Quantum Graphs I. Some Basic Structures

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1   Introduction

We use the name "quantum graph" for a graph considered as a one-dimensional singular variety and equipped with a self-adjoint differential (in some cases pseudo-differential) operator ("Hamiltonian"). There are manifold reasons for studying quantum graphs. They naturally arise as simplified (due to reduced dimension) models in mathematics, physics, chemistry, and engineering (nanotechnology), when one considers propagation of waves of different nature (electromagnetic, acoustic, etc.) through a "mesoscopic" quasi-one-dimensional system that looks like a thin neighborhood of a graph. One can mention in particular the free-electron theory of conjugated molecules in chemistry, quantum chaos, quantum wires, dynamical systems, photonic crystals, scattering theory, and a variety of other applications. We will not discuss any details of these origins of quantum graphs, referring the reader instead to [54] for a recent survey and literature. The problems addressed in the quantum graph theory include justifications of quantum graphs as approximations for more realistic (and complex) models of waves in complex structures, analysis of various direct and inverse spectral problems (coming from quantum chaos, optics, scattering theory, and other areas), and many others. This paper does not contain discussion of most of these topics and the reader is referred to the survey [54] and to papers presented in the current issue of Waves in Random Media for more information and references.

In this paper we address some basic notions and results concerning quantum graphs and their spectra. While the spectral theory of combinatorial graphs is a rather well established topic (e.g., books [12, 21, 22, 23, 62] and

references therein), the corresponding theory of quantum graphs is just developing (e.g., examples of such studies in [3, 5, 6, 7, 8, 9, 15], [16] - [20], [25], [29] - [35], [39], [43] - [49], [56] - [58], [64, 65, 70, 74, 79, 80] and further references in [54]).

Let us describe the contents of the following sections. Section 2 is devoted to introducing basic notions of a metric and quantum graph. The largest Section 3 deals with the detailed description of self-adjoint vertex conditions for second derivative Hamiltonians on quantum graphs. Treatment of infinite graphs required some restrictions on their structure. The vertex conditions are written in the form that enables one to describe easily the quadratic forms of the operators and to classify all permutation-invariant conditions. Section 4 is devoted to relations between quantum and combinatorial spectral problems that will be seen as especially helpful in the planned next part [56] of this article. The paper ends with short sections containing remarks and acknowledgments.

The reader should note that this paper is of the survey nature and hence most of the results are not new (although the exposition might differ from other sources). Some references are provided throughout the text, albeit the bibliography was not intended to be comprehensive, and the reader is directed to the surveys [54, 55] for more detailed bibliography. It was initially planned to address several new issues in this paper, among which one can mention above all a more detailed spectral treatment of infinite graphs (bounds for generalized eigenfunctions, Schnol's theorems, periodic graphs, some gap opening effects, and discussion of bound states), however the article size limitations resulted in the necessity of postponing those to the next paper [56]. For the same reason, the author has also restricted considerations to the case of the second derivative Hamiltonian only, while one can extend these without much of a difficulty to more general Schrödinger operators (e.g., [46]). This, as well as some other topics will be dealt with elsewhere. So, the paper is planned to serve as an introduction that could be useful while reading other articles of this issue of Waves in Random Media, and also as the first part of [56].

2   Quantum graphs

As it was mentioned in the introduction, we will be dealing with *quantum graphs*, i.e. graphs considered as one-dimensional singular varieties rather

than purely combinatorial objects and correspondingly equipped with differential (or sometimes "pseudo-differential") operators (Hamiltonians) rather than discrete Laplace operators.

2.1 Metric graphs

A **graph** Γ consists of a finite or countably infinite set of vertices $V = \{v_i\}$ and a set $E = \{e_j\}$ of edges connecting the vertices. Each edge e can be identified with a pair (v_i, v_k) of vertices. Although in many quantum graph considerations directions of the edges are irrelevant and could be fixed arbitrarily (we will not need them in this paper), it is sometimes more convenient to have them assigned. Loops and multiple edges between vertices are allowed, so we avoid saying that E is a subset of $V \times V$. We also denote by E_v the set of all edges incident to the vertex v (i.e., containing v). It is assumed that the degree (valence) $d_v = |E_v|$ of any vertex v is finite and positive. We hence exclude vertices with no edges coming in or going out. This is natural, since for the quantum graph purposes such vertices are irrelevant.

So far all our definitions have dealt with a combinatorial graph. Here we introduce a notion that makes Γ a topological and metric object.

Definition 1. *A graph Γ is said to be a **metric graph** (sometimes the notion of a **weighted graph** is used instead), if its each edge e is assigned a positive length $l_e \in (0, \infty]$ (notice that edges of infinite length are allowed).*

Having the length assigned, an edge e will be identified with a finite or infinite segment $[0, l_e]$ of the real line with the natural coordinate x_e along it. In most cases we will drop the subscript in the coordinate and call it x, which should not lead to any confusion. This enables one to interpret the graph Γ as a topological space (simplicial complex) that is the union of all edges where the ends corresponding to the same vertex are identified.

The reader should note that we do not assume the graph to be embedded in any way into an Euclidean space. In some applications such a natural embedding does exist (e.g., in modeling quantum wire circuits or photonic crystals), and in such cases the coordinate along an edge is usually the arc length. In some other applications (e.g., in quantum chaos) the graph is not assumed to be embedded.

Graph Γ can be equipped with a natural metric. If a sequence of edges $\{e_j\}_{j=1}^M$ forms a path, its length is defined as $\sum l_j$. For two vertices v and w, the distance $\rho(v, w)$ is defined as the minimal path length between them.

Since along each edge the distance is determined by the coordinate x, it is easy to define the distance $\rho(x, y)$ between two points x, y of the graph that are not necessarily vertices. We leave this to the reader.

We also impose some additional conditions:

• **Condition A.** The "infinite" ends of infinite edges are assumed to have degree one. Thus, the graph can be thought of as a graph with finite length edges with additional infinite "leads" or "ends" going to infinity attached to some vertices. This situation arises naturally for instance in scattering theory. Since these "infinite" vertices will never be treated as regular vertices (in fact, in this paper such vertices will not arise at all), one can just assume that each infinite edge is a ray with a single vertex.

• **Condition B.** When studying infinite graphs, we will impose some assumptions that will imply in particular that for any positive number r and any vertex v there is only a finite set of vertices w at a distance less than r from v. In particular, the distance between any two distinct vertices is positive, and there are no finite length paths of infinitely many edges. This obviously matters only for infinite graphs (i.e., graphs with infinitely many edges) and is automatically satisfied for the class of infinite metric graphs that will be introduced later.

So, now one can imagine the graph Γ as a one-dimensional simplicial complex, each $1D$ simplex (edge) of which is equipped with a smooth structure, with singularities arising at junctions (vertices) (see Fig. 1).

The reader should notice that now the points of the graph are not only its vertices, but all intermediate points x on the edges as well. One can define in the natural way the Lebesgue measure dx on the graph. Functions $f(x)$ on Γ are defined along the edges (rather than at the vertices as in discrete models). Having this and the measure, one can define in a natural way some function spaces on the graph:

Definition 2. *1. The space $L_2(\Gamma)$ on Γ consists of functions that are measurable and square integrable on each edge e and such that*

$$\|f\|^2_{L_2(\Gamma)} = \sum_{e \in E} \|f\|^2_{L_2(e)} < \infty.$$

In other words, $L_2(\Gamma)$ is the orthogonal direct sum of spaces $L_2(e)$.

