LECTURE 1

How to define differential operators on metric graphs

1.1. Schrödinger operators on metric graphs

The main subject of our studies will be magnetic Schrödinger operators on metric graphs. Every such operator is determined by triple consisting of

(1) a metric graph,
(2) a differential operator acting on the edges,
(3) certain vertex conditions.

The three components of such a triple are not completely independent, and we are going to describe all members in detail. Our studies will be mostly restricted to self-adjoint operators, but the same methods can successfully be applied even to certain non-self-adjoint problems.

1.1.1. Metric graphs. In discrete mathematics, graphs are usually defined as ordered pairs of vertices and edges with the emphasis on the *first component* - the set of vertices. This reflects the fact that one is interested in a certain jump processes between the vertices, almost neglecting the dynamics on the edges. For differential operators, the edges play the crucial role which makes it necessary to turn the standard definition of graphs 'up side down' and start the whole construction with the edges.

Let us recall first the definition of a graph used in discrete mathematics:

A graph G consists of a set V of vertices and a set E of edges. Every edge connects two vertices and therefore can be seen as an element of $V \times V$. Then E is a subset of $V \times V$.

To represent a graph, one often makes a drawing like it is done in Fig. 1.2 and 1.3. Here fat points correspond to vertices, while lines represent the edges. It is natural to generalise this definition and consider every edge as an interval on the real line having a certain length. Only the lengths of the intervals will be important for us. In this way we obtain a new object called a **metric graph**. Any two points on such a graph have a distance - the length of the shortest path connecting the points. Even in this approach, the edges seem to play a secondary role as they appear as weights attached to the edges. We prefer to change the point of view and start the whole construction with the edges. Here we are going to give a rigorous definition for graphs formed by a finite number of edges.

Consider N compact or semi-infinite intervals E_n, each belonging to a separate copy of the real line $\mathbb{R}$:

$$E_n = \begin{cases} [x_{2n-1}, x_{2n}], & n = 1, 2, ..., N_c \\ [x_{2n-1}, \infty), & n = N_c + 1, ..., N_c + N_i = N, \end{cases} \tag{1.1}$$

where N_c (respectively N_i) denotes the number of compact (respectively infinite) intervals. Each of these numbers could be equal to zero. The intervals E_n are called **edges**. It will be convenient to assume that $x_{2n-1} \le x_{2n}$.

Consider the set $\mathbf{V} = \{x_j\} = \left(\cup_{n=1}^{N_c} \{x_{2n-1}, x_{2n}\} \right) \cup \left(\cup_{n=N_c+1}^{N} x_{2n-1} \right)$ of all endpoints, and an arbitrary its partition into M equivalence classes $V^m, m = 1, 2, \dots, M$, called **vertices**. In other words, we divide the set $\mathbf{V}$ into M nonintersecting sets V^m

$$\begin{aligned} &\mathbf{V} = V^1 \cup V^2 \cup \dots \cup V^M, \\ &V^{m_1} \cap V^{m_2} = \emptyset, \text{ provided } m_1 \neq m_2. \end{aligned} \tag{1.2}$$

The endpoints belonging to the same equivalence class will be identified

$$x, y \in V^m \Rightarrow x \sim y, \tag{1.3}$$

where $\sim$ denotes the equivalence relation induced by the partition.

Definition 1.1. *Consider N finite or semi-infinite closed intervals E_n belonging to separate copies of $\mathbb{R}$, called* **edges**, *and a partition of the set $\mathbf{V}$ of their endpoints into equivalence classes V^m, called* **vertices**: $\mathbf{V} = \cup_{m=1}^{M} V^m$. *The corresponding* **metric graph** Γ *is the union of the edges with the endpoints belonging to the same vertex identified.*

Two points x and y are **equivalent** ($x \sim y$) if and only if either they belong to the same edge E_n and are equal, or they belong to the same vertex V^m:

$$x \sim y \Leftrightarrow \left[\begin{array}{l} \exists E_n : x, y \in E_n \text{ and } x = y, \\ \\ \exists V^m : x, y \in V^m. \end{array} \right. \tag{1.4}$$

With this notation the graph Γ can formally be seen as the quotient metric space

$$\Gamma = \bigcup_{n=1}^{N} E_n / x \sim y. \tag{1.5}$$

A metric graph is called **connected** if any two points x and y in Γ can be connected by a **path** - a finite sequence of compact intervals $I_j = [y_{2j-1}, y_{2j}], j = 1, 2, \dots, J$ each belonging to a certain edge E_n, $n = n(j)$, such that the endpoints in subsequent intervals are equivalent (belong to the same vertex)

$$y_{2j} \sim y_{2j+1}, \;\; j = 1, 2, \dots, J-1,$$

and

$$x = y_1, \;\; y = y_{2J}.$$

Note that such a path need not be unique. If the graph is not connected, then it is straightforward to define the **number β_0 of connected components** (the zero-th Betti number). We shall often restrict our studies to connected graphs.

