# Quantum graphs: an introduction and a brief survey

This article is dedicated to the memory of Professor V. Geyler

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#### Abstract

The purpose of this text is to set up a few basic notions concerning quantum graphs, to indicate some areas addressed in the quantum graph research, and to provide some pointers to the literature. The pointers in many cases are secondary, i.e. they refer to surveys in [77] or elsewhere.

# 1 Introduction

We use the name "quantum graph" for a graph considered as a one-dimensional singular variety and equipped with a 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 (e.g., nanotechnology and microelectronics), when one considers propagation of waves of various nature (electromagnetic, acoustic, etc.) through a quasi-one-dimensional system (often a "mesoscopic" one) that looks like a thin neighborhood of a graph. One can mention in particular the free-electron

theory of conjugated molecules in chemistry, quantum wires, dynamical systems, photonic crystals, thin waveguides, and many other applications. We will provide the necessary references later on in this text. The paper is intended to serve as a survey, a literature guide, and an introduction that could be useful for reading other articles of this volume that are devoted to quantum graphs and their applications. One can find surveys and collections of papers on quantum graphs and related issues in [27, 31, 109, 123, 124, 128, 129, 140–144, 188].

# 2 Graphs and metric graphs

A graph  $\Gamma$  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, its endpoints. In most cases of interest, directions of the edges will be irrelevant, although it is sometimes more convenient to have them assigned arbitrarily<sup>1</sup>. Loops and multiple edges are allowed.

We denote by  $E_v$  the set of edges incident to the vertex v (i.e., containing v) and will always assume that the degree (valence)  $d_v = |E_v|$  of any vertex v is finite and positive. Thus, vertices with no incident edges are not allowed (it will be clear later that for the quantum graph purposes such vertices are irrelevant).

We introduce now an additional structure that makes  $\Gamma$  a topological and metric, rather than purely combinatorial, object.

**Definition 1.** A graph  $\Gamma$  is said to be a **metric graph**<sup>2</sup>, if its each edge e is assigned a positive length  $l_e \in (0, \infty]$  (edges of infinite length are allowed).

An edge e can be identified with a finite or infinite segment  $[0, l_e]$  of the real line. We will fix such an identification for each edge, which introduces a coordinate  $x_e$  along it<sup>3</sup>. When this cannot lead to confusion, the subscript e will be omitted and the coordinate will be denoted x. This defines natural

<sup>&</sup>lt;sup>1</sup>In studies devoted to quantum chaos on graphs, it is common to count each edge twice, i.e. with both directions.

<sup>&</sup>lt;sup>2</sup>Sometimes the notions of a weighted graph or  $\mathbb{R}$ -graph are used instead.

<sup>&</sup>lt;sup>3</sup>This also introduces a preferred direction on the edge. As we have mentioned before, in some cases it is convenient to introduce two copies of each edge, which are equipped with opposite directions and correspondingly reversed coordinates.

topology on the graph, which makes  $\Gamma$  a topological space (1D simplicial complex). This space is the union of all edges, where the ends corresponding to the same vertex are identified. Graph  $\Gamma$  can also be equipped with a natural metric. If a sequence of edges  $\{e_j\}_{j=1}^M$  forms a path, its length can be defined 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. It is also easy to define the natural distance  $\rho(x,y)$  between two points x,y of the graph that are not necessarily vertices. We leave this to the reader.

In the case of infinite graphs (i.e., graphs with infinitely many vertices), sometimes the following additional condition of finiteness arises:

• Finite ball volume. 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 matters only for graphs with infinitely many edges and is usually satisfied in applications.

In some cases (e.g., when studying fractals or infinite quantum trees), this assumption is too restrictive and needs to be abandoned.

If infinite edges are present, in most cases the following condition is assumed:

• Infinite leads. 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 one or more additional infinite "leads" or "ends" going to infinity attached to some vertices. This situation arises naturally for instance in scattering theory. These "infinite" vertices are usually not treated as vertices, so one can just assume that each infinite edge is a ray with a single vertex.

The graph is not assumed to be embedded into an Euclidean space (or Riemannian manifold). In some applications such a natural embedding does exist (e.g., in modeling quantum wire circuits or photonic crystals, see further sections), and in such cases the coordinate along an edge is usually the arc length. In some other applications, there is no natural embedding.