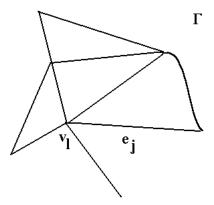*2. The Sobolev space $H^1(\Gamma)$ consists of all **continuous** functions on Γ*

Figure 1: Graph Γ.

that belong to $H^1(e)$ for each edge e and such that

$$\sum_{e \in E} \|f\|_{H^1(e)}^2 < \infty.$$

Note that continuity in the definition of the Sobolev space means that the functions on all edges adjacent to a vertex v assume the same value at v.

There seem to be no natural definition of Sobolev spaces $H^k(\Gamma)$ of order k higher than 1, since boundary conditions at vertices depend on the Hamiltonian (see details later on in this paper).

The last step that is needed to finish the definition of a quantum graph is to introduce a self-adjoint (differential or more general) operator (Hamiltonian) on Γ. This is done in the next section.

2.2 Operators

The operators of interest in the simplest cases are:
the negative second derivative

$$f(x) \rightarrow -\frac{d^2 f}{dx^2}, \tag{1}$$

a more general Schrödinger operator

$$f(x) \rightarrow -\frac{d^2 f}{dx^2} + V(x)f(x), \tag{2}$$

or a magnetic Schrödinger operator

$$f(x) \rightarrow \left(\frac{1}{i}\frac{d}{dx} - A(x)\right)^2 + V(x)f(x). \tag{3}$$

Here x denotes the coordinate x_e along the edge e.

Higher order differential and even pseudo-differential operators arise as well (see, e.g. the survey [54] and references therein). We, however, will concentrate here on second order differential operators, and for simplicity of exposition specifically on (1). In order for the definition of the operators to be complete, one needs to describe their domains. The natural conditions require that f belongs to the Sobolev space $H^2(e)$ on each edge e. One also clearly needs to impose boundary value conditions at the vertices. These will be studied in the next section.

3   Boundary conditions and self-adjointness

We will discuss now the boundary conditions one would like to add to the differential expression (1) in order to create a self-adjoint operator.

3.1   Graphs with finitely many edges

In this section we will consider **finite graphs** only. This means that we assume that the number of edges $|E|$ is finite (and hence the number of vertices $|V|$ is finite as well, since we assume all vertex degrees to be positive). Notice that edges are still allowed to have infinite length.

We will concentrate on local (or vertex) boundary conditions only, i.e. on those that involve the values at a single vertex only at a time. It is possible to describe all the vertex conditions that make (1) a self-adjoint operator (see [43, 41] and a partial description in [34]). This is done by either using the standard von Neumann theory of extensions of symmetric operators (as for instance described in [1]), or by its more recent version that amounts to finding Lagrangian planes with respect to the complex symplectic boundary form that corresponds to the maximal operator (see for instance

[3, 26, 27, 28, 41, 42, 43, 69, 71] for the accounts of this approach that goes back at least as far as [63], where it was presented without use of words "symplectic" or "Lagrangian"). One of the most standard types of such boundary conditions is the "Kirchhoff" condition:

$$\begin{cases} f(x) \text{ is continuous on } \Gamma \\ \text{and} \\ \text{at each vertex } v \text{ one has } \sum_{e \in E_v} \frac{df}{dx_e}(v) = 0 \end{cases}, \qquad (4)$$

where the sum is taken over all edges e containing the vertex v. Here the **derivatives are taken in the directions away from the vertex (we will call these "outgoing directions")**, the agreement we will adhere to in all cases when these conditions are involved. Sometimes (4) is called the Neumann condition. It is clear that at "loose ends" (vertices of degree 1) it turns into the actual Neumann condition. Besides, as the Neumann boundary condition for Laplace operator, it is natural. Namely, as it will be seen a little bit later, the domain of the quadratic form of the corresponding operator does not require any conditions on a function besides being in $H^1(\Gamma)$ (and hence continuous). It is also useful to note that under the boundary conditions (4) one can eliminate all vertices of degree 2, connecting the adjacent edges into one smooth edge.

There are many other plausible vertex conditions (some of which will be discussed later), and the question we want to address now is how to describe all of those that lead to a self-adjoint realization of the second derivative along the edges.

Since we are interested in local vertex conditions only, it is clear that it is sufficient to address the problem of self-adjointness for a single junction of d edges at a vertex v. Because along each edge our operator acts as the (negative) second derivative, one needs to establish two conditions per an edge, and hence at each vertex the number of conditions must coincide with the degree d of the vertex. For functions in H^2 on each edge, the conditions may involve only the boundary values of the function and its derivative. Then the most general form of such (homogeneous) condition is

$$A_v F + B_v F' = 0. \qquad (5)$$

Here A_v and B_v are $d \times d$ matrices, F is the vector $(f_1(v), ..., f_d(v))^t$ of the vertex values of the function along each edge, and $F' = (f_1'(v), ..., f_d'(v))^t$

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is the vector of the vertex values of the derivatives taken along the edges in the outgoing directions at the vertex v, as we have agreed before. The rank of the $d \times 2d$ matrix (A_v, B_v) must be equal to d (i.e., maximal) in order to ensure the correct number of independent conditions. When this would not lead to confusion, we will drop the subscript v in these matrix notations, remembering that the matrices depend on the vertex (in fact, for non-homogeneous graphs they essentially have no other choice).

Now one is interested in the necessary and sufficient conditions on matrices A and B in (5) that would guarantee self-adjointness of the resulting operator. All such conditions were completely described in [43] (see also the earlier paper [33] for some special cases and [41, 48]for an alternative consideration that represents the boundary conditions in terms of vertex scattering matrices). We will formulate the corresponding result in the form taken from [43].

Theorem 3. *[43] Let Γ be a metric graph with finitely many edges. Consider the operator $\mathcal{H}$ acting as $-\dfrac{d^2}{dx_e^2}$ on each edge e, with the domain consisting of functions that belong to $H^2(e)$ on each edge e and satisfy the boundary conditions (5) at each vertex. Here $\{A_v,\, B_v \mid v \in V\}$ is a collection of matrices of sizes $d_v \times d_v$ such that each matrix $(A_v\, B_v)$ has the maximal rank. In order for $\mathcal{H}$ to be self-adjoint, the following condition at each vertex is necessary and sufficient:*

$$\text{the matrix } A_v B_v^* \text{ is self-adjoint.} \tag{6}$$

The proof of this theorem can be found in [43].

We would like now to describe the quadratic form of the operator $\mathcal{H}$ corresponding to the (negative) second derivative along each edge, with self-adjoint vertex conditions (5) (we assume in particular that (6) is satisfied). In order to do so, we will establish first a couple of simple auxiliary statements.

In the next two lemmas and a corollary we will consider matrices A and B as in (8). Since we will be concerned with a single vertex here, we will drop for this time the subscripts v in A_v, B_v, and d_v. Let us introduce some notations. We will denote by P and P_1 the orthogonal projections in $\mathbb{C}^d$ onto the kernels $K = \ker B$ and $K_1 = \ker B^*$ respectively. The complementary orthogonal projectors onto the ranges $R = R(B^*)$ and $R_1 = R(B)$ are denoted by Q and Q_1 (here $R(M)$ denotes the range of a matrix M).

