this cycle. On every edge Δ_j is has to be equal to $\sin(\sqrt{\lambda_0}x)$. The existence of such non-trivial function is guaranteed by the fact that the edge lengths are rationally dependent. The case of a loop is treated analogously. □

Remark 2.24. In terms of the operator of Dirichlet decoupling A_D defined in (10) it is easy to see that eigenvalues of $A_{\min}$ (if any) might occur only at points $(\frac{\pi m}{l_j})^2$, where $m \in \mathbb{Z}\backslash\{0\}$, $j = 1, \dots, n$. Moreover, the eigenfunctions (if any) of $A_{\min}$ are equal to those eigenfunctions of A_D which satisfy the matching conditions for the normal derivatives in (4).

Remark 2.25. If Γ is a finite compact metric graph, the operator $A_{\max}$ is the negative second derivative on the domain (2) and the boundary triple for $A_{\max}$ is chosen as $(\mathbb{C}^N, \Gamma_0, \Gamma_1)$, where N is the number of vertices of Γ and the operators Γ_0 and Γ_1 are defined by (3), the generalized Weyl-Titchmarsh M-function has poles precisely at the points of the spectrum of the operator A_D of Dirichlet decoupling (10) provided that the graph Γ has no loops *and* the edge lengths along every cycle of Γ are rationally independent.

The elementary proof of this is based on the explicit form of the M-function, see Theorem 2.16, and the work done in the proof of Theorem 2.22.

If instead of the operator $A_{\max}$ treated by Theorem 2.22 one considers the operator of the negative second derivative on Γ defined on the domain (5), Lemma 2.23 continues to hold (with an elementary substitution of Dirichlet decoupling by the Neumann one). Unfortunately, in this situation Theorem 2.22 fails. Instead, one can prove the following modification of it.

Theorem 2.26. *Suppose that* Γ *is a finite compact metric graph. Let the operator* $A_{\max}$ *be negative second derivative on the domain* (5). *Let* $A_{\min} = A^*_{\max}$ *(the domain of* $A_{\min}$ *is then described by* (7)*). Then the symmetric operator* $A_{\min}$ *has no eigenvalues* away from zero *if and only if (i) the graph* Γ *has no loops* and *(ii) every cycle belonging to the graph* Γ *has rationally independent edge lengths.*

The *proof* follows essentially the same lines as the proof of Theorem 2.22. The only difference comes when one considers the candidate for an eigenfunction on the cyclic part of the graph. On a cycle with an even number of edges, even despite the fact that the edge lengths are chosen to be rationally independent, one can construct an eigenfunction of the operator $A_{\min}$ corresponding to the point $\lambda = 0$ by putting it to be equal to 1 on all odd edges and -1 on all even edges.

It follows that in the situation of graph Laplacians with δ' matching even the condition that the graph Γ contains no loops and the edge lengths over all cycles are rationally independent does not in general guarantee that the matrix-function $B - M(\lambda)$ carries all the spectral information about the extension A_B. Nevertheless, it still carries full information about the spectrum away from zero.

3. Trace formulae for a pair of graph Laplacians

In the present section, we apply the mathematical apparatus developed in Section 2 in order to study isospectral (i.e., having the same spectrum, counting multiplicities) quantum Laplacians defined on a finite compact metric graph Γ. In order to do so, we will assume that the graph itself is given. Moreover, we will assume that the matching conditions at all its vertices are of δ type (δ' type, respectively).

Considering a pair of such Laplacians which differ only in coupling constants defining the matching conditions we will derive an infinite series of trace formulae.

We proceed with our main theorem of this section.

Theorem 3.1. *Let Γ be a finite compact metric graph having N vertices. Let A_{B_1} and A_{B_2} be two graph Laplacians on the graph Γ with δ-type matching conditions ($B_1 = \operatorname{diag}\{\tilde\alpha_1, \dots, \tilde\alpha_N\}$ and $B_2 = \operatorname{diag}\{\alpha_1, \dots, \alpha_N\}$, where both sets $\{\tilde\alpha_m\}$ and $\{\alpha_m\}$ are the sets of coupling constants in the sense of Definition 2.2). Let the (point) spectra of these two operators (counting multiplicities) be equal, $\sigma(A_{B_1}) = \sigma(A_{B_2})$.*

Then the following infinite series of trace formulae holds:

$$\sum_{j=1}^{m} \frac{1}{j} C_{m-1}^{m-j} \operatorname{Tr}(D^j B_2^{m-j} \Gamma_N^{-m}) = 0, \quad m = 1, 2, \dots ,$$

where $D := B_1 - B_2$ and the matrix Γ_N is the matrix of valences, $\Gamma_N = \operatorname{diag}\{\gamma_1, \dots, \gamma_N\}$, γ_k being the valence of the vertex V_k.