It is useful to picture a metric graph  $\Gamma$  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 points of a metric graph are not only its vertices, but all intermediate points x on the edges as well. When we say a "function f(x) on  $\Gamma$ ," we mean that the values f(x) are defined along the edges, not just at the vertices, as is the case in discrete models. Having the coordinate x, one can define the natural Lebesgue measure dx on  $\Gamma$ . The notions of measurability

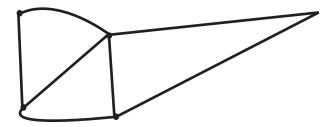


Figure 1: A metric graph  $\Gamma$ .

and integrability can be now introduced, which enable one to define some standard function spaces on the graph:

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

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

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

The finiteness of the sum condition is relevant for infinite graphs only.

Due to the presence of the coordinate x along the edges, one can discuss differentiability of a function f on each edge (but not on the whole graph). This leads to the following definition:

**Definition 3.** The Sobolev space  $H^1(\Gamma)$  consists of all **continuous** functions on  $\Gamma$  that belong to  $H^1(e)$  for each edge e and such that

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

The continuity requirement in the definition of the Sobolev space  $H^1$  means that the functions on all edges adjacent to a vertex v assume the same value at v. This is a natural condition for one-dimensional  $H^1$ -functions. However, there seems to be no natural definition of Sobolev spaces  $H^k(\Gamma)$  of order k higher than 1, due to the lack of natural conditions at vertices. As we will see, these conditions might be different for different Hamiltonians (see details later on in the following sections). Again, the finiteness of the sum condition is superfluous, unless the graph is infinite.

An interesting moduli space of metric graphs<sup>4</sup> with a fixed fundamental group was introduced twenty years ago in [56] (see also [34, 136] and the survey [210]). It was used for studying outer automorphisms of free groups (that is why the name "Outer space" is common). In particular, various natural compactifications of this space have been introduced and studied. Although this space has never been used in quantum graphs research, the author has a feeling that in some problems its use might become beneficial.

# 3 Quantum graphs

In order to make a metric graph a quantum one, an additional structure is needed: a differential (or sometimes more general) operator (Hamiltonian) on  $\Gamma$ , which is mostly, but not always, required to be self-adjoint. The most frequently studied operators of interest are acting as follows: the negative second derivative

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

a more general Schrödinger operator

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

or a still more general magnetic Schrödinger operator

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

It is clear that the definition of such an operator is not complete, till its domain is described. For "decent" potentials V and A, the natural requirement coming from the standard ODE theory is that f belongs to the Sobolev space  $H^2(e)$  on each edge e. What is still missing, is having appropriate boundary value conditions at the vertices (**vertex conditions**). We will address these in the next section.

Possibilities of more general scalar or matrix differential or pseudo-differential operators will be mentioned at a later stage. We will concentrate here on the most common scalar second order differential operators, and for simplicity of exposition on (1).

 $<sup>{}^{4}</sup>$ The name  $\mathbb{R}$ -graphs was used there.

**Definition 4.** A quantum graph is a metric graph equipped with the operator  $\mathcal{H}$  (Hamiltonian) that acts as the negative second order derivative along edges<sup>5</sup> and is accompanied by "appropriate" vertex conditions.

### 4 Vertex conditions

We will describe now what kind of boundary conditions one can add to the differential expression (1) in order to create a "reasonable" operator. In most cases, being "reasonable" will mean being self-adjoint.

Standard Sobolev trace theorems say that a function  $f \in H^2(e)$  and its first derivative have correctly defined values at the endpoints of the edge e. Already the second order derivatives of  $H^2$  functions do not have traces at the vertices. It is thus clear that the vertex conditions may involve only the values of f and df/dx at a vertex v. In principle, the conditions can mix the values at different vertices (e.g., periodicity condition for a function f on a segment e does exactly that). We, however, will concentrate at the moment on the **local vertex conditions** only, i.e. those that involve the values of functions and their derivatives at a single vertex at a time. We will see soon that the general, non-local, case can be reduced to the local one.

To avoid some technical details, we restrict ourselves here to **finite graphs**. I.e., we assume that the number of edges |E| (and hence the number of vertices |V|) is finite. The edges are still allowed to have infinite length. One can find discussion of infinite graphs in [47, 75, 145, 150, 180, 204, 205], as well as in Section 7.3.

A typical vertex condition is what is often called the "Kirchhoff"  $^6$  condition:

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

Here the sum is taken over all edges e incident to the vertex v and the derivatives are taken in the directions away from the vertex (we will call these "outgoing directions")<sup>7</sup>. Sometimes (4) is called by the more

<sup>&</sup>lt;sup>5</sup>More general Hamiltonians also arise and will be discussed later in this text.

