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GEOMETRIC PROPERTIES OF QUANTUM GRAPHS AND VERTEX SCATTERING MATRICES

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Abstract. Differential operators on metric graphs are investigated. It is proven that vertex matching (boundary) conditions can be successfully parameterized by the vertex scattering matrix. Two new families of matching conditions are investigated: hyperplanar Neumann and hyperplanar Dirichlet conditions. Using trace formula it is shown that the spectrum of the Laplace operator determines certain geometric properties of the underlying graph.

Keywords: scattering theory, quantum graphs, matching (boundary) conditions.

Mathematics Subject Classification: 35R30, 47A10, 81U40, 81Q10.

1. INTRODUCTION

Quantum graphs is a rapidly developing area of research in mathematical physics with important prospective applications in nanotechnology and modern engineering. By the term quantum graph we understand an ordinary differential operator on a metric graph coupled via *matching*, or also called *boundary*, conditions at the vertices. These operators are studied in the current article using methods of spectral analysis of self-adjoint operators concentrating on the relations between their spectral properties and the geometric structure of the underlying graph. To calculate an eigenfunction of such an operator one needs to solve first a certain ordinary differential equation on every edge separately, but solutions on different edges are connected through the matching conditions and thus the spectral problem on the whole graph reminds us about partial differential equations. From the mathematical point of view quantum graphs are precisely the area of research, where ordinary and partial differential equations meet each other, in other words where methods developed originally for ordinary and for partial differential equations are used simultaneously.

In a series of papers [14–16] it was proven that in the case of a compact graph the spectrum determines the Euler characteristic of the underlying graph as well as the number of connected components in the special case of so-called standard matching conditions at the vertices. The main analytic tool developed there is the celebrated trace formula proposed independently by J.-P. Roth [18] and T. Kottos and U. Smilansky [12]. The aim of the current article is to develop this approach further in order to include more general matching conditions at the vertices. Therefore the first part of the article is devoted to the discussion of the most general matching conditions that can be imposed at the vertices. In order to simplify our presentation only a star graph is considered in Section 2. During these studies we found it useful to use a new parameterization of matching conditions by the matrix S, which is the vertex scattering matrix for the energy parameter equal to 1. The advantage of this parameterization is that it is unique and that the parameter has a clear physical interpretation. This parameterization is a slight modification of M. Harmer's parameterization [9], which is unique as well, but the parameter used there has not been given a clear interpretation so far. The set of matching conditions leading to energy independent vertex scattering matrices is characterized and relations with known parameterizations due to M. Harmer and P. Kuchment are established [9, 13]. We propose to call such matching conditions *non-resonant*.

In Section 3 we discuss which families of matching conditions reflect the connectivity of the graph in a proper way. All such matching conditions are classified. We select two particular families of matching conditions: *Hyperplanar Neumann* and *Hyperplanar Dirichlet* conditions (see formulas (3.1) and (3.2)). The first family is a direct generalization of standard boundary conditions. The second family generalizes the so-called δ'_s boundary conditions considered *e.g.* by P. Exner, P. Kuchment, S. Fulling and J. Wilson in [4, 6, 13].

In Sections 4 and 5 arbitrary finite compact graphs are considered. The corresponding Laplace operator is defined on the domain of functions satisfying matching conditions at the vertices that are properly connecting and lead to energy independent vertex scattering matrices, *i. e.* are non-resonant. These operators have a pure discrete spectrum consisting of eigenvalues tending to $+\infty$. Following methods developed in [12, 15, 16, 18] we prove the trace formula for arbitrary non-resonant matching conditions. This formula connects the set of eigenvalues (*the energy spectrum*) with the set of periodic orbits on the metric graph (*the length spectrum*). In addition it includes so-called spectral and algebraic multiplicities of the eigenvalue zero. The first number is just the multiplicity of the eigenvalue zero whereas the second number is the multiplicity of the eigenvalue given by the characteristic equation used in the derivation of the trace formula. These numbers may be different and Section 5 is devoted to explicit calculation of these numbers for the special case of hyperplanar Neumann and Dirichlet conditions at the vertices. Both the spectral and algebraic multiplicities of the eigenvalue zero can be calculated from the spectrum. The first number is trivially given as the multiplicity of $\lambda = 0$, the second number is determined by the asymptotics of the spectrum (see [14]). After accomplishing our studies we have learned about paper [6], where the relation between algebraic and spectral multiplicities and the index of the Laplacian were obtained. We believe that our approach provides a new insight to the problem, since in our calculations one can see straightforwardly a connection between the multiplicities of the eigenvalue zero and the cycles in a geometric graph.