Proof. We will use the apparatus developed in Section 2. Namely, we choose the maximal operator $A_{\max}$ as in (2), the boundary triple (3) and use the expression for the Weyl-Titchmarsh M-function of $A_{\max}$ obtained in Theorem 2.16. Then w.r.t. the chosen boundary triple the operators A_{B_1} and A_{B_2} are both almost solvable extensions of the operator $A_{\min} = A^*_{\max}$, parameterized by the matrices B_1 and B_2, respectively. Throughout we of course assume that $D \neq 0$.

We will now show that provided that the spectra of both given operators coincide, $\det(B_1 - M(\lambda))(B_2 - M(\lambda))^{-1} \equiv 1$. This is done by a Liouville-like argument. Indeed, consider two matrix-functions $M_j = (B_j - M(\lambda)) \left(\frac{\sin(\sqrt{\lambda} l_1) \sin(\sqrt{\lambda} l_2) \cdots \sin(\sqrt{\lambda} l_n)}{(\sqrt{\lambda})^N} \right)$, $j = 1, 2$. Put $F_j := \det M_j$. Then, as can be easily seen from Theorem 2.16, F_1, F_2 are two scalar analytic entire functions in $\mathbb{C}$. By Theorem 2.11 their fraction F_1/F_2 has no poles and no zeroes, since the spectra of operators A_{B_1} and A_{B_2} coincide.

Now it can be easily ascertained that both F_1 and F_2 are of normal type and of order at least not greater than 1 [18]. Then their fraction is again an entire function of order not greater than 1 [18]. Finally, by Hadamard's theorem $\frac{F_1}{F_2} = e^{a\lambda + b}$.

It remains to be seen that $a = b = 0$. This follows immediately from the asymptotic behavior of the matrix-function $M(\lambda)$ as $\lambda \to -\infty$. Namely, $M(\sqrt{\lambda}) = \sqrt{\lambda} A(\sqrt{\lambda})$ (see Theorem 2.16), where $A(\sqrt{\lambda}) \to i\Gamma_N$ as $\lambda \to -\infty$. In fact, $A(\sqrt{\lambda}) = i\Gamma_N + \bar{o}(\frac{1}{|\sqrt{\lambda}|^M})$ for any $M > 0$, which essentially makes the rest of the proof work.

We have thus obtained the following identity:

$$1 \equiv \det(B_1 - M(\lambda))(B_2 - M(\lambda))^{-1} = \det(I + D(B_2 - M(\lambda))^{-1}).$$

Since the analytic matrix-function $(B_1 - M(\lambda))(B_2 - M(\lambda))^{-1}$ tends to I as $\lambda \to -\infty$, it is can be diagonalized there. We are then able to apply the standard formula connecting determinant and trace

$$\ln \det(I + D(B_2 - M(\lambda))^{-1}) = \operatorname{Tr} \ln(I + D(B_2 - M(\lambda))^{-1}).$$

Then

$$0 = \operatorname{Tr} \ln(I + D(B_2 - M(\lambda))^{-1}) = \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{j} \operatorname{Tr} \left(D(B_2 - M)^{-1} \right)^j . \tag{11}$$

The sum is absolutely convergent since $\left\| (B_2 - M(\lambda))^{-1} \right\| \ll 1$ as $\lambda \to -\infty$, which again follows from the asymptotic behavior of $M(\lambda)$ outlined above.