<sup>&</sup>lt;sup>6</sup>This name, albeit often used, is not too appropriate.

<sup>&</sup>lt;sup>7</sup>We will adhere to this agreement about outgoing differentiations in all cases when these conditions are involved.

appropriate name **Neumann condition** (to satisfy all the parties, we will use the conciliatory name **Neumann-Kirchhoff conditions**). Indeed, at the "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. I.e., as we will see 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 thus continuous). Another useful remark is that under the boundary conditions (4) one can eliminate all vertices of degree 2, connecting the two adjacent edges into one smooth edge.

For local vertex conditions, it is sufficient to address the problem of describing the conditions for a single junction of d edges at a vertex v (a "star graph"). Since along each edge our operator acts as a second order operator, one expects 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. As we have already mentioned, 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 clearly is

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

Here  $A_v$  and  $B_v$  are  $d \times d$  matrices, F(v) is the column vector  $(f_1(v), ..., f_d(v))^t$  of the values at the vertex v that function f attains along all edges incident to v (e.g., if f is continuous, all these values will be the same), and  $F'(v) = (f'_1(v), ..., f'_d(v))^t$  is the column vector of the values at v of the derivatives taken along these edges in the outgoing directions. 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.

One can describe completely all conditions (5) that guarantee self-adjointness of the resulting operator. This can be done by either using the von Neumann theory of extensions of symmetric operators (as for instance described in [6]), 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 [66–68, 116, 176, 182, 189] for the accounts of this approach that goes back at least as far as [169]). The next theorem contains three different descriptions of all self-adjoint vertex conditions. It combines the results from [104, 116, 128, 144]. Experience shows that all three of these descriptions are useful in various circumstances.

Theorem 5. Let  $\Gamma$  be a metric graph with finitely many edges. Consider the operator  $\mathcal{H}$  acting as  $-\frac{d^2}{dx_e^2}$  on each edge e, with the domain consisting of functions that belong to  $H^2(e)$  and certain local vertex conditions involving vertex values of functions and their derivatives. The operator is self-adjoint, if and only if the vertex conditions can be written in one (and thus any) of the following three forms:

- **A** Conditions (5) at each vertex, where  $\{A_v, B_v | v \in V\}$  is a collection of matrices of sizes  $d_v \times d_v$  such that
  - The  $d_v \times 2d_v$  matrix  $(A_v B_v)$  has the maximal rank.
  - The matrix  $A_v B_v^*$  is self-adjoint.
- **B** For every vertex v of degree  $d_v$ , there exists a unitary  $d_v \times d_v$  matrix  $U_v$  such that the vertex conditions at v are

$$i(U_v - \mathbb{I})F(v) + (U_v + \mathbb{I})F'(v) = 0,$$
 (6)

where  $\mathbb{I}$  is the  $d_v \times d_v$  identity matrix.

C For every vertex v of degree  $d_v$ , there are two orthogonal (and mutually orthogonal) projectors  $P_v$ ,  $Q_v$  operating in  $\mathbb{C}^{d_v}$  and an invertible self-adjoint operator  $\Lambda_v$  operating in the subspace  $(1 - P_v - Q_v)\mathbb{C}^{d_v}$  (either  $P_v$ ,  $Q_v$ , or  $C_v := 1 - P_v - Q_v$  might be zero), such that the functions f in the operator domain satisfy at each vertex v the following boundary conditions:

$$\begin{cases} P_v F(v) = 0 - the "Dirichlet part", \\ Q_v F'(v) = 0 - the "Neumann part", \\ C_v F'(v) = \Lambda_v C_v F(v) - the "Robin part". \end{cases}$$
(7)

### Remark 6.

- 1. It is not hard to notice that the representation (5) of vertex conditions is not unique: multiplying matrices A and B from the left by any invertible matrix C does not alter the conditions. On the other hand, (6) or (7), which clearly are particular cases of (5), parametrize conditions uniquely.
- 2. Equivalence of (6) and (7) is rather straightforward. It is also not hard to show that (5) can be reduced to (6) or (7).

Vertex conditions can be described also in a different manner, usually adopted in studying quantum chaos on graphs [109, 132, 133]. It involves prescribing how waves scatter at each vertex. One can find discussion of relations between these descriptions and of the ones in the theorem above in the paper [25] in [77].

### 4.1 Quadratic form

It is easy to describe the quadratic form of the operator  $\mathcal{H}$  corresponding to the (negative) second derivative along each edge, with self-adjoint vertex conditions written in the form (C) of the preceding theorem.