2. MATCHING CONDITIONS VIA THE VERTEX SCATTERING MATRIX

2.1. PARAMETERIZATION OF THE MATCHING CONDITIONS

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

Consider a star graph Γ with v semi–infinite nodes $\Delta_j = [0, \infty)$, $j = 1, 2, \ldots, v$, connected at one vertex V. Let $\mathcal{H} \equiv L^2(\Gamma) = \oplus_{n=1}^{v} L^2([0, \infty))$ be the Hilbert space of square integrable functions on Γ and let L be the Laplace operator

$$L = \bigoplus_{j=1}^{v} \left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} \right). \tag{2.1}$$

This differential expression does not determine the self-adjoint operator uniquely. Consider the maximal operator $L_{\max}$ associated with (2.1) which is defined on the domain $\mathrm{Dom}\,(L_{\max}) = \oplus_{j=1}^{v} W_2^2((0, \infty))$, where W_2^2 denotes the Sobolev space. All self-adjoint operators associated with (2.1) can now be obtained as restrictions of the maximal operator by imposing certain matching conditions connecting boundary values of the functions at the vertex V. This procedure is equivalent to describing all self-adjoint extensions of the minimal (symmetric) operator $L_{\min} = L_{\max}^*$, which can be carried out using von Neumann theory. Let $\partial_n \psi$ denote the normal derivative in the direction outside the vertex, then $\boldsymbol{\psi}(V), \partial_n \boldsymbol{\psi}(V)$ denote the vectors of boundary values for ψ and its normal derivative at the vertex V. Thus the following Theorem can be proven.

Theorem 2.1. *The family of all self-adjoint extensions of the minimal operator $L_{\min}$ can uniquely be parameterized by an arbitrary $v \times v$ unitary matrix S, so that the operator $L(S)$ is the restriction of $L_{\max} = L_{\min}^*$ to the set of functions satisfying the matching conditions*

$$i(S - I)\boldsymbol{\psi}(V) = (S + I)\partial_n \boldsymbol{\psi}(V). \tag{2.2}$$

We propose to use this parameterization of the matching conditions instead of Harmer's one (see [9]). The advantage of the current parameterization is that it is unique and the parameter S has a clear physical meaning: it is equal to the value of the vertex scattering matrix at $k = 1$.

The research on matching (or boundary) conditions and self-adjoint operators on graphs goes back to 80-ies with works by B. Pavlov and N. Gerasimenko [7] and P. Exner and P. Šeba [5] and is described in detail by P. Kuchment [13]. An efficient description of such boundary conditions using two quadratic matrices was obtained in 1999 by V. Kostrykin and R. Schrader [10] with the disadvantage of not being unique. In 2004 P. Kuchment has noticed that this parameterization can be made unique by using certain orthogonal projections [13]. Harmer's parameterization proposed already in 2000 [9] is also unique, but no clear physical interpretation for the unitary parameter is given.

2.2. MATRIX S AND THE VERTEX SCATTERING MATRIX

Any solution to the differential equation

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

can be written in the basis of incoming and outgoing waves as follows

$$\psi_j(x) = b_j e^{-ikx} + a_j e^{ikx}, \quad x \in \Delta_j, \quad k > 0. \tag{2.3}$$

The relation between the vectors of waves' amplitudes $\boldsymbol{a}$ and $\boldsymbol{b}$ is given by the vertex scattering matrix $S_v(k)$: $\boldsymbol{a} = S_v(k)\boldsymbol{b}$. The scattering matrix has to be chosen so that the function in (2.3) satisfies the matching conditions (2.2) at the vertex. The values of the functions and of normal derivatives at the vertex are:

$$\boldsymbol{\psi}(V) = \boldsymbol{b} + \boldsymbol{a} = (I + S_v(k))\boldsymbol{b} \text{ and } \partial_n\boldsymbol{\psi}(V) = -ik\boldsymbol{b} + ik\boldsymbol{a} = ik(-I + S_v(k))\boldsymbol{b}.$$

After substitution into equation (2.2) we obtain

$$S_v(k) = \frac{k(S+I) + (S-I)}{k(S+I) - (S-I)}. \tag{2.4}$$

One can show that the matrix appearing in the denominator is invertible, so $S_v(k)$ is well defined. From equation (2.4) we can easily observe that $S_v(1) = S$. Using the spectral representation for the unitary matrix $S = \sum_{j=1}^{v} e^{i\theta_j}\langle\cdot,\phi_j\rangle\phi_j$ the scattering matrix can be written as

$$\begin{aligned} S_v(k)\psi &= \sum_{j=1}^{v} \frac{k(e^{i\theta_j}+1) + (e^{i\theta_j}-1)}{k(e^{i\theta_j}+1) - (e^{i\theta_j}-1)}\langle\psi,\phi_j\rangle\phi_j = \\ &= \sum_{j:\theta_j=\pi}(-1)\langle\psi,\phi_j\rangle\phi_j + \sum_{j:\theta_j=0} 1\langle\psi,\phi_j\rangle\phi_j + \\ &\quad + \sum_{j:\theta_j\neq\pi,0} \frac{k(e^{i\theta_j}+1) + (e^{i\theta_j}-1)}{k(e^{i\theta_j}+1) - (e^{i\theta_j}-1)}\langle\psi,\phi_j\rangle\phi_j. \end{aligned} \tag{2.5}$$