Lemma 4. *Let $d \times d$ matrices A and B be such that the $d \times 2d$ matrix $(A\,B)$ has maximal rank and AB^* is self-adjoint. Then*

1. *Operator A maps the range R of B^* into the range R_1 of B.*

2. *The mapping $P_1AP : K \to K_1$ is invertible.*

3. *The mapping $Q_1BQ : R \to R_1$ is invertible (we denote its inverse by $B^{(-1)}$).*

4. *The matrix $B^{(-1)}AQ$ is self-adjoint.*

Proof. Self-adjointness of AB^* means $AB^* = BA^*$, which immediately implies the first statement of the lemma. In order to prove the next two statements, let us decompose the space $\mathbb{C}^d$ into the orthogonal sum $R_1 \oplus K_1$ and $\mathbb{C}^{2d}$ into $\mathbb{C}^d \oplus \mathbb{C}^d = R \oplus K \oplus R \oplus K$. Then the matrix $(A\,B)$ representing an operator from $\mathbb{C}^{2d}$ into $\mathbb{C}^d$ can be written in a 2×4 block-matrix form with respect to these decompositions. Taking into account the definitions of the subspaces $R, R_1, K,$ and K_1 and the already proven first statement of the lemma, this leads to the block matrix

$$(A\,B) = \begin{pmatrix} A_{11} & A_{12} & B_{11} & 0 \\ 0 & A_{22} & 0 & 0 \end{pmatrix}. \tag{7}$$

For this matrix to have maximal rank, the entry A_{22} must be invertible, which gives the second statement of the lemma. The third statement is obvious, since the matrix B_{11} is square and has no kernel (which has already been eliminated and included into K). Immediate calculation shows that self-adjointness of AB^* means that the square matrix $A_{11}B_{11}^*$ is self-adjoint, i.e. $A_{11}B_{11}^* = B_{11}A_{11}^*$. Since invertibility of B_{11} has already been established (recall that its inverse is denoted by $B^{(-1)}$), we can multiply the previous equality by appropriate inverse matrices from both sides to get

$$B^{(-1)}A_{11} = A_{11}^* B^{(-1)*}.$$

This means that the matrix $B^{(-1)}A_{11}$ is self-adjoint and hence the last statement of the lemma is proven.

Corollary 5. *Let the conditions of Lemma 4 be satisfied. Then the boundary condition (5) $AF + BF' = 0$ is equivalent to the pair of conditions $PF = 0$*

and $LQF + QF' = 0$, where P, as before, is the orthogonal projection onto the kernel of matrix B, Q is the complementary projector, and L is the self-adjoint operator $B^{(-1)}A$.

Proof. We will employ the notations used in the preceding lemma. It is clear that (5) is equivalent to the pair of conditions $P_1 AF + P_1 BF' = 0$ and $Q_1 AF + Q_1 BF' = 0$. The lemma now shows that the first of them can be rewritten as $A_{22}PF = 0$, which by the second statement of the lemma is equivalent to $PF = 0$. The second equality, again by the lemma, can be equivalently rewritten as $AQF + B_{11}QF' = 0$, or after inverting B_{11} as $LQF + QF' = 0$, which finishes the proof of the corollary.

We can now re-phrase general self-adjoint boundary conditions in a fashion that is sometimes more convenient (for instance, for describing the quadratic form of the operator).

Theorem 6. *All self-adjoint realizations $\mathcal{H}$ of the negative second derivative on Γ with vertex boundary conditions can be described as follows. For every vertex v there are an orthogonal projector P_v in $\mathbb{C}^{d_v}$ with the complementary projector $Q_v = Id - P_v$ and a self-adjoint operator L_v in $Q_v \mathbb{C}^{d_v}$. The functions f from the domain $D(\mathcal{H}) \subset \bigoplus_e H^2(e)$ of $\mathcal{H}$ are described by the following conditions at each (finite) vertex v:*

$$P_v F(v) = 0$$
$$Q_v F'(v) + L_v Q_v F(v) = 0. \tag{8}$$

In terms of the matrices A_v and B_v of Theorem 3, P_v is the orthogonal projector onto the kernel of B_v and $L_v = B_v^{(-1)} A_v$ (where $B_v^{(-1)}$ has been defined previously).

Proof. Adopting the definitions of P_v and L_v provided in the theorem, one can see that the theorem's statement is just a simple consequence of Theorem 3, Lemma 4, and Corollary 5 combined.

Remark 7. *1. In view of the first condition in (8), the second one can be equivalently written as $Q_v F'(v) + L_v F(v) = 0$.*

2. Conditions (8) say that the P_v-component of the vertex values $F(v)$ of f must be zero (kind of a "Dirichlet" part), while the P_v-part of the derivatives $F'(v)$ is unrestricted. The Q_v-part of the derivatives $F'(v)$ is determined by the Q_v-part of the function $F(v)$.

We will need also the following well known trace estimate that we prove here for completeness.

Lemma 8. *Let $f \in H^1[0, a]$, then*

$$|f(0)|^2 \leq \frac{2}{l}\|f\|^2_{L_2[0,a]} + l\|f'\|^2_{L_2[0,a]} \tag{9}$$

for any $l \leq a$.

Proof. Due to H^1-continuity of both sides of the inequality, it is sufficient to prove it for smooth functions. Start with the representation

$$f(0) = f(x) - \int_0^x f'(t)dt, \ x \in [0, l] \tag{10}$$

and estimate by Cauchy-Schwartz inequality

$$|\int_0^x f'(t)dt|^2 \leq \|f'\|^2_{L_2[0,a]}\|\chi_{[0,x]}\|^2_{L_2[0,a]} = x\|f'\|^2_{L_2[0,a]}.$$

This implies

$$\|\int_0^x f'(t)dt\|^2_{L_2[0,l]} \leq \|f'\|^2_{L_2[0,a]} \int_0^l x\,dx = \frac{l^2}{2}\|f'\|^2_{L_2[0,a]}.$$

Now taking $L_2[0, l]$-norms in both sides of (10) and using triangle inequality and $(a + b)^2 \leq 2a^2 + 2b^2$, we get the estimate

$$|f(0)|^2 l \leq 2\|f\|^2_{L_2[0,a]} + l^2\|f'\|^2_{L_2[0,a]},$$

which implies the statement of the lemma.

We are ready now for the description of the quadratic form of the operator $\mathcal{H}$ on a finite graph Γ. Let as before Γ be a metric graph with finitely many vertices. The selfadjoint operator $\mathcal{H}$ in $L_2(\Gamma)$ acts as $-\dfrac{d^2}{dx^2}$ along each edge, with the domain consisting of all functions $f(x)$ on Γ that belong to the

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Sobolev space $H^2(e)$ on each edge e and satisfy at each vertex v conditions (8):

$$P_v F(v) = 0$$
$$Q_v F'(v) + L_v Q_v F(v) = 0. \tag{11}$$

Here, as always $F(v) = (f_1(v), ... f_{d_v}(v))^t$ is the column vector of the values of the function f at v that it attains when v is approached from different edges e_j adjacent to v, $F'(v)$ is the column vector of the corresponding outgoing derivatives at v, the $d_v \times d_v$-matrix P_v is an orthogonal projector and L_v is a self-adjoint operator in the kernel $Q_v \mathbb{C}^{d_v}$ of P_v.

Theorem 9. *The quadratic form h of $\mathcal{H}$ is given as*

$$
\begin{aligned}
h[f, f] &= \sum_{e \in E} \int_e |\tfrac{df}{dx}|^2 dx - \sum_{v \in V} \sum_{e_j, e_k \in E_v} (L_v)_{jk} \, f_j(v) \overline{f_k(v)} \\
&= \sum_{e \in E} \int_e |\tfrac{df}{dx}|^2 dx - \sum_{v \in V} \langle L_v F, F \rangle,
\end{aligned} \tag{12}
$$

where $\langle , \rangle$ denotes the standard hermitian inner product in $\mathbb{C}^d$. The domain of this form consists of all functions f that belong to $H^1(e)$ on each edge e and satisfy at each vertex v the condition $P_v F = 0$.