**Theorem 7.** The quadratic form h of  $\mathcal{H}$  is given as

$$h[f, f] = \sum_{e \in E} \int_{e} \left| \frac{df}{dx} \right|^{2} dx + \sum_{v \in V} \langle \Lambda_{v} C_{v} F, C_{v} F \rangle, \tag{8}$$

where  $\langle , \rangle$  denotes the standard hermitian inner product in  $\mathbb{C}^{\dim C_v}$ . 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  $P_vF = 0$ .

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

$$h[f,g] = \sum_{e \in E} \int_{e} \frac{df}{dx} \frac{\overline{dg}}{dx} dx + \sum_{v \in V} \langle \Lambda_v C_v F, C_v G \rangle.$$
 (9)

# 4.2 Examples of boundary conditions

In this section we list some examples of vertex conditions that arise rather often.

### 4.2.1 $\delta$ -type conditions

These vertex conditions are defined as follows:

$$\begin{cases} f(x) \text{ is continuous on } \Gamma \\ \text{and} \\ \text{at each vertex } v, \sum_{e \in E_v} \frac{df}{dx_e}(v) = \alpha_v f(v) \end{cases}$$
 (10)

Here  $\alpha_v$  are some fixed numbers. One can recognize these conditions as an analog of conditions one obtains for the Schrödinger operator on the line

with a  $\delta$  potential, which explains the name. The self-adjointness condition is satisfied if and only if all numbers  $\alpha_v$  are real. When  $\alpha_v = 0$ , one arrives to the previously considered Neumann-Kirchhoff conditions.

### 4.2.2 $\delta'$ -type conditions

These are similar to the  $\delta$ -type ones, with the roles of the vertex values of functions and their derivatives switched:

$$\begin{cases}
\text{The values} \frac{df}{dx_e}(v) \text{ are independent of } e \text{ at any vertex } v. \\
\text{and} \\
\text{at each vertex } v, \sum_{e \in E_v} f_e(v) = \alpha_v \frac{df}{dx_e}(v)
\end{cases}$$
(11)

When  $d_v = 2$ , these conditions correspond to the symmetrized version of what is usually called  $\delta'$  conditions at a point. The true counterpart is provided in [71].

### 4.2.3 Decoupling conditions

There exist vertex conditions that essentially split the graph into unrelated edges. One can consider for instance the **vertex Dirichlet conditions**, that force the functions from the domain of the operator to vanish at all vertices. Then the operator is the direct sum of the operators on each edge e with Dirichlet conditions at the ends. Similar thing happens if one enforces **vertex Neumann conditions** (not to be mixed up with the Neumann-Kirchhoff conditions), requesting that derivatives along each edge vanish at the vertices. In both these cases, the topology of the graph is irrelevant from the quantum graph point of view.

# 4.3 Non-local conditions and turning a quantum graph into a single "rose"

The above discussion of the decoupling conditions leads to the understanding that the whole topology of the quantum graph is contained in the vertex conditions only. In particular, one can identify all vertices of a quantum graph into one "super-vertex"  $v_0$ , so the graph becomes just a "rose" of several petals (each edge bends into a loop), and all vertex conditions are written at this single vertex (see Fig. 2). If one starts with some special type

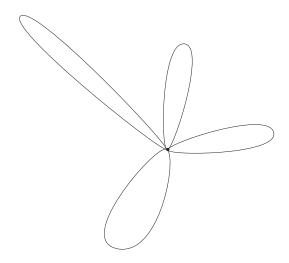


Figure 2: Graph  $\Gamma$  turned into a single "rose."

of vertex conditions, for instance Neumann-Kirchhoff ones, this procedure will not preserve this special type. On the other hand, if one needs to work with most general vertex conditions, then one can as well assume that the graph is just a rose of several loops at a single vertex. This also shows that non-local conditions can be turned into local ones at this single "supervertex", and thus description of self-adjoint local conditions given in Theorem 5 can be applied to non-local conditions as well.

# 4.4 Non-selfadjoint conditions

It is sometimes needed to consider more general Hamiltonians than the self-adjoint ones. For instance, one might be interested in accretive or dissipative Hamiltonians. The paper [131] in [77] provides criteria under which the vertex conditions lead to such operators.

# 4.5 Conditions involving spectral parameter

Sometimes vertex conditions arise that involve the spectral parameter  $\lambda$ . This usually happens when the ideal vertex corresponds to an object with some internal structure in a real world problem, see [79, 80, 140, 147, 151] for various examples.