Consider $\operatorname{Tr}(D(B_2 - M(\lambda))^{-1})^j$. First, again using the explicit formula for $M(\lambda)$ obtained in Theorem 2.16, we note that

$$B_2 - M(\lambda) = B_2 + \tau\Gamma_N + \bar{o}(\tau^{-M}) \quad \text{for arbitrarily large} \quad M > 0,$$

where for the sake of convenience we have put $\tau := -i\sqrt{\lambda}$ so that $\sqrt{\lambda} = i\tau$, $\tau \to +\infty$. Now from the second Hilbert identity we immediately derive

$$(B_2 - M(\lambda))^{-1} = (B_2 + \tau\Gamma_N)^{-1} + \bar{o}(\tau^{-M})$$

for an arbitrarily large positive M. Then, clearly,

$$(D(B_2 - M(\lambda))^{-1})^j = (D(B_2 + \tau\Gamma_N)^{-1})^j + \bar{o}(\tau^{-M}) \quad \text{for all} \quad j.$$

Substituting this expression into (11), we have for an arbitrary large natural M

$$0 = \sum_{j=1}^{M} \frac{(-1)^{j+1}}{j} \operatorname{Tr} \left(D(B_2 + \tau\Gamma_N)^{-1}\right)^j + \bar{o}(\tau^{-M}).$$

Note, that all the matrices D, B_2 and Γ_N are diagonal and thus commute. We will then expand $(B_2 + \tau\Gamma_N)^{-j}$ into the power series and substitute the result into the last formula. One has

$$\begin{aligned}(B_2 + \tau\Gamma_N)^{-j} &= \frac{1}{\tau^j}\left(I + \frac{\Gamma_N^{-1}B_2}{\tau}\right)^{-j}\Gamma_N^{-j}\\ &= \frac{1}{\tau^j}\sum_{i=0}^{\infty}\frac{1}{\tau^i}C_{i+j-1}^{i}\Gamma_N^{-i}B_2^i\Gamma_N^{-j}(-1)^i = \sum_{m=j}^{\infty}\frac{1}{\tau^m}C_{m-1}^{m-j}\Gamma_N^{-m}B_2^{m-j}(-1)^{m-j}\\ &= \sum_{m=j}^{M}\frac{1}{\tau^m}C_{m-1}^{m-j}\Gamma_N^{-m}B_2^{m-j}(-1)^{m-j} + \bar{o}(\tau^{-M}).\end{aligned}$$

The identity (11) then yields

$$\begin{aligned}(12)\quad 0 &\equiv \operatorname{Tr}\ln(I + D(B_2 - M(\lambda))^{-1})\\ &= -\sum_{j=1}^{M}\frac{1}{j}\sum_{m=j}^{M}\frac{1}{\tau^m}C_{m-1}^{m-j}(-1)^m \operatorname{Tr}(D^j\Gamma_N^{-m}B_2^{m-j}) + \bar{o}(\tau^{-M})\\ &= -\sum_{m=1}^{M}\frac{(-1)^m}{\tau^m}\sum_{j=1}^{m}\frac{1}{j}C_{m-1}^{m-j}\operatorname{Tr}(D^j\Gamma_N^{-m}B_2^{m-j}) + \bar{o}(\tau^{-M}).\end{aligned}$$

Identity (12) holds for any natural $M \gg 1$ and thus in the last sum each term of the form $\beta_m\tau^{-m}$ ought to be equal to zero. This immediately yields the claim. □

Leaving the analysis of full countable set of trace formulae thus obtained for a forthcoming publication, we derive a few corollaries from the last Theorem restricting consideration to just the first formula.

Corollary 3.2. *(i) Suppose that the matrices B_1 and B_2 are scalar (i.e., all the coupling constants in matching conditions coincide for the operators A_{B_1}, A_{B_2}, respectively). Then if $\sigma(A_{B_1}) = \sigma(A_{B_2})$, we obtain $B_1 = B_2$. In other words, different graph Laplacians have under the assumption made different spectra, or, to put it the other way around, the spectrum of graph Laplacian uniquely determines the coupling constants, provided that all the coupling constants are equal.*

(ii) If $B_1 = 0$ (which corresponds to the case of a graph Laplacian with standard, or Kirchhoff, matching conditions) and $B_2 \geq 0$, the corresponding operators A_{B_1} and A_{B_2} cannot have identical spectra.

(iii) If $B_1 \geq B_2$ or $B_2 \geq B_1$, the corresponding operators A_{B_1} and A_{B_2} again cannot have identical spectra. Thus under the assumption that, roughly speaking, the strength of matching condition is ordered, the spectrum of graph Laplacian uniquely determines all the coupling constants.