Correspondingly, the sesqui-linear form of $\mathcal{H}$ is:

$$
h[f, g] = \sum_{e \in E} \int_e \frac{df}{dx} \frac{\overline{dg}}{dx} dx - \sum_{v \in V} \langle L_v F, G \rangle. \tag{13}
$$

Proof. Notice that Lemma 8 shows that (12) with the domain described in the theorem defines a closed quadratic form. It hence corresponds to a self-adjoint operator $\mathcal{M}$ in $L_2(\Gamma)$. Integration by parts in (13) against smooth functions g that vanish in a neighborhood of each vertex shows that on its domain $\mathcal{M}$ acts as the negative second derivative along each edge. So, the remaining task is to show that its domain $D(\mathcal{M})$ consists of all functions that belong to H^2 on each edge and satisfy the vertex conditions (8). This would imply that $\mathcal{M} = \mathcal{H}$. So, let us assume $f \in D(\mathcal{M})$. In particular, $f \in \bigoplus_e H^1(e)$. It is the standard conclusion then that $f \in H^2(e)$ for any edge e (we leave to the reader to fill in the details, see also the section concerning infinite graphs). We need now to verify that f satisfies the vertex conditions (8). The condition $P_v F(v) = 0$ does not need to be checked, since

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it is satisfied on the domain of the quadratic form. Integration by parts transforms (13) into

$$-\sum_{e \in E} \int_e \frac{d^2 f}{dx^2} \overline{g} dx - \sum_{v \in V} \langle F' + L_v F, G \rangle. \tag{14}$$

The second term must vanish for any g in the domain of the quadratic form. Taking into account that then $G(v)$ can be an arbitrary vector such that $P_v G(v) = 0$, this means that for each v the equality

$$Q_v F'(v) + Q_v L_v F(v) = 0 \tag{15}$$

needs to be satisfied, where Q_v is the complementary projection to P_v. This gives us the needed conditions (8) for the function f.

It is also easy to check in a similar fashion that as soon as a function f belongs to H^2 on each edge and satisfies (8), it belongs to the domain of $\mathcal{M}$. This proves that $\mathcal{M}$ in fact coincides with the previously described operator $\mathcal{H}$. The proof is hence completed.

Corollary 10. *The operator $\mathcal{H}$ is bounded from below. Moreover, let $S = \max\limits_v \{\|L_v\|\}$, then*

$$\mathcal{H} \geq -C \, Id, \tag{16}$$

where

$$C = 4S \max\{2S, \max\limits_e \{l_e^{(-1)}\}\}.$$

Proof. One can choose $l := \min\{l_e\}$ in (9) applied to any edge e. Then, due to (9) one has:

$$\sum_v \langle L_v F(v), F(v) \rangle \leq S \sum_v |F(v)|^2$$
$$\leq 2S \left(\tfrac{2}{l} \|f\|^2_{L_2(\Gamma)} + l \|f'\|^2_{L_2(\Gamma)} \right). \tag{17}$$

If now $2lS \leq 1$, then (17) and the definition of the quadratic form h show that the statement of the Corollary holds.

Although one can (and often needs to) consider quantum graphs with more general Hamiltonian operators (e.g. Schrödinger operators with electric and magnetic potentials, operators of higher order, pseudo-differential operators, etc.), **for the purpose of this article only** we adopt the following definition:

Definition 11. *A **quantum graph** is a metric graph equipped with the operator $\mathcal{H}$ that acts as the negative second order derivative along edges and is accompanied by the vertex conditions (8).*

3.2 Examples of boundary conditions

In this section we take a brief look from the prospective of the previous section at some examples of vertex conditions and corresponding operators. The reader can find more examples in [34, 43, 59].

3.2.1 δ-type conditions

are defined as follows:

$$
\begin{cases}
f(x) \text{ is continuous on } \Gamma \\
\text{and} \\
\text{at each vertex } v, \ \sum_{e \in E_v} \frac{df}{dx_e}(v) = \alpha_v f(v)
\end{cases}
. \tag{18}
$$

Here α_v are some fixed numbers. One can recognize these conditions as an analog of conditions one obtains from a Schrödinger operator on the line with a δ potential, which explains the name. In this case the conditions can be obviously written in the form (5) with

$$
A_v = \begin{pmatrix}
1 & -1 & 0 & .... & 0 \\
0 & 1 & -1 & ... & 0 \\
... & ... & 0 & 1 & -1 \\
-\alpha_v & 0 & ... & 0 & 0
\end{pmatrix}
$$

and

$$
B_v = \begin{pmatrix}
0 & 0 & .... & 0 \\
... & ... & ... & ... \\
0 & 0 & .... & 0 \\
1 & 1 & ... & 1
\end{pmatrix}.
$$

Since

$$
A_v B_v^* = \begin{pmatrix}
0 & 0 & .... & 0 & 0 \\
... & ... & ... & ... & ... \\
0 & 0 & ... & 0 & -\alpha_v
\end{pmatrix},
$$

the self-adjointness condition (6) is satisfied if and only if α is real.

In order to write the vertex conditions in the form (8), one needs to find the orthogonal projection P_v onto the kernel of B_v and the self-adjoint operator $L_v = B_v^{(-1)} A_v Q_v$. It is a simple exercise to find that Q_v is the one-dimensional projector onto the space of vectors with equal coordinates and correspondingly the range of P_v is spanned by the vectors r_k, $k = 1, ..., d_v - 1$, where r_k has 1 as the k-th component, -1 as the next one, and zeros otherwise. Then a straightforward calculation shows that L_v is the multiplication by the number $-\dfrac{\alpha_v}{d_v}$. In particular, the description of the projector P_v shows that the quadratic form of the operator $\mathcal{H}$ is defined on functions that are continuous throughout all vertices (i.e., $F(v) = (f(v), ..., f(v))^t$) and hence belong to $H^1(\Gamma)$. The form is computed as follows:

$$
\begin{aligned}
&\sum_{e \in E} \int_e |\tfrac{df}{dx}|^2 dx - \sum_{v \in V} \langle L_v F, F \rangle \\
&= \sum_{e \in E} \int_e |\tfrac{df}{dx}|^2 dx + \sum_{v \in V} \alpha_v |f(v)|^2.
\end{aligned}
\tag{19}
$$

It is obvious from (19) that the operator is non-negative if $\alpha_v \geq 0$ for all vertices v.

3.2.2 Neumann (Kirchhoff) conditions

These conditions (4) that have already been mentioned, represent probably the most common case of the δ-type conditions (18) when $\alpha_l = 0$, i.e.

$$
\begin{cases}
f(x) \text{ is continuous on } \Gamma \\
\text{and} \\
\text{at each vertex } v, \ \sum_{e \in E_v} \tfrac{df}{dx_e}(v) = 0
\end{cases}
\tag{20}
$$

The discussion above shows that the quadratic form of $\mathcal{H}$ is

$$
\sum_{e \in E} \int_e |\frac{df}{dx}|^2 dx,
\tag{21}
$$

defined on $H^1(\Gamma)$, and the operator is non-negative

3.2.3 Conditions of δ'-type

These conditions remind the δ-type ones, but with the roles of functions and the derivatives are reversed at each vertex (see also [2]). In order to describe

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them, let us introduce the notation f_v for the restriction of a function f onto the edge e. Then the conditions at each vertex v can be described as follows:

$$\left\{ \begin{array}{l} \text{The value of the derivative } \frac{df_e}{dx_e}(v) \text{ is the same for all edges } e \in E_v \\ \text{and} \\ \sum_{e \in E_v} f_e(v) = \alpha_v \frac{df}{dx}(v) \end{array} \right. .$$

$$(22)$$

Here, as before, $\frac{df_e}{dx_e}(v)$ is the derivative in the outgoing direction at the vertex v. It is clear that in comparison with δ-type case the matrices A_v and B_v are switched:

$$B_v = \begin{pmatrix} 1 & -1 & 0 & .... & 0 \\ 0 & 1 & -1 & ... & 0 \\ ... & ... & 0 & 1 & -1 \\ -\alpha_v & 0 & ... & 0 & 0 \end{pmatrix}$$

and

$$A_v = \begin{pmatrix} 0 & 0 & .... & 0 \\ ... & ... & ... & ... \\ 0 & 0 & .... & 0 \\ 1 & 1 & ... & 1 \end{pmatrix}.$$

Since

$$A_v B_v^* = \begin{pmatrix} 0 & 0 & .... & 0 & 0 \\ ... & ... & ... & ... & ... \\ 0 & 0 & ... & 0 & -\alpha_v \end{pmatrix},$$

the self-adjointness condition (6) is satisfied again for real α_v only.