### 4.6 Realization of vertex conditions

It is an interesting, and not completely resolved question of which of all possible vertex conditions can arise in practical problems leading to quantum graph models. See, for instance, [51, 70, 87] for some partial results.

# 5 Motivations for quantum graph models

As it has already been mentioned, quantum graph models (often under different names, e.g. quantum networks) come from various areas of mathematics, physics, and engineering, e.g. see the survey [140] for details. Here we just provide some token (and incomplete) pointers to applications in dynamical systems and probability theory [93–95], spectral theory of differential operators on manifolds and in singular domains [53, 64, 65], chemistry (including studying carbon nanostructures) [9, 73, 111, 112, 126, 127, 149, 192, 197, 198], superconductivity theory [8, 61, 194–196], photonic crystal theory [14, 89, 90, 139, 146, 147, 177], microelectronics and waveguide theory [78, 82, 84, 88, 122, 135, 161, 162, 164, 184, 185, 213], biology [48, 49, 171], acoustics [42], quantum Hall effect [41], and many others. Another reason for studying quantum graphs is that they often offer a simplified, but still non-trivial models for complex phenomena, such for instance as electron propagation in multiply connected media [11, 13], Anderson localization [1–5, 76, 120], quantum chaos [109, 124, 132–134], and some problems of quantum field theory [19, 28, 101– 103, 105, 211]. Quantum graph (also called quantum network) models have also been used for quite a while as toy models for quantum mechanics [166].

# 6 Justification of the quantum graph model for waves in narrow branching media

One of the most important sources of quantum graphs is an attempt to model waves of various nature (acoustic, electromagnetic, electron, etc.) propagating in thin (often mesoscopic or nano-scale) branching media by waves propagating on graphs. Mathematically speaking, one deals with a partial differential operator (say, Laplace operator, or more general Schrödinger operator with Dirichlet or Neumann boundary conditions) in a narrow branching domain that resembles a fattened graph (see Fig. 3). Since studying such an

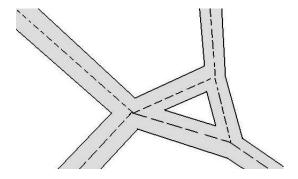


Figure 3: A narrow branching domain (shaded) with the approximating graph (dotted lines.)

operator is very hard both analytically and numerically, one wonders whether one can approximate properties (e.g., the spectrum) of the operator by those of an operator on a graph itself. This turns out to be a highly non-trivial question, which has attracted attention of many researchers. Survey [110] in [77] provides a nice overview of the exciting recent developments in this problem and of the mathematics involved, as well as comprehensive references.

# 7 Spectral properties

Among the properties of quantum graph Hamiltonians that have attracted most attention are those related to their spectra: the types of spectra that can arise, spectral gaps, spectral asymptotics and statistics, regular and generalized eigenfunctions, scattering theory, etc. In this section, we will glance over the various topics that have been considered.

# 7.1 Finite graphs

In the case of a compact graph (i.e., a finite graph with all edges of a finite length), standard Sobolev embedding theorems imply discreteness of the spectrum (see, e.g., [144] for this trivial folklore result). One of the main achievements have been explicit trace formulas that can be derived for the quantum graph case and which are the cornerstone for many further developments, e.g. inverse problems and quantum chaos studies. See, for instance,

[109, 132–134, 193, 212] and the survey [32] in [77].

Another large area of research is "quantum chaology" on quantum graphs, which deals with the spectral statistics of quantum graph operators. It is surveyed in [109], as well as in [124] in [77].

Generic and extremal properties of quantum graph spectra, e.g. simplicity were studied in [98, 99].

Determinants of quantum graph Hamiltonians are considered in [7, 100]. Index theorems for quantum graphs in relation to heat kernel asymptotics were considered in [104].

### 7.2 Finite graphs with infinite leads attached

Assume now that several infinite leads are attached to a compact graph. One can think of this situation as of a simple "star graph", where an "obstacle" (a compact graph) is inserted into the vertex. Then the natural questions to study are about limiting absorption and scattering. These have been addressed in quite a few publications, e.g. in [106, 107, 130, 160, 174–176, 179, 183]. One of the simple but crucial ideas in this topic in particular, and in quantum (as well as combinatorial) graph research in general, is usage of the so called Dirichlet-to-Neumann map that enables one to eliminate the scatterer sitting at the vertex and replace it with an energy dependent vertex condition, see for instance [92, 145, 161, 179] for the quantum and [113] for the combinatorial graph case. This trick, also well known in matrix theory as Schur complement and in physics as Feshbach formula, is particularly useful when treating self-similar (e.g., fractal) structures. It is also responsible for the "decoration" mechanism for spectral gap opening, discussed below.