(iv) If all the coupling constants in the matching conditions are known to be zero but for exactly one, the spectrum of graph Laplacian uniquely determines the operator.

Proof. The first trace formula obtained in the last Theorem reads

$$\operatorname{Tr} D\Gamma_N^{-1} = 0.$$

All the assertions follow immediately from this since $\Gamma_N > 0$ and has no zero diagonal entries. □

The situation of graph Laplacian with δ' type matching conditions is similar, but somewhat different.

Theorem 3.3. *Let Γ be a finite compact metric graph having N vertices. Let A_{B_1} and A_{B_2} be two graph Laplacians on the graph Γ with δ'-type matching conditions ($B_1 = \operatorname{diag}\{\tilde{\alpha}_1, \dots, \tilde{\alpha}_N\}$ and $B_2 = \operatorname{diag}\{\alpha_1, \dots, \alpha_N\}$, where both sets $\{\tilde{\alpha}_m\}$ and $\{\alpha_m\}$ are the sets of coupling constants in the sense of Definition 2.2). Let the (point) spectra of these two operators (counting multiplicities) be equal, $\sigma(A_{B_1}) = \sigma(A_{B_2})$. Let further B_1 and B_2 be invertible.*

Then the following infinite series of trace formulae holds:

$$\sum_{j=1}^{m} \frac{1}{j} C_{m-1}^{m-j} \operatorname{Tr}(D^j B_2^{-m+j} \Gamma_n^{j+m}) = 0, \quad m = 1, 2, \dots ,$$

where $D := B_2^{-1} - B_1^{-1}$ and the matrix Γ_N is the matrix of valences, $\Gamma_N = \operatorname{diag}\{\gamma_1, \dots, \gamma_N\}$, γ_k being the valence of the vertex V_k.

A sketch of the proof. Certain minor technical differences compared to the proof of previous Theorem are due to the fact that in the case of δ' type matching conditions the diagonal of the matrix $M(\lambda)$ decays as $\lambda \to -\infty$ instead of growing there. In order to cope with this situation, one considers $B_1^{-1}(B_1 - M(\lambda))$ instead of $B_1 - M(\lambda)$ and $B_2^{-1}(B_2 - M(\lambda))$ instead of $B_2 - M(\lambda)$. This is possible since by assumption both matrices B_1 and B_2 are invertible.

Then

$$\det\left[B_1^{-1}(B_1 - M(\lambda))(B_2^{-1}(B_2 - M(\lambda)))^{-1}\right] = \det(I + DM(\lambda)(I - B_2^{-1}M(\lambda))^{-1})$$

with the argument of determinant on the right having the required form of identity plus a vanishing term. The rest of the proof is carried along the same lines as the proof of Theorem 3.1. □

Due to the requirement that B_1 and B_2 are invertible, only the following two assertions based on the first trace formula remain valid in the situation of graph Laplacians with δ' type matching conditions.

Corollary 3.4. *(i) Suppose that the matrices B_1 and B_2 are scalar (i.e., all the coupling constants in matching conditions coincide for the operators A_{B_1}, A_{B_2}, respectively). Then if $\sigma(A_{B_1}) = \sigma(A_{B_2})$, we obtain $B_1 = B_2$.*

(ii) If $B_1 \geq B_2$ or $B_2 \geq B_1$, the corresponding operators A_{B_1} and A_{B_2} cannot have identical spectra.

The corollaries derived above from Theorems 3.1 and 3.3 are formulated implicitly, i.e., they do not provide an explicit procedure of reconstruction for the matrix B based on the spectrum of the corresponding graph Laplacian A_B. Yet the approach suggested by us above can be utilized in order to obtain, at least in some special cases, such procedures. We will discuss these elsewhere as in our view this discussion is beyond the scope of the present paper.

Acknowledgments. The authors express their deep gratitude to Prof. Yurii Samoilenko and to Prof. Sergey Naboko for their constant attention to the authors' work and for fruitful discussions. The second author also thanks the School of Mathematics of Cardiff University, where parts of the work were done, and personally Prof. Marco Marletta for hospitality.