We see once more time that the scattering matrix $S_v(k)$ is unitary for every real value of k. The scattering matrix $S_v(k)$ does not depend on the energy if and only if S has just eigenvalues ± 1, *i. e.* the subspaces

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

span $\mathbb{C}^v$: $N_{+1} \oplus N_{-1} = \mathbb{C}^v$. The corresponding matching conditions will be called **non-resonant** underlying the fact that the vertex scattering matrices have no singularities in this case. Following [13] all non-resonant matching conditions can be written in the form

$$P_{N_1}\partial_n\boldsymbol{\psi}(V) = 0, \;\; P_{N_{-1}}\boldsymbol{\psi}(V) = 0, \tag{2.6}$$

where P_N denotes the orthogonal projector on the subspace N.

3. VERTEX SCATTERING MATRIX AND CONNECTIVITY

3.1. PROPERLY CONNECTING MATCHING CONDITIONS

In this section we will discuss which additional properties (beyond unitarity) of the matrix S should be required so that the matching conditions correspond to the situation where the vertex V does connect together all edges. We required so far that the matching conditions involve the boundary values at the vertex V, but it might happen that the end points can be divided into two nonintersecting classes $V = V_1 \cup V_2, V_1 \cap V_2 = \emptyset$ so that matching conditions (2.2) connect together the boundary values at V_1 and V_2 separately. Such matching conditions do not correspond to the vertex V but rather to two (independent) vertices V_1 and V_2. In other words, if the vertex V can be chopped into two vertices so that the matching conditions are preserved, then such conditions are not properly connecting and should be excluded from our consideration if no further special reason exists. This problem has been discussed in details in [17] and in [11], but uniqueness of our new parameterization makes this discussion much more transparent.

Summing up the following definition appears natural

Definition 3.1. Matching conditions are called **properly connecting** if and only if the vertex cannot be divided into two (or more) vertices so that the matching conditions connect together only boundary values belonging to each of the new vertices.

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

Proposition 3.2. *Matching conditions* (2.2) *are properly connecting if and only if the unitary matrix S is irreducible, i.e. S cannot be turned into block-diagonal form by permutation of the basis vectors.*

Proof. If the matching conditions connect together just the boundary values associated with two nonintersecting sets $V_1, V_2,\ V_1 \cup V_2 = V$, then the corresponding matrix S is reducible. It is also clear that if S is reducible, then the set V can be divided into V_1 and V_2, so that the matching conditions connect separately boundary values from these two subsets. $\square$

3.2. CONNECTIVITY OF NON-RESONANT CONDITIONS

Whether or not non-resonant matching conditions are properly connecting can be characterized using the notions of coordinate subspaces and perpendicularity. The first one is a straightforward generalization of coordinate planes in $\mathbb{R}^3$, the second one is closely connected to but is different from orthogonality.

Definition 3.3. A subspace $K \subset \mathbb{C}^n$ is called a **coordinate subspace** if and only if it is spanned by a certain number of basic vectors from the standard basis in $\mathbb{C}^n$, but does not coincide with $\mathbb{C}^n$. We say that a subspace N is **perpendicular** to a subspace K if and only if $P_K N \subset N \cap K$ and $P_N K \subset N \cap K$, where P denotes the orthogonal projection.

Theorem 3.4. *The non-resonant matching conditions described by the matrix S are properly connecting if and only if $N_{-1}(S)$ is not perpendicular to any coordinate subspace.*

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

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

The non-resonant matching conditions are *not* properly connecting for example in the following two cases:

1. Dirichlet conditions at the vertex: $N_1 = \{0\}, N_{-1} = \mathbb{C}^v$.
2. Neumann conditions at the vertex: $N_1 = \mathbb{C}^v, N_{-1} = \{0\}$.

These matching conditions correspond to the case where the vertex V is maximally decomposed.