# 7.3 Infinite graphs

The case of an infinite quantum graph (i.e., a graph with infinitely many edges), even under the finite ball volume condition, is rather complex and not much can be said about it in general. For instance, all kinds of spectra can arise: pure point, singular continuous, and absolutely continuous. There are only a few general things that can be established. First of all, due to the presence of continuous spectrum, one cannot test whether a given point  $\lambda$  belongs to the spectrum by checking existence of a corresponding eigenfunction. However, there exist two types of PDE theorems that help with this difficulty, allowing one to test the spectrum by looking for **generalized** 

**eigenfunctions**, i.e. those that do not decay fast enough (or do not decay at all) to be true eigenfunctions.

The first type are the generalized eigenfunction expansions (see [24, 202] and references therein) which say that under some conditions on a self-adjoint partial differential operator in  $\mathbb{R}^n$ , there exists a set of values of  $\lambda$  of the full spectral measure and for each point of this set a generalized eigenfunction of a controlled (usually polynomial) growth, which form a complete family in  $L^2$ . One can find a general framework of this kind of theorems nicely described in an appendix to [202]. This general technique can be, and has been applied to quantum graphs [120].

In a converse direction, Schnol' type theorems [59, 108, 200] claim that existence for some  $\lambda$  of a sub-exponentially growing generalized eigenfunction implies that  $\lambda$  is in the spectrum. A Schnol' type theorem holds also for infinite graphs under some mild conditions [145]. Notice that Schnol' theorem needs to be transferred from PDEs in  $\mathbb{R}^n$  to infinite graphs with some modification [145]. Direct transfer would lead to the requirement that the volume of the ball of radius r grows sub-exponentially with the radius, which would exclude the case of trees.

Another statement that does not depend on the specific structure of an infinite graph is the "decoration" method of gap opening, due to [199] (in the combinatorial case)<sup>8</sup>. Assume that one "decorates" a combinatorial or quantum, finite or infinite graph  $\Gamma_0$  by attaching to its each vertex a fixed finite graph  $\Gamma_1$  (Fig. 4). Then, under mild conditions, the spectrum of the so

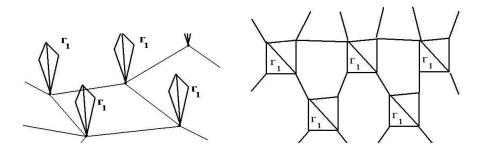


Figure 4: Two types of "decorations" of a graph  $\Gamma_0$ . On the left, a copy of  $\Gamma_1$  is attached to each vertex of  $\Gamma_0$ . In the one shown on the right, each vertex of a **regular** graph  $\Gamma_0$  is replaced by a fixed graph  $\Gamma_1$ .

<sup>&</sup>lt;sup>8</sup>Some indications of the presence of this effect were discussed previously in [12, 182]

decorated graph has mandatory gaps near the eigenvalues of the decoration. The reason is that one can eliminate the decorations, as it was described before, by replacing them with their Dirichlet-to-Neumann maps. These maps depend on the spectral parameter in a singular way: they are meromorphic with poles on the spectrum of the decoration. This introduces a vertex "potential" that blows up at some points, thus preventing the spectrum from appearing near these points. One can find the details for the combinatorial case in [199] and for the quantum one in [145].

These are probably the only general results about spectra of infinite quantum graphs that are known to the author. However, for special subclasses of infinite graphs, a more detailed analysis is possible, which usually dwells on some kind of a symmetry.

### 7.3.1 Radial trees

In the case when the graph is a rooted tree, whose properties (degrees of vertices and lengths of edges) depend only on the distance from the root, a simple harmonic analysis is possible, which essentially reduces the problem to a weighted ODE problem on the half line. One can find the corresponding results in [167, 168, 203–205].