References

1. S. Avdonin and P. Kurasov, *Inverse problems for quantum trees*, Inverse Problems and Imaging **2** (2008), no. 1, 1–21.
2. S. Avdonin, P. Kurasov, and M. Nowaczyk, *Inverse problems for quantum trees* II*: Recovering matching conditions for star graphs*, Inverse Problems and Imaging **4** (2010), no. 4, 579–598.
3. M. Sh. Birman, M. Z. Solomjak, *Spectral Theory of Self-Adjoint Operators in Hilbert Space*, Mathematics and its Applications (Soviet Series), D. Reidel Publishing Co., Dordrecht, 1987.
4. V. A. Derkach and M. M. Malamud, *Generalized resolvents and the boundary value problems for Hermitian operators with gaps*, J. Funct. Anal. **95** (1991), 1–95.
5. P. Exner, *A duality between Schrödinger operators on graphs and certain Jacobi matrices*, Ann. Inst. H. Poincare **66** (1997), 359–371.
6. P. Exner, *Lattice Kronig-Penney models*, Phys. Rev. Lett. **74** (1995), 3503–3506.
7. V. I. Gorbachuk and M. L. Gorbachuk, *Boundary Value Problems for Operator Differential Equations*, Kluwer Academic Publishers, Dordrecht—Boston—London, 1991. (Russian edition: Naukova Dumka, Kiev, 1984)
8. B. Gutkin and U. Smilansky, *Can one hear the shape of a graph?* J. Phys. A **34** (2001), 6061–6068.
9. V. Kostrykin, J. Potthoff, and R. Schrader, *Heat kernels on metric graphs and a trace formula*, Adventures in Mathematical Physics, Contemporary Mathematics, vol. 447, Amer. Math. Soc., 2007, pp. 175–198.
10. V. Kostrykin and R. Schrader, *Kirchhoff's rule for quantum wires*, J. Phys. A **32** (1999), 595–630.
11. T. Kottos and U. Smilansky, *Periodic orbit theory and spectral statistics for quantum graphs*, Ann. Physics **274** (1999), 76–124.
12. A. N. Kochubei, *On extension of symmetric operators and symmetric binary relations*, Mat. Zametki **17** (1975), 41–48. (Russian); English transl. Math. Notes **17** (1975), 25–28.
13. A. N. Kochubei, *Characteristic functions of symmetric operators and their extensions*, Izv. Akad. Nauk Arm. SSR, Ser. Mat. **15** (1980), no. 3, 219–232. (Russian)
14. P. Kuchment, *Quantum graphs: an introduction and a brief survey*, Analysis on Graphs and its Applications, Proc. Symp. Pure. Math., Amer. Math. Soc., 2008, pp. 291–314.
15. P. Kurasov and M. Nowaczyk, *Inverse spectral problem for quantum graphs*, J. Phys. A: Mathematical and General **38** (2005), 4901–4915; correction: J. Phys. A: Mathematical and General **39** (2006), 993.
16. P. Kurasov, *Graph Laplacians and topology*, Arkiv för Matematik **46** (2008), 95–111.
17. P. Kurasov, *Inverse problem for Aharonov-Bohm rings*, Math. Proc. Cambridge Philosophical Society **148** (2010), 331–362.
18. B. Ya. Levin, *Lectures on Entire Functions*, Translations of Mathematical Monographs, vol. 150, Amer. Math. Soc., Providence, RI, 1996.
19. J. P. Roth, *Le spectre du Laplacien sur un graphe*, Théorie du Potentiel (Orsay, 1983), Lecture Notes in Math., vol. 1096, Springer, Berlin, 1984, pp. 521–539. (French)
20. V. Ryzhov, *Functional model of a class of nonselfadjoint extensions of symmetric operators*, Operator Theory: Adv. Appl. **174** (2007), 117–158.

Institute of Mathematics, National Academy of Science of Ukraine, 3 Tereshchenkivs'ka, Kyiv, 01601, Ukraine
E-mail address: julija.ershova@gmail.com

Department of Higher Mathematics and Mathematical Physics, St. Petersburg State University, 1 Ulianovskaya, St. Petersburg, St. Peterhoff, 198504, Russia
E-mail address: alexander.v.kiselev@gmail.com

Received 22/08/2012