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

1. **Hyperplanar Neumann conditions**:
$$\begin{cases} \boldsymbol{\psi}(V) \parallel \boldsymbol{w}, \\ \partial_n \boldsymbol{\psi}(V) \perp \boldsymbol{w}, \end{cases} \tag{3.1}$$
where $\boldsymbol{w} \in \mathbb{C}^v$ is any vector with all components different from zero;
2. **Hyperplanar Dirichlet conditions**:
$$\begin{cases} \boldsymbol{\psi}(V) \perp \boldsymbol{u}, \\ \partial_n \boldsymbol{\psi}(V) \parallel \boldsymbol{u}, \end{cases} \tag{3.2}$$
where $\boldsymbol{u} \in \mathbb{C}^v$ is any vector with all components different from zero.

These matching conditions correspond to the case where one of the subspaces N_1 or N_{-1} is one dimensional and is spanned by either $\boldsymbol{w}$ or $\boldsymbol{u}$. Since all components of these vectors are different from zero, the corresponding subspaces are not perpendicular to any coordinate subspace. It is then clear that both hyperplanar Neumann and Dirichlet conditions are non-resonant properly connecting matching conditions. In the case of a vertex formed by one end point hyperplanar Neumann and Dirichlet conditions reduce to classical Neumann and Dirichlet conditions respectively, which motivates their name. The word "hyperplanar" reflects the fact that one of the corresponding subspaces N_1 or N_{-1} has codimension 1. Note that if the vector $\boldsymbol{w}$ is chosen equal to $(1, 1, \ldots, 1)$, then hyperplanar Neumann conditions coincide with the standard matching (boundary) conditions (which are sometimes called Neumann conditions in the literature). At the same time if the vector $\boldsymbol{u}$ is equal to $(1, 1, \ldots, 1)$, then hyperplanar Dirichlet conditions become the so-called δ_s' matching conditions. Introducing these new families of matching conditions allows us to enlarge the number of parameters and to fit new physical systems.

4. TRACE FORMULA FOR NON-RESONANT MATCHING CONDITIONS

The trace formula connects together the spectrum of a quantum graph and the set of periodic orbits for the underlying metric graph. It was first suggested independently by J.-P. Roth and B. Gutkin, T. Kottos and U. Smilansky [8, 12, 18]. In 2005 the authors provided a rigorous proof of this formula [16] discovering important relations with the Euler characteristic of the graph [14]. For considered there standard matching conditions it was used that the vertex scattering matrix S_v is independent of the energy. Thus one can easily generalize the proof of the trace formula for any Laplace operator on a metric graph with any properly connecting non-resonant matching conditions. The only difficulty appears when one tries to calculate the spectral and algebraic multiplicities of the zero eigenvalue.

Let L be the Laplace operator defined by (2.1) on a connected metric graph Γ formed by N edges joined at M vertices V_m of valence v_m. The set of all edges will be denoted by $E = \{\Delta_1, \ldots, \Delta_N\}$, $\Delta_j = [x_{2j-1}, x_{2j}]$ and the set of vertices $V = \{V_1, \ldots V_M\}$ is a partition of the set of endpoints $\{x_j\}_{j=1}^{2N}$. The Euler characteristic of a graph will be denoted by $\chi = M - N$. The maximal Laplace operator $L_{\max}$ is defined by (2.1) on the Sobolev space $W_2^2(\Gamma \setminus V)$. Consider the vectors of boundary values and normal derivatives associated with each vertex V_m, *i. e.* v_m-dimensional vectors $\boldsymbol{\psi}(V_m)$ and $\partial_n \boldsymbol{\psi}(V_m)$ with components $\psi(x_j)$ and $\partial_n \psi(x_j)$ respectively for $x_j \in V_m$. The Theorem 2.1 for star graphs can now be easily generalized for arbitrary graphs.

Theorem 4.1. *The family of self-adjoint restrictions of $L_{\max}$ can be described by matching conditions connecting the boundary values $\boldsymbol{\psi} = (\boldsymbol{\psi}(V_1), \ldots, \boldsymbol{\psi}(V_M))$ and $\partial_n \boldsymbol{\psi} = (\partial_n \boldsymbol{\psi}(V_1), \ldots, \partial_n \boldsymbol{\psi}(V_M))$*

$$i(S - I)\boldsymbol{\psi} = (S + I)\partial_n \boldsymbol{\psi}, \tag{4.1}$$

where S is an arbitrary $2N \times 2N$ unitary matrix. These matching conditions are properly connecting if and only if they have the form

$$i(S^m - I)\boldsymbol{\psi}(V_m) = (S^m + I)\partial_n \boldsymbol{\psi}(V_m), \quad m = 1, \ldots, M, \tag{4.2}$$

where S^m are unitary $v_m \times v_m$ irreducible matrices. The properly connecting non-resonant matching conditions are given by:

$$P_{N_1^m} \partial_n \boldsymbol{\psi}(V_m) = 0, \;\; P_{N_{-1}^m} \boldsymbol{\psi}(V_m) = 0, \quad m = 1, 2, \ldots, M, \tag{4.3}$$

where N_1^m and N_{-1}^m are not perpendicular to any coordinate subspace in $\mathbb{C}^{v_m}$.