### 7.3.2 Periodic graphs

If an abelian group acts freely and co-compactly on the graph, abelian harmonic analysis (akin to the standard Floquet theory for PDEs [63, 138, 191]) is possible, which proves completeness of the so called Floquet-Bloch generalized eigenfunctions, the band-gap structure of the spectrum, Liouville type theorems, etc. There are some differences with the continuous case, though. For instance, while in the periodic elliptic PDE case the spectrum is absolutely continuous [138, 191], this is not true anymore in the graph case, where compactly supported eigenfunctions arise [137, 145]. Also, localized perturbations of periodic structures and operators can lead to existence of eigenvalues embedded into the continuous spectrum, which does not happen in the PDE case. One can find these and other discussions of periodic graph problems in [12, 22, 69, 71, 86, 92, 118, 137, 139, 145–149, 178].

### 7.3.3 Other classes of infinite graphs

There are studies of spectral properties on some other classes of infinite combinatorial and quantum graph structures, such as the so called limit operators, operators of quasi-crystal type, random operators, etc. (e.g., [1–5,76,114,120,190] and references therein).

### 7.4 Inverse problems

One can ask the natural question, analogous to the famous problem of spectral geometry "Can one hear the shape of the drum?" In the quantum graph setting, the question is of whether one can reconstruct the topology, vertex conditions, and potentials of the Hamiltonian of a finite quantum graph from the spectral data, or, if some infinite leads are attached, from scattering data. It is known that in general this is impossible (see [23, 33, 153]). However, the beautiful construction of [115] shows that "one can hear the shape of a quantum graph" if one assumes rational independence of edges' lengths. See also [17, 18, 45, 97, 152, 187, 214] for the control theory approach and other discussions of the inverse problem.

### 7.5 Nodal domains

An important part of spectral theory of differential operators is studying nodal domains of eigenfunctions of a differential operator with discrete spectrum. In dimension one, i.e. on a finite interval, this is done by the well known oscillation theorems that essentially claim that the nth eigenfunction has n nodal domains. In higher dimensions, this becomes an upper bound (and not a sharp one) for the number of nodal domains [55,119]. Many "simplest" questions still do not have their answers, e.g. that the number of nodal domains cannot be bounded over the whole spectrum, or that the nodal set for the second eigenfunction in a simply-connected domain always hits the boundary (Payne conjecture). Many researchers have been interested in studying nodal domains of eigenfunctions on combinatorial or quantum graphs. Recently, counting of nodal domains was suggested as a tool to resolve the problem of isospectrality of non-isomorphic graphs. See [26, 30] and [15] in [77] for surveys, recent results, and references.

### 7.6 Relations to discrete operators

This introductory survey is devoted to the new area of quantum graphs and their spectra. On the other hand, the combinatorial counterpart of this theory, which is sometimes called **discrete geometric analysis**, is a rather well established topic (see e.g., books [29, 52, 54, 57, 58, 207] and the surveys [121, 163, 208]). One wonders whether there is a relation between the two. The answer is a "yes," although the relation is not always straightforward.

We will show now how spectral problems for quantum graphs can sometimes be transformed into the ones for difference operators on combinatorial graphs. This observation goes back at least to [8, 61] (see also [50, 72, 145, 180] for more detailed considerations).

Let us consider the simplest case of  $\Gamma$  a finite graph (the procedure works for infinite graphs as well, but needs to be done more carefully [180]) with the Hamiltonian  $\mathcal{H}$  defined as the negative second derivative with Neumann-Kirchhoff conditions (4). Since the spectrum  $\sigma(\mathcal{H})$  is discrete, we need to look for eigenfunctions, i.e. solutions of the equation

$$\mathcal{H}f = \lambda f \tag{12}$$

with  $f \in L_2(\Gamma)$ . Let v be a vertex and e one of the outgoing edges of length  $l_e$  with the coordinate x counted from v. Let us denote by  $w_e$  the other end of e. Then along this edge one can solve (12):

$$f_e(x) = \frac{1}{\sin\sqrt{\lambda}l_e} \left( f_e(v) \sin\sqrt{\lambda}(l_e - x) + f_e(w_e) \sin\sqrt{\lambda}x \right). \tag{13}$$

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 be interpreted for  $\lambda = 0$ ), i.e. when  $\lambda$  does not belong to the spectrum of the operator on the edge e with Dirichlet conditions at the edge's ends.

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

$$f'_e(v) = \frac{\sqrt{\lambda}}{\sin l_e \sqrt{\lambda}} \left( f_e(w_e) - f_e(v) \cos l_e \sqrt{\lambda} \right). \tag{14}$$

Substituting these relations into (4) to eliminate the derivatives, one reduces (4) to a system of discrete equations that involve only the vertex values:

$$T(\lambda)F = 0. (15)$$

Here  $T(\lambda)$  is a square matrix of dimension  $\sum_{v} d_{v}$ .