Consider first the case when $\alpha_v = 0$ for some vertex v. Then the kernel of B_v consists of all vector with equal coordinates, and the projector Q_v projects orthogonally onto the subspace of vectors that have the sum of their coordinates equal to zero. On this subspace operator A_v is equal to zero, and hence $L_v = 0$. This leads to no non-integral contribution to the quadratic form coming from the vertex v. In particular, if $\alpha_v = 0$ for all vertices, we get the quadratic form

$$\sum_e \int_e |\frac{df}{dx}|^2 dx$$

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with the domain consisting of all functions from $\bigoplus\limits_{e} H^1(e)$ that have at each vertex the sum of the vertex values along all entering edges equal to zero. In this case the operator is clearly non-negative.

Let us look at the case when for a vertex v the value α_v is non-zero. In this case the operator B_v is invertible and so $P_v = 0, Q_v = Id$. It is not hard to compute that $(L_v)_{ij} = -(\alpha d)^{(-1)}$ for all indices i, j. This leads to the non-integral term

$$\frac{1}{\alpha_v} | \sum_{\{e \in E_v\}} f_e(v)|^2.$$

One can think that the case when $\alpha_v = 0$ is formally a "particular case" of this one, if one assumes that the denominator being equal to zero forces the condition that the sum in the numerator also vanishes.

The quadratic form for a general choice of real numbers α can be written as follows:

$$\sum_{e \in E} \int_e |\frac{df}{dx}|^2 dx + \sum_{\{v \in V \,|\, \alpha_v \neq 0\}} \frac{1}{\alpha_v} | \sum_{\{e \in E_v\}} f_e(v)|^2.$$

The domain consists of all functions in $\bigoplus\limits_{e} H^1(e)$ that have at each vertex v where $\alpha_v = 0$ the sum of the vertex values along all entering edges equal to zero.

When all numbers α_v are non-negative, the operator is clearly non-negative as well.

3.2.4   Vertex Dirichlet and Neumann conditions

The **vertex Dirichlet conditions** are those where at each vertex it is required that the boundary values of the function on each edge are equal to zero. In this case the operator completely decouples into the direct sum of the negative second derivatives with Dirichlet conditions on each edge. There is no communication between the edges. The quadratic form is clearly

$$\sum_{e \in E} \int_e |\frac{df}{dx}|^2 dx$$

on functions $f \in H^($Γ$)$ with the additional condition $f(v) = 0$ for all vertices v. The spectrum $\sigma(\mathcal{H})$ is then found as

$$\sigma(\mathcal{H}) = \{n^2 \pi^2 / l_e^2 \mid e \in E, \, n \in \mathbb{Z} - 0\}.$$

Another type of conditions under which the edges completely decouple and the spectrum can be easily found from the set of edge lengths, is the **vertex Neumann conditions**. Under these conditions, no restrictions on the vertex values $f_e(v)$ are imposed, while all derivatives $f'_e(v)$ are required to be equal to zero. Then on obtains the Neumann boundary value problem on each edge separately. The formula for the quadratic form is the same as for the vertex Dirichlet conditions, albeit on a larger domain with no vertex conditions imposed whatsoever.

3.2.5   Classification of all symmetric vertex conditions

The reader might have noticed that in all examples above the conditions were invariant with respect to any permutations of edges at a vertex. We will now classify all such conditions (8). The list of symmetric vertex conditions includes several popular classes. However, quantum graph models arising as approximations for thin structures sometimes involve non-symmetric conditions as well, which preserve some memory of the geometry of junctions (see, e.g. [58, 59, 60]). As it has already been mentioned, one can find discussion of other examples of boundary conditions in [34, 43].

Let us repeat for the reader's convenience the boundary conditions (8) at a vertex v, dropping for simplicity of notations all subscripts indicating the vertex:

$$
\begin{aligned}
PF(v) &= 0 \\
QF'(v) + LQF(v) &= 0.
\end{aligned}
\tag{23}
$$

Here, as before, P is an orthogonal projector in $\mathbb{C}^d$, $Q = I - P$, and L is a self-adjoint operator in $Q\mathbb{C}^d$.

We are now interested in the case when these conditions are invariant with respect to the symmetric group S_d acting on $\mathbb{C}^d$ by permutations of coordinates. Notice that this action has only two non-trivial invariant subspaces: the one-dimensional subspace U consisting of the vectors with equal components, and its orthogonal complement $U^\perp$, since the representation of S_d in $U^\perp$ is irreducible (e.g., Section VI.4.7 in [13] or VI.3 in [78]). Here $U^\perp$ consists of all vectors with the sum of components equal to zero. Let us denote by ϕ the unit vector $\phi = (d^{-1/2}, ..., d^{-1/2}) \in \mathbb{C}^d$. This is a unit basis vector of U. Then the orthogonal projector onto U is $\phi \otimes \phi$ (a physicist would denote it $|\phi\rangle\langle\phi|$) acting on a vector a as $\langle a, \phi\rangle\phi$. Then the complementary

projector onto $U^\perp$ is $I - \phi \otimes \phi$. In order for (23) to be S_d-invariant, operators P and L must be so. Due to the just mentioned existence of only two non-trivial S_d-invariant subspaces, there are only four possible orthogonal projectors that commute with S_d: $P = 0$, $P = \phi \otimes \phi$, $P = I - \phi \otimes \phi$, and $P = I$. Let us study each of these cases:

- **Let first $P = 0$.** In this case $Q = I$ and L acting on $\mathbb{C}^d$ must commute with the representation of the symmetric group by permutations of coordinates. As it was discussed above, this implies that $L = \alpha \phi \otimes \phi + \beta I$. This shows that there are no restrictions imposed on the vertex values F and the restrictions on F' are given as $F' + \alpha \langle F, \phi \rangle + \beta F = 0$. In other words, one can say that the expression $f'_e(v) + \beta f_e(v)$ is edge-independent and $-\alpha \sum\limits_{e \in E_v} f_e(v) = (f'(v) + \beta f(v))$. In the particular case when $\alpha \neq 0$, $\beta = 0$, we conclude that all the values of the outgoing derivatives $f'_e(v)$ are the same, and $\sum\limits_{e \in E_v} (f_e(v)) = -\alpha^{(-1)} f'(v)$. One recognizes this as the δ'-**type conditions**. If $\alpha = \beta = 0$, one ends up with the **vertex Neumann condition**.

- **Let now $P = I$.** Then $Q = 0$ and hence L is irrelevant. We conclude that $F = 0$ and no more conditions are imposed. This is the **vertex Dirichlet condition**, under which the edges decouple.