In what follows only the case of non-resonant matching conditions will be considered. The corresponding operator will be denoted by $L(\Gamma)$. Every eigenfunction $\psi(x,k)$, corresponding to the energy $\lambda = k^2$ is a solution to the differential equation

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2}\psi(x,k) = k^2\psi(x,k), \quad x \in [x_{2j-1}, x_{2j}], \tag{4.4}$$

on the edges, satisfying the matching conditions (4.2) at the vertices. For $k \neq 0$ every solution to (4.4) can be written using either a basis of incoming or one of outgoing waves (see [8, 12] and later [16])

$$\begin{aligned} \psi(x,k) &= a_{2j-1}e^{ik|x-x_{2j-1}|} + a_{2j}e^{ik|x-x_{2j}|}, \qquad x \in \Delta_j = [x_{2j-1}, x_{2j}]. \\ &= b_{2j-1}e^{-ik|x-x_{2j-1}|} + b_{2j}e^{-ik|x-x_{2j}|} \end{aligned} \tag{4.5}$$

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

$$\boldsymbol{b} = \mathbf{S}_e\boldsymbol{a}, \text{ where } \mathbf{S}_e(k) = \left(\begin{array}{c|c|c} S_e^1 & 0 & \cdots \\ \hline 0 & S_e^2 & \cdots \\ \hline \vdots & \vdots & \ddots \end{array}\right), \; S_e^j(k) = \begin{pmatrix} 0 & e^{ikd_j} \\ e^{ikd_j} & 0 \end{pmatrix}, \tag{4.6}$$

where d_j denotes the length of the edge Δ_j. The amplitudes are also related by the vertex scattering matrices, which are obtained from the requirement that $\psi(x,k)$ satisfies (4.2). For that purpose it is convenient to use the following representation for the solution to (4.4), using only amplitudes related to every end point x_i from V_m

$$\psi(x,k) = a_je^{ik|x-x_j|} + b_je^{-ik|x-x_j|}$$

and the corresponding vectors of amplitudes $\boldsymbol{a}^m, \boldsymbol{b}^m \in \mathbb{C}^{v_m}$. Then for all $k \neq 0$ the matching conditions (4.3) are equivalent to

$$\begin{cases} P_{N_{-1}^m}(\boldsymbol{a}^m + \boldsymbol{b}^m) = 0, \\ P_{N_1^m}(\boldsymbol{a}^m - \boldsymbol{b}^m) = 0. \end{cases} \tag{4.7}$$

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

$$\boldsymbol{a}^m = S_v^m\boldsymbol{b}^m, \quad m = 1, 2, ..., M. \tag{4.8}$$

The last equation implies that

$$\begin{pmatrix} \boldsymbol{a}^1 \\ \boldsymbol{a}^2 \\ \vdots \\ \boldsymbol{a}^M \end{pmatrix} = \mathbf{S}_v \begin{pmatrix} \boldsymbol{b}^1 \\ \boldsymbol{b}^2 \\ \vdots \\ \boldsymbol{b}^M \end{pmatrix}, \text{ with } \mathbf{S}_v = \left(\begin{array}{c|c|c} S_v^1 & 0 & \cdots \\ \hline 0 & S_v^2 & \cdots \\ \hline \vdots & \vdots & \ddots \end{array}\right). \tag{4.9}$$

Note that the matrices $\mathbf{S}_e(k)$ and $\mathbf{S}_v$ possess the block representations (4.6) and (4.9) in different bases. Clearly a vector $\boldsymbol{a}$ determines an eigenfunction of the Laplace operator if and only if the following equation holds

$$\det(\mathbf{S}(k) - I) = 0, \text{ where } \mathbf{S}(k) = \mathbf{S}_v \mathbf{S}_e(k). \tag{4.10}$$

Equation (4.10) determines the spectrum of $L(\Gamma)$ with correct multiplicities for all nonzero values of the energy, but the multiplicity $m_a(0)$ of the zero eigenvalue given by this equation, *i. e.* the dimension of $\ker(\mathbf{S}(k) - I)$, 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.*