One can notice that (15) is a system of second order **difference** equations on the **combinatorial** version of the graph  $\Gamma$ , where at each vertex v we have a  $d_v$ -dimensional value F(v) of the vector function F assigned. The components of this vector are labeled by the edges adjacent to v. Notice that if the graph is not regular (i.e., if  $d_v$  is not constant throughout  $\Gamma$ ), then the dimensions of the vector values are changing from vertex to vertex. One concludes that the following statement holds:

**Theorem 8.** A point  $\lambda \neq n^2 \pi^2 l_e^{(-2)}$  belongs to the spectrum of  $\mathcal{H}$  if and only if zero belongs to the spectrum of the matrix pencil  $T(\lambda)$ .

This theorem shows that spectral problems for quantum graph Hamiltonians can be rewritten as spectral problems for some difference operators on the combinatorial counterpart of the graph. In general, though, (15) might look complicated. It simplifies significantly for some frequently arising situations. Indeed, if we assume that all edges are of same length l, then (15) becomes at each vertex

$$\sum_{e=(v,w)\in E_v} f_e(w_e) = \cos l\sqrt{\lambda} F(v). \tag{16}$$

This means that  $\lambda \neq n^2\pi^2 l^{(-2)}$  belongs to the spectrum of the quantum graph Hamiltonian if and only if  $\cos l\sqrt{\lambda}$  belongs to the spectrum of the discrete Laplace operator that maps  $\{f(v)\}$  into  $\{\sum_{e=(v,w)\in E_v}f_e(w_e)\}$ . This enables

one to transfer known spectral results from discrete geometric analysis to the quantum graph situation. In the case of infinite graphs, though, the question arises of whether the various types (pure point, singular continuous, absolutely continuous) of the spectrum are preserved under this transformation. The positive answer can be found in [180].

The author would like to take this opportunity to mention the often forgotten important paper [201], where a discrete analog of pseudodifferential operator technique is developed with important applications to spectral theory and Greens function estimates in discrete setting.

# 8 PDE and Control problems

Problem of boundary control of partial differential equations on graphs has been considered by several authors, due to many applications in engineering.

Here as the boundary of a graph one considers its vertices of degree 1. The bottom line of these studies can be roughly summarized as follows: presence of cycles in a graph prohibits controllability, so one tries to apply control on trees only; on trees, one should control either all, or all but one boundary vertices. One can find the details and references in [16, 60, 62, 154, 173] and in the survey [10] in [77].

A variety of other PDE problems on quantum graphs have been considered, see details and references in [20, 21, 43, 44, 46, 131, 156–159, 172, 186, 188].

# 9 Various generalizations of quantum graphs

Many generalizations of quantum graphs have been studied due to various applications. The operators we have considered so far were scalar (i.e., spin was not taken into account). However, **matrix operators** such as Dirac operators and Rashba Hamiltonians have also been considered, see the survey [117] in [77] for details and references.

Differential operators of orders higher than 2 were considered, due to the needs of photonic crystal theory, in [147].

Both photonic crystal theory and quantum waveguide theory have lead (albeit in somewhat different manner) to the necessity of considering the problems, where the particle is not strictly confined to a graph, but rather attracted to it by a delta-type potential along the graph. This, in particular, allows for tunneling between distant parts of the graph, rather than forcing the quantum particle to move through the vertices, as in the standard quantum graph theory. This explains why these systems are sometimes called leaky graphs. One can find a detailed survey on leaky graphs in [74] in [77] and considerations of such systems as coming from the photonic crystals in [89, 90, 146, 147]. The leaky graph operators can usually be written as "pseudo-differential" operators of first order on graphs [90, 147, 177].

In many applications, it is interesting to study analogs of quantum graphs that consist of cells of a higher dimension, for instance branching surface structures (sometimes called "open book structures"). Such necessity arises in dynamical systems, fluid dynamics, as well as in photonic crystal theory. It is also interesting to allow combinations of cells of different dimension, e.g. one-dimensional edges attached to two-dimensional surfaces or three-dimensional volumes. These are the so called **multistructures**. One can find

some information on such objects in [35, 36, 81, 85, 96, 155, 159, 188], although the theory here is not nearly as well developed as for quantum graphs.

Another interesting direction related to quantum graphs both in spirit and in terms of some shared techniques, is **analysis on fractals**. One can find basic introduction to this analysis and references in [125, 206] and a survey of some exciting recent developments in [170] in [77].

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