- **Let $P = \phi \otimes \phi$.** Then $Q = I - \phi \otimes \phi$ and L is equal to a scalar α, due to irreducibility of the representation in $Q\mathbb{C}^d$. Then $\sum\limits_{e \in E_v} f_e(v) = 0$ and

$$F'(v) - \langle F'(v), \phi \rangle \phi + \alpha F(v) = 0.$$

The last equality shows that the expression $f'_e(v) + \alpha f_e(v)$ is edge-independent and equal to $\sum\limits_{e \in E_v} f'_e(v)$. This, together with $\sum\limits_{e \in E_v} f_e(v) = 0$ gives all the conditions in this case. There appears to be no common name for these conditions.

- **The last case is $P = I - \phi \otimes \phi$.** Then $Q = \phi \otimes \phi$ and L is a scalar α again. In this case the condition $PF = 0$ means that the values $f_e(v)$ are edge independent, or in other words f is continuous through the vertex v. The other condition easily leads to $\sum\limits_{e \in E_v} f'_e(v) = -\alpha f(v)$, which one recognizes as the δ-**type conditions**.

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This completes our classification of symmetric vertex conditions. These conditions were found previously in [34] by a different technique.

As we have already mentioned before, non-symmetric conditions arise sometimes as well (e.g., [34, 43, 58, 59, 60]).

One of the natural questions to consider is which of the conditions (6) arise in the asymptotic limits of problems in thin neighborhoods of graphs. This issue was discussed in [54], however it has not been resolved yet. One might think that when quantum graph models are describing the limits of thin domains, different types of vertex conditions could probably be obtained by changing the geometry of the domain near the junctions around vertices. This guess is based in particular on the results of [59, 60].

3.3   Infinite quantum graphs

We will now allow the number of vertices and edges of a metric graph Γ to be (countably) infinite. Our goal is to define a self-adjoint operator $\mathcal{H}$ on Γ in a manner similar to the one used for finite graphs. In other words, $\mathcal{H}$ should act as the (negative) second derivative along each edge, and the functions from its domain should satisfy (now infinitely many) vertex conditions (5) or equivalently (8). This would turn a metric graph Γ into a quantum graph. However, unless additional restrictions on the graph and vertex conditions are imposed, the situation can become more complex than in the finite graph case. This is true even for such "simple" graphs as trees, where additional boundary conditions at infinity may or may not be needed depending on geometry (see [19, 79]). On the other hand, if one looks at the naturally arising infinite graphs, one can notice that in many cases there is an automorphism group acting on the graph such that the orbit space (which is a graph by itself) is compact. This is the case for instance with periodic graphs and Cayley graphs of groups. We do not need exactly the homogeneity, but rather that the geometry does not change drastically throughout the graph. The assumptions that we introduce below captures this idea and covers all cases mentioned above. It also enables one to establish nice properties of the corresponding Hamiltonians. We would also like to notice that this class of graphs is in some sense an analog of the so called manifolds of bounded geometry [76]. On such manifolds studying elliptic operators is easier than on more general ones.

Assumption 1. *The lengths of all edges e are uniformly bounded from below:*

$$0 < l_0 \le l_e \le \infty. \tag{24}$$

Remark 12. *1. This assumption makes sense for infinite graphs only.*

   2. There is no upper bound assumed on the lengths of edges. In fact, some edges may be of infinite length, as they often are, e.g. in scattering problems.

Let us now equip a metric graph Γ with the negative second derivative operator and boundary conditions (8). We will say that the Hamiltonian $\mathcal{H}$ is defined, although its precise definition will be provided only a little bit later in this section. This makes Γ a quantum graph.

Assumption 2. *The following estimate holds uniformly for all vertices v:*

$$\|L_v\| \le S < \infty. \tag{25}$$

The norms in (25) are the operator norms with respect to the standard l_2 norms on spaces $\mathbb{C}^d$.

Remark 13. *If the vertex conditions are given in the form (5), then the condition above should be replaced by the following:*

$$\|B_v^{(-1)} A_v Q_v\| \le S < \infty.. \tag{26}$$

Here, as before, Q_v is the orthogonal projection onto the range of B_v^* and $B_v^{(-1)}$ is the inverse to the operator B_v acting from the range of B_v^* to the range of B_v.

Let us now define the operator $\mathcal{H}$ more precisely.

Definition 14. *The (unbounded) Hamiltonian $\mathcal{H}$ in $L_2(\Gamma)$ acts as the negative second derivative along the edges, defined on the domain $D(\mathcal{H})$ consisting of functions f such that:*

   1. $f \in H^2(e)$ for each edge e,

   2.

$$\sum_e \|f\|^2_{H_2(e)} < \infty,$$

3. for each vertex v, conditions (8) are satisfied:

$$L_v F(v) + Q_v F'(v) = 0, \ P_v F(v) = 0.$$

It will be shown below that this operator is self-adjoint and in fact is the only "reasonable" self-adjoint realization of our Hamiltonian (i.e., its restriction to the appropriate subspace of compactly supported functions is essentially self-adjoint). We, however, want to describe the corresponding quadratic form first. The definition will be similar to the one we gave in the case of finite graphs:

Definition 15. *The quadratic form h is defined as*

$$h[f, f] = \sum_{e \in E} \int_e |\frac{df}{dx}|^2 dx - \sum_{v \in V} \langle L_v F, F \rangle, \qquad (27)$$

where $\langle , \rangle$ denotes the standard hermitian inner product in $\mathbb{C}^{d_v}$.

The domain of this form consists of all functions f that belong to $H^1(e)$ for each edge e, satisfy at each vertex v the condition $P_v F = 0$, and such that

$$\sum_e \|f\|^2_{H^1(e)} < \infty. \qquad (28)$$

One can easily write the sesquilinear form for h:

$$h[f, g] = \sum_{e \in E} \int_e \frac{df}{dx} \frac{\overline{dg}}{dx} dx - \sum_{v \in V} \langle L_v F, G \rangle. \qquad (29)$$

Some remarks are due concerning this definition.

Remark 16.   *1. Analogous formulas can be written in terms of the matrices A_v, B_v of conditions (5), one just needs to replace L_v by $B_v^{(-1)} A_v$ and remember that P_v is the orthogonal projection onto the kernel of B_v.*

2. Due to the lower bound on the lengths of the edges, the norms of the trace operators that associate to each function $f \in H^1(e)$ for $e \in E_v$ its value at the vertex v are bounded uniformly with respect to v and e:

$$|f(v)| \leq C \|f\|_H^1(e). \qquad (30)$$

3. *In order for the definition to be correct, one needs to make sure that both infinite sums in the formula for h converge. The first one (the sum of the integrals) converges due to Cauchy-Schwartz inequality and (28). Moreover, (28) and (30) imply that for any f from the domain of the form one has for its traces $F(v)$ (recall that $F(v)$ is a vector in $\mathbb{C}^{d_v}$) the inequality*

$$\sum_v \|F(v)\|^2 \leq C \sum_e \|f\|^2_{H^1(e)} < \infty. \tag{31}$$

Since the same applies to the function g, this, (25), and the Cauchy-Schwartz inequality secure convergence of the second sum.

We are now prepared for the discussion of the Hamiltonian.

Theorem 17. *Let Γ be a quantum graph satisfying Assumptions 1 and 2. Under the definitions given above for the quadratic form h and operator $\mathcal{H}$, the following statements hold:*

1. *The operator $\mathcal{H}$ is self-adjoint and its quadratic form is h.*

2. *Let $\mathcal{H}_0$ be the restriction of $\mathcal{H}$ onto the sub-domain consisting of all functions from $D(\mathcal{H})$ with compact support. Then $\mathcal{H}_0$ is symmetric, essentially self-adjoint, and its closure is $\mathcal{H}$.*

Before we proceed to the proof of the theorem, let us mention that its second statement implies that under the prescribed vertex conditions there is only one reasonable way to define our self-adjoint Hamiltonian $\mathcal{H}$, and it is the one we choose. One can also notice that according to [19, 79] this is not true anymore for graphs that do not have "bounded geometry" in terms of the Assumptions 1 and 2, even for trees, where some boundary conditions at infinity might be needed.