Theorem 4.2 (Trace formula)**.** *Let Γ be a compact finite metric graph with the total length $\mathcal{L}$ and let L be the Laplace operator in $L_2(\Gamma)$ determined by properly connecting non-resonant matching conditions at the vertices. Then the following two trace formulae establish the relation between the spectrum $\{k_n^2\}$ of $L(\Gamma)$ and the set $\mathcal{P}$ of closed paths on the metric graph Γ*

$$\begin{aligned} u(k) \equiv 2m_s(0)\delta(k) + \sum_{k_n \neq 0} (\delta(k-k_n) + \delta(k+k_n)) = \\ = (2m_s(0) - m_a(0))\delta(k) + \frac{\mathcal{L}}{\pi} + \\ + \frac{1}{2\pi} \sum_{p\in\mathcal{P}} l(\mathrm{prim}\,(p)) \big(S(p)e^{ikl(p)} + S^*(p)e^{-ikl(p)}\big), \end{aligned} \tag{4.11}$$

and

$$\begin{aligned} \sqrt{2\pi}\hat{u}(l) = 2m_s(0) + \sum_{k_n\neq 0} 2\cos k_n l = \\ = 2m_s(0) - m_a(0) + 2\mathcal{L}\delta(l) + \\ + \sum_{p\in\mathcal{P}} l(\mathrm{prim}\,(p)) \Big(S(p)\delta(l - l(p)) + S^*(p)\delta(l + l(p))\Big), \end{aligned} \tag{4.12}$$

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

The proof follows step by step the proof of Theorem 2 from [14], see also [3].

This theorem shows, that both spectral and algebraic multiplicities of the eigenvalue zero may be calculated from the spectrum of the Laplace operator: the spectral multiplicity is trivially equal to the multiplicity of $\lambda = 0$, the algebraic multiplicity is determined by the spectral asymptotics (see [14, 15]). Therefore in the following section we are going to study spectral and algebraic multiplicites for different types of matching conditions.

5. SPECTRAL AND ALGEBRAIC MULTIPLICITIES

5.1. ON THE GROUND STATE EIGENFUNCTION

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

Lemma 5.1. *Let L be the Laplace operator on a metric graph defined on the functions satisfying non-resonant matching conditions. Then every eigenfunction corresponding to $\lambda = 0$ is a piecewise constant function.*

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

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

Consider the corresponding Dirichlet integral

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

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

$$\begin{aligned}\int_\Gamma |\psi'(x)|^2 dx &= -\int_\Gamma \psi''(x)\overline{\psi(x)} dx - \sum_{x_j} \partial_n \psi(x_j)\overline{\psi(x_j)} = \\ &= -\sum_{m=1}^M \sum_{x_j \in V_m} \partial_n \psi(x_j)\overline{\psi(x_j)} = -\sum_{m=1}^M \langle \partial_n \boldsymbol{\psi}(V_m), \boldsymbol{\psi}(V_m)\rangle_{\mathbb{C}^{v_m}} = 0,\end{aligned}$$

since for every V_m the vectors $\boldsymbol{\psi}(V_m)$ and $\partial_n \boldsymbol{\psi}(V_m)$ belong to two mutually orthogonal subspaces. Hence $\alpha_j = 0$, $j = 1, 2, \ldots, N$ and every eigenfunction corresponding to $\lambda = 0$ is piecewise constant. □

5.2. HYPERPLANAR NEUMANN MATCHING CONDITIONS

Let us calculate the spectral and algebraic multiplicities of the eigenvalue zero for connected graphs. We assume that at every vertex V_m the matching conditions are given by formula (3.1) with $\boldsymbol{w}$ substituted with $\boldsymbol{w}^m$. Consider a closed path $p_{(x_{l_1}, x_{l_2}, \ldots, x_{l_{2n(p)}})}$ of the discrete length $n(p)$. Every such path can be characterized by the sequence of endpoints $(x_{l_1}, x_{l_2}, \ldots, x_{l_{2n(p)}})$ that the path comes across and that every pair $(x_{l_{2k}}, x_{l_{2k+1}})$ (as well as $(x_{l_{2n(p)}}, x_{l_1})$) belongs to a certain vertex on the path, while elements of every pair $(x_{l_{2k-1}}, x_{l_{2k}})$ are endpoints of a certain edge on the path. Every endpoint x_j is associated with the unique component of some vector $\boldsymbol{w}^m$, so that $w(x_j)$ is uniquely defined.

Definition 5.2. Hyperplanar Neumann matching conditions are called **coherent** if and only if for every nonintersecting closed path $p_{(x_{l_1},x_{l_2},\ldots,x_{l_{2n(p)}})}$ it holds

$$\prod_{k=1}^{n(p)} w(x_{l_{2k}}) = \prod_{k=0}^{n(p)-1} w(x_{l_{2k+1}}). \tag{5.1}$$

For coherent conditions there is a nontrivial eigenfunction corresponding to $\lambda = 0$.