Proof. First of all, it is immediate to check that both operators $\mathcal{H}$ and $\mathcal{H}_0$ are symmetric. Next, the form h is closed. Indeed, the estimate (31) shows that the norm

$$\sqrt{M\|f\|^2_{L^2(\Gamma)} + h[f, f]}$$

with a sufficiently large M on the domain of h is equivalent to the norm of the space $H = \bigoplus_e H^1(e)$. This implies closedness. Now, the form h corresponds

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to a self-adjoint operator $\mathcal{M}$. We will show that $\mathcal{M}$ coincides with $\mathcal{H}$, which would prove the first statement of the theorem. According to the definition of operator $\mathcal{M}$, for any $f \in D(\mathcal{M}) \subset H$ there exists $p \in L_2(\Gamma)$ (which is then denoted by $\mathcal{M}f$) such that for any $g \in D(h)$ one has

$$h[f,g] = \sum_e \int_e p(x)\overline{g(x)}dx.$$

Let now g be any compactly supported function smooth on each edge and equal to zero in a neighborhood of each vertex. Then clearly $g \in D(h)$. Choosing only such functions in the previous equality, substituting the definition of h for the left hand side, and integrating by parts, one concludes that

$$p(x) = \mathcal{M}f(x) = -\frac{d^2f}{dx^2}$$

on each edge, where the derivatives are meant in the distributional sense. This means that $\frac{d^2f}{dx^2} \in L^2(\Gamma)$, and due to $f \in D(h) \subset H$, we conclude that $f \in \bigoplus_e H^2(e)$ and $\sum_e \|f\|_{H^2(e)} < \infty$. Since $f \in D(h)$, this function satisfies the conditions $P_v F(v) = 0$ at each vertex v. We need to show that it satisfies also the remaining vertex conditions (those containing derivatives). One does this using a test function $g \in D(h)$ that is non-zero in small neighborhood of a single vertex v. Then integration by parts shows that

$$\langle F'(v) + L_v F(v), G(v) \rangle = 0.$$

Since this equality must hold for any vector $G(v)$ such that $P_v G(v) = 0$, this implies the complete boundary condition (8). This shows that $\mathcal{M} \subset \mathcal{H}$.

It is a straightforward calculation of exactly same nature that shows that in fact any $f \in D(\mathcal{H})$ belongs to $D(\mathcal{M})$. Hence, $\mathcal{M} = \mathcal{H}$ and the first statement of the theorem is proven.

Let now $f \in D(\mathcal{H})$. Our goal is to create a sequence of cut-off functions $\phi_n(x)$ such that $f_n = \phi_n f \in D(\mathcal{H}_0)$ and

$$\|f - f_n\|_{L_2(\Gamma)} \to 0, \ \|\mathcal{H}f - \mathcal{H}_0 f_n\|_{L_2(\Gamma)} \to 0. \tag{32}$$

If this were accomplished, then we would know that $\mathcal{H}$ were the closure of $\mathcal{H}_0$ and hence $\mathcal{H}_0$ were essentially self-adjoint.

The idea of how functions ϕ_n should behave is clear: they must be equal to 1 on an expanding and exhausting sequence $\Gamma_n \subset \Gamma$ of compacta, must

have compact supports, must be constant in a neighborhood of each vertex (in order not to destroy the vertex conditions), and must fall off to zero "not too fast," so that their first and second order derivatives are uniformly bounded. Now, if a sequence of such functions is constructed, then (32) is straightforward. The graph nature of our variety causes some superficial complications, so we will describe this construction (which could certainly be done in many different ways). Let us first describe a convenient expanding sequence of compacta in Γ that exhaust the whole graph. Let us fix a vertex $o \in \Gamma$ and consider for any natural n the set $\Gamma_n \subset \Gamma$ that contains all (finite) edges e whose both endpoints are at a distance at most n from o and all points x of infinite edges such that $\rho(x, o) \leq n$ (here ρ is the previously defined metric on Γ). This is clearly an expanding sequence of compact sets that exhausts Γ. Let $\phi(x)$ be any smooth function on $[0, l_0/4]$ such that it is identically equal to 1 in a neighborhood of 0 and identically equal to zero close to $l_0/4$. Here l_0 is the lower bound for the lengths of all edges of Γ, which is positive due to our assumptions. We are ready to define the cut-off function ϕ_n on Γ. It is equal to 1 on Γ_n and to 0 on all edges which do not have vertices in Γ_n. We only need to define it along the edges that have only one vertex in Γ_n. Let e be a finite edge whose one vertex v is contained in Γ_n. The function ϕ_n is defined to be equal to 1 along e starting from v till the middle of the edge, then it is continued by an appropriately shifted copy of $\phi(x)$ (which by construction will become zero at least at the distance $l_e/4$ from the end of the edge), and stays zero after that. If e is an infinite edge starting at $v \in \Gamma_n$, then ϕ_n is defined to be equal to 1 along e starting from v till the the distance n from o, then it is continued by an appropriately shifted copy of $\phi(x)$, and stays zero after that. It is clear that all our requirements for the sequence of functions are satisfied.

Let now $f \in D(\mathcal{H})$ and $f_n = \phi_n f$. Then f_n is in $H^2(e)$ for any edge e and satisfies the boundary conditions. The reason for the latter is that ϕ_n is constant around each vertex, and so multiplication by it does not destroy the vertex conditions. In other words, $f_n \in D(\mathcal{H}_0)$. One gets the following simple conclusion:

$$\lim_{n \to \infty} \|f - f_n\|_{L_2(\Gamma)} = \lim_{n \to \infty} \|(1 - \phi_n)f\|_{L_2(\Gamma)}$$
$$\leq C \lim_{n \to \infty} \|f\|_{L_2(\Gamma - \Gamma_n)} = 0.$$

Here C is the maximal value of $|\phi(x) - 1|$. We also have

$$\mathcal{H}f - \mathcal{H}_0 f_n = (1 - \phi_n)f'' - \phi_n' f' - \phi_n'' f.$$

Since f, f', and f'' all belong to $L_2(\Gamma)$ and the functions $1 - \phi_n$, ϕ_n', and ϕ_n'' are uniformly bounded and supported outside Γ_n, we also obtain the second required limit

$$\lim_{n \to \infty} \|\mathcal{H}f - \mathcal{H}_0 f_n\|_{L_2(\Gamma)} = 0.$$

This finishes the proof of the theorem.

4   Relations between spectra of quantum and discrete graph operators

In many (if not most) cases when a quantum graph is involved, one is interested in the spectrum of the corresponding Hamiltonian $\mathcal{H}$. This is true for quantum chaos studies, scattering theory, photonics, etc. (see the references in [54]).

We have emphasized throughout the text the difference between combinatorial graphs and corresponding difference operators on one hand and metric graphs equipped with differential operators on the other. However, we will show now that spectral problems for quantum graphs can sometimes be transformed into the ones for difference operators on combinatorial graphs. This observation goes back probably to the paper [4].

We will address here the cases of finite graphs with edges of finite lengths only. Due to the article size limitations, more complex situation of infinite graphs will be treated in [56]. The situation of interest for scattering theory when several infinite leads are attached to a finite graph will also be considered elsewhere.

Let us start with the following simple result.

Theorem 18. *Let Γ be a finite quantum graph with finite length edges equipped with a Hamiltonian given by the negative second derivative along the edges and vertex conditions (8). Then its resolvent is of trace class, and in particular the spectrum is discrete.*

Proof. The domain of $\mathcal{H}$ is a closed subspace of the direct sum of the Sobolev spaces $H^2(e)$ on all edges. Hence, for non-real λ the resolvent $R(\lambda) = (\mathcal{H} - \lambda)^{-1}$ maps $L_2(\Gamma)$ continuously into this direct sum. Now the statement follows form the standard embedding theorem for the Sobolev spaces on finite intervals.

According to Theorem 18, the spectrum $\sigma(\mathcal{H})$ is discrete. We are interested therefore in solving the equation

$$\mathcal{H}f = \lambda f \tag{33}$$

with $f \in L_2(\Gamma)$. Let v be a vertex and e be one of the outgoing edges of length l_e and with the coordinate x counted from v. We will also denote by w_e the other end of e. Then along this edge one can solve (33) as follows:

$$f_e(x) = \frac{1}{\sin \sqrt{\lambda} l_e} \left(f_e(v) \sin \sqrt{\lambda}(l_e - x) + f_e(w_e) \sin \sqrt{\lambda} x \right). \tag{34}$$

This can be done as long as $\lambda \neq n^2 \pi^2 l_e^{-2}$ with an integer $n \neq 0$ (the formula can also be naturally interpreted for $\lambda = 0$), i.e. when λ does not belong to the spectrum of the negative second derivative with Dirichlet conditions on e (identified with $[0, l_e]$).

The last formula allows us to find the derivative at v:

$$f_e'(v) = \frac{\sqrt{\lambda}}{\sin l_e \sqrt{\lambda}} \left(f_e(w_e) - f_e(v) \cos l_e \sqrt{\lambda} \right). \tag{35}$$

Substituting these relations into (23) to eliminate the derivatives, one reduces (23) to a system of discrete equations that involve only the vertex values:

$$T(\lambda)F = 0. \tag{36}$$

Here F is the vector of dimension $D = \sum_v d_v$ that combines all the vector values $F(v)$ of function f and $T(\lambda)$ is a $D \times D$ matrix.

The reader can notice that (36) is a system of second order difference equations on the **combinatorial** version of the graph Γ, where at each vertex v we have a d_v-dimensional value $F(v)$ of the vector function F assigned. One easily concludes that the following statement holds:

Theorem 19. *A point* $\lambda \neq n^2 \pi^2 l_e^{(-2)}$, $n \in \mathbb{Z} - \{0\}$ *belongs to the spectrum of* $\mathcal{H}$ *if and only if zero belongs to the spectrum of the matrix* $T(\lambda)$.

This theorem shows that spectral problems for quantum graph Hamiltonians can be rewritten as spectral problems for some difference operators. One can notice that when computed, the system (36) often looks rather complex. However, it simplifies significantly for some frequently arising situations.

Consider for instance a quantum graph with all edges of same length l and with δ-type vertex conditions. In this case the function is continuous, and hence the values $F_e(v) = f(v)$ do not depend on the edge $e \in E_v$. Then (36) after some simple arithmetic becomes

$$\sum_{\{w \mid e = (v,w) \in E_v\}} f(w) = \left(\alpha \frac{\sin l\sqrt{\lambda}}{l\sqrt{\lambda}} + d_v \cos \sqrt{\lambda} \right) f(v). \qquad (37)$$

In the particular case when all vertices have same degree d (i.e., the graph is regular), we conclude that $\lambda \neq n^2\pi^2/l^2$ belongs to the spectrum $\sigma(\mathcal{H})$ of the quantum graph if and only if $\left(\alpha \frac{\sin l\sqrt{\lambda}}{l\sqrt{\lambda}} + d \cos \sqrt{\lambda} \right)$ belongs to the spectrum $\sigma(\Delta)$ of the discrete Laplace Δ operator on Γ that is defined by the left hand side of (37). This provides a very useful relation of the spectra that enables one to pass information between the continuous and discrete models. The full advantage of using this correspondence will be shown in particular in [56].

One can ask what happens to the excluded Dirichlet eigenvalues $n^2\pi^2/l_e^2$. The following examples show that it is hard to answer this question in general terms.

- Consider the vertex Dirichlet conditions case. Here the whole spectrum obviously consists of the above Dirichlet eigenvalues only.

- Consider a ring consisting of two edges of lengths l_1, l_2 connected at two vertices of degree 2 into a loop of length $L = l_1 + l_2$ and equipped with the Kirchhoff conditions (4). As it has been mentioned before, this means that we can eliminate the two vertices of the graph and consider it as a circle of length L equipped with the negative second derivative Hamiltonian $\mathcal{H}$. In this case, the spectrum $\sigma(\mathcal{H})$ is the set of numbers $\{(2n\pi/L)^2\}$. If the numbers l_j are rationally independent, then none of the edge Dirichlet eigenvalues are in the spectrum.

- Choosing in the previous example the lengths l_j commensurate, one can make sure that only a non-empty part of the set of edge Dirichlet eigenvalues belongs to $\sigma(\mathcal{H})$.

One should beware these edge Dirichlet eigenvalues. For instance, in the case of an integer lattice graph $\Gamma = \mathbb{Z}^n$, one can apply standard Floquet theory used for periodic PDEs (e.g., [51, 52, 53, 73]) to find the spectrum.

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At the first glance, this leads to the usual picture of a band-gap absolutely continuous spectrum of a periodic problem. However, there is a danger (that has materialized in several publications) to overlook the point spectrum that does arise at the edge Dirichlet eigenvalues.

5 Remarks

1. We have considered for the sake of simplicity the second derivative Hamiltonians only. One can analogously deal with more general Schrödinger operators on graphs that involve electric and magnetic potentials [46]. Sometimes matrix or higher order differential and even pseudo-differential operators on graphs need to be considered [15, 36, 57, 58, 70]. We hope to address some of these issues elsewhere.

2. The results of Section 4 concerning relations between spectra of quantum and combinatorial graph operators in the case of infinite graphs require more analysis, since the spectra might not be discrete anymore. In particular, one should be able to identify points of the spectrum with those where some growing solutions (generalized eigenfunctions) exist. This requires analogs of the so called Schnol's theorems and estimates on generalized eigenfunctions (see the PDE versions of these correspondingly in [24, 40, 75, 76] and [10, 77, 38]). Such analogs will be provided in [56].

3. It was mentioned that in situation the discrete equations (36) that one gets when switching from a quantum to a combinatorial graph look rather complex. It would be nice to fit those into some algebraic framework that would allow a thorough analysis like the one available for discrete Laplace operators. One can interpret (36) in terms of graph representations [11, 37], although we have not found this useful so far. A vertex scattering matrix approach [48] might also prove to be useful here.

4. The results of this paper do not provide any details of the structure of the spectrum that would reflect specific graph geometry. This is a problem definitely worth studying and the one that has been addressed from various points of view in several publications (e.g. [3, 5, 6, 7, 8], [16]-[20], [29]-[32], [39], [43]-[49], [54]-[61], [64, 65, 74, 79, 80], other

papers of the current issue of Waves in Random Media, and references therein). We plan to address some of the related problems (e.g., spectral gaps, bound states, etc.) in [56] and other papers.

5. An interesting and useful generalization that deserves consideration concerns operators on multi-structures that involve cells of different dimensions (see, e.g. [14, 50, 66, 72]). Among those one can mention for instance, $2D$ or $3D$ quantum wells joined by $1D$ quantum wires, or three-dimensional photonic band gap media that sometimes look as $2D$ surface structures in $\mathbb{R}^3$.

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