Lemma 5.3. *The spectral multiplicity $m_s^N(0)$ of the eigenvalue $\lambda = 0$ of the Laplace operator with hyperplanar Neumann matching conditions on a connected graph Γ is equal to one if the conditions are coherent and to zero otherwise.*

Proof. Let ψ be any zero energy eigenfunction. Lemma 5.1 implies that ψ is piecewise constant and therefore the second condition in (3.1) is trivially satisfied.

Choose any edge Δ_j and let $\psi(x)|_{x\in\Delta_j} = c$, where c is a certain complex number. Let V_l be one of the two vertices that Δ_j connects. Then the values of ψ on all the other edges connected at V_l can be calculated since one of the coordinates of the vector $\boldsymbol{\psi}(V_l)$ is known and the vector is proportional to $\boldsymbol{w}^l$. In this way the values of the function ψ on all neighboring edges may be calculated. In the coherent case this procedure can be continued until we get a unique function on Γ. The set of such functions can be parameterized by c and therefore the spectral multiplicity $m_s^N(0)$ is equal to one.

In the case of non coherent conditions we are going to get a contradiction considering the edges from the path p for which (5.1) does not hold. It follows that ψ is identically equal to zero and hence $m_s^N(0) = 0$ in this case. □

Now to calculate the algebraic multiplicity it is enough to determine the difference $m_a^N(0) - m_s^N(0)$.

Lemma 5.4. *Consider the Laplace operator on a connected graph Γ defined by the hyperplanar Neumann matching conditions at the vertices. Then it holds*

$$m_a^N(0) - m_s^N(0) = \begin{cases} g, & \text{if the matching conditions are coherent,} \\ g-1, & \text{if the matching conditions are not coherent,} \end{cases} \tag{5.2}$$

where $g = N - M + 1$ is the number of cycles in Γ.

Proof. The algebraic multiplicity of $\lambda = 0$ is equal to the dimension of the space of solutions to the system of equations (4.7) and (4.6) with

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

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

$$\begin{cases} a_j + a_{j-(-1)^j} = \alpha_m w^m(x_j), \quad x_j \in V_m \\ \sum_{x_j\in V_m} (a_j - a_{j-(-1)^j})\overline{w^m(x_j)} = 0 \end{cases} \qquad m = 1, \ldots, M. \tag{5.3}$$

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

The equations on s_j are just the same as the equations determining the eigenfunction ψ, the corresponding dimension $m_s^N(0)$ has already been calculated in Lemma 5.3.

The equations on f_j can be written as a "balance of flows" (see equations (3.11) and (3.12) in [14]):

$$\sum_{j, x_{2j} \in V_m} f_j \, \overline{w^m(x_{2j})} = \sum_{j, x_{2j-1} \in V_m} f_j \, \overline{w^m(x_{2j-1})}. \tag{5.4}$$

1) Assume that the matching conditions are coherent, *i.e.* (5.1) holds for any cycle in the graph.

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

An arbitrary graph Γ can be turned into a tree T by deleting exactly $g = N - M + 1$ edges. Let us denote those edges by $\Delta_1, \Delta_2, \ldots, \Delta_g$. For every such edge denote by C_j the shortest closed path on $T \cup \Delta_j$. Then there exists a flow $\boldsymbol{\varphi}^j$ supported just by C_j. It will be convenient to normalize it so that $\varphi^j|_{\Delta_j} = 1$. Assume that $\boldsymbol{f}$ is any solution of (5.4) on a graph Γ and let us consider

$$\boldsymbol{f} - \sum_{j=1}^{g} f_j \, \boldsymbol{\varphi}^j, \tag{5.5}$$

which is supported by T. Since the function satisfies (4.7), it is zero and it follows that every $\boldsymbol{f}$ can be written as a combination of $\boldsymbol{\varphi}^j$ which of course are linearly independent. Thus $m_a^N(0) - m_s^N(0) = g$ for coherent matching conditions.

2) Consider now the case of incoherent matching conditions. Without loss of generality we may assume that already matching conditions on the cycle C_1 are incoherent. Consider any other cycle C_j, $j = 2, 3, \ldots, g$. If the matching conditions on this cycle are coherent then as before there exists a nonzero flow $\boldsymbol{\varphi}^j$ supported by C_j. If the matching conditions on C_j are incoherent then there exists a flow $\boldsymbol{\varphi}^j$ supported by $T \cup C_1 \cup C_j$. This can easily be seen in the case where C_1 and C_j have no common points. Let us denote by s_{1j} the shortest path connecting these two cycles. Then the flow $\boldsymbol{\varphi}^j$ can be constructed as a combination of the flows on the open cycles C_1 and C_j and on the path s_{1j}. The case where the two cycles have common points is similar. Thus we have $g - 1$ linearly independent flows $\boldsymbol{\varphi}^2, \ldots, \boldsymbol{\varphi}^g$, which can be normalized by the condition $\boldsymbol{\varphi}^j|_{\Delta_j} = 1$.

As before for arbitrary flow $\boldsymbol{f}$ satisfying the matching conditions on Γ consider

$$\boldsymbol{f} - \sum_{j=2}^{g} f_j \, \boldsymbol{\varphi}^j. \tag{5.6}$$

By construction the support of every such flow belongs to $T \cup C_1$. It is clear that the flow vanishes everywhere outside C_1 (this can be proven as in the coherent case) but the matching conditions for C_1 are incoherent. Hence this flow is identically equal to zero. It follows that any flow $\boldsymbol{f}$ can be written as a linear combination of $\boldsymbol{\varphi}^j$, $j = 2, \ldots, g$, which are obviously linearly independent. Hence $m_a^N(0) - m_s^N(0) = g - 1$ for incoherent matching conditions. $\square$

Two previous lemmas imply the following theorem (see Theorem 20 and Corollary 15 in [6]).

Theorem 5.5. *Consider the Laplace operator on a connected metric graph Γ defined by hyperplanar Neumann matching conditions. Let $m_s^N(0)$, respectively $m_a^N(0)$, denote the spectral, respectively algebraic, multiplicities of the eigenvalue zero. Then it holds*

$$2m_s^N(0) - m_a^N(0) = \chi, \tag{5.7}$$

where $\chi = 1 - g$ is the Euler characteristic of the graph Γ.

5.3. HYPERPLANAR DIRICHLET MATCHING CONDITIONS

Similar analysis can be done for hyperplanar Dirichlet matching conditions and we are going to present the results on spectral and algebraic multiplicities in this case. Instead of calculating directly the number of linearly independent solutions to corresponding systems of equations, we are going to use already obtained multiplicities for hyperplanar Neumann matching conditions and make a one-to-one mapping between the solutions.

Theorem 5.6. *Consider the Laplace operator on a connected metric graph Γ defined by hyperplanar Dirichlet matching conditions. Let $m_s^D(0)$, respectively $m_a^D(0)$, denote the spectral, respectively algebraic, multiplicities of the eigenvalue zero. Then it holds*

$$2m_s^D(0) - m_a^D(0) = -\chi, \tag{5.8}$$

where $\chi = 1 - g$ is the Euler characteristic of the graph Γ.

Proof. For hyperplanar Dirichlet matching conditions each subspace N_{-1}^m is spanned by one vector $\boldsymbol{u}^m = (u_1, \ldots, u_{v_m})$ with all components different from zero. To calculate the spectral and algebraic multiplicities one has to perform the same steps as for hyperplanar Neumann matching conditions arriving at the following system (instead of (5.3)):

$$\begin{cases} \tilde{a}_j - \tilde{a}_{j-(-1)^j} = \beta_m u^m(x_j), & x_j \in V_m \\ \sum_{x_j \in V_m} (\tilde{a}_j + \tilde{a}_{j-(-1)^j}) \overline{u^m(x_j)} = 0 \end{cases} \qquad m = 1, \ldots, M, \tag{5.9}$$

where $\tilde{a}_j$ denote the corresponding amplitudes in representation (4.5).

Consider the following mapping:

$$\begin{cases} a_k = (-1)^k \tilde{a}_k, \\ w(x_k) = (-1)^{k+1} u(x_k), \end{cases} \tag{5.10}$$

which establishes a one-to-one correspondence between solutions to (5.3) and (5.9). As a result of mapping (5.10) we get the following relations between the spectral $m_s^D(0)$ and algebraic $m_a^D(0)$ multiplicities of the zero eigenvalue for hyperplanar Dirichlet matching conditions:

$$\begin{aligned} m_s^D(0) &= m_a^N(0) - m_s^N(0), \\ m_a^D(0) - m_s^D(0) &= m_s^N(0). \end{aligned} \tag{5.11}$$

Therefore $2m_s^D(0) - m_a^D(0) = -\chi$. $\square$

Formulas (4.11) and (4.12) show that the knowledge of the spectrum allows one to calculate $m_s(0)$ and $2m_s(0) - m_a(0)$ following ideas of [14] and [15]. This means that the algebraic multiplicity $m_a(0)$ is determined by the spectrum of the Laplacian. In particular the Euler characteristics is determined by the spectrum for both hyperplanar Neumann and Dirichlet matching conditions without knowing a priori which class of conditions occurs, provided $\chi \leq -2$. It might be important to study also the case where hyperplanar Dirichelt and Nuemann matching conditions are introduced simultaneously at different vertices. In this way new classes of isospectral quantum graphs may be obtained (see [1,2], where the first such examples are constructed using representation theory).

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