The **distance** $d(x, y)$ between any two points $x, y \in \Gamma$ is the length of the shortest path connecting the points. Note that the distance between two points on the same edge may be less than $|x - y|$. We formally put $d(x, y) = \infty$ if x and y belong to different connected components.

Every metric graph can also be seen as a singular one-dimensional manifold with the singular set given by the vertices.

The number d^m of elements in the class V^m will be called the **valence** or **degree of** V^m. If the graph has no loops (edges attached by both endpoints to the

same vertex), then the degree of a vertex is equal to the number of edges joined together at it. In what follows we are going to identify the set of all endpoints $\mathbf{V} = \{x_{2n-1}, x_{2n}\}_{n=1}^{N_c} \cup \{x_{2n-1}\}_{n=N_c+1}^{N}$ and the set of all vertices $\{V^m\}_{m=1}^{M}$. It is clear that

$$D := \sum_{m=1}^{M} d^m = 2N_c + N_i = \#\mathbf{V}, \tag{1.6}$$

where $\#\mathbf{V}$ denotes the total number of endpoints.

The main part of this book will be devoted to **compact finite graphs**, which occur when $N_i = 0$, *i.e.* all edges are finite closed intervals: $N = N_c$. On the other hand, non-compact graphs appear in applications related to scattering phenomena, and it is hard to avoid such graphs while speaking about vertex conditions.

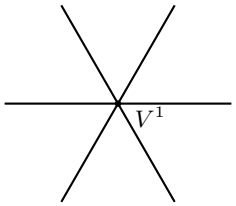

FIGURE 1.1. Non-compact connected graph (star graph)

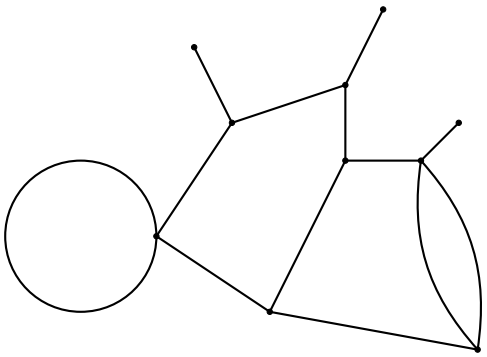

FIGURE 1.2. Connected compact graph

For compact graphs, the **Euler characteristic** χ is given by the formula

$$\chi = M - N, \tag{1.7}$$

where M and N are the number of vertices and edges respectively. The Euler characteristic determines the first Betti number β_1 – the number of (homotopically) independent cycles in the graph

$$\beta_1 = \beta_0 - \chi. \tag{1.8}$$

For metric **trees** - connected graphs without cycles - the Euler characteristic is equal to one. For all other connected graphs, χ is nonpositive: $\chi \leq 0$.

The graphs presented in Figures 1.2 and 1.3 have the same Euler characteristic equal to -3, but the number of independent cycles is different, namely 4 and 6, since they do not have the same number of connected components.

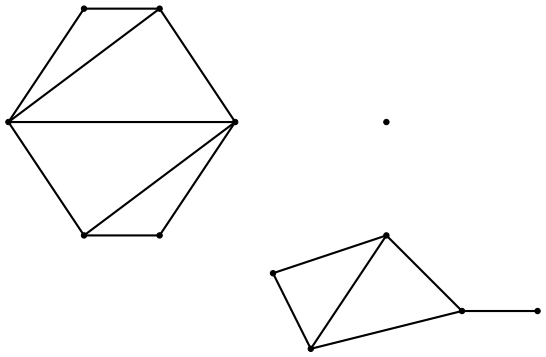

FIGURE 1.3. Compact graph with three connected components

Only the lengths $l_n = x_{2n} - x_{2n-1}$, $n = 1, 2, \dots, N_c$, of the finite edges are going to play a role in our studies not their particular parametrization. Therefore graphs with equal lengths of the edges will be identified, of course provided the edges are connected in the same way. For compact graphs we define their **total length** $\mathscr{L}$ as

$$\mathscr{L} = \sum_{n=1}^{N} \ell_n. \tag{1.9}$$

It is clear that isometric compact graphs have the same total length.

A parametrization of the edges naturally induces a measure on the graph Γ. Consider complex valued functions on Γ and the corresponding Hilbert space

$$L_2(\Gamma) = \bigoplus_{j=1}^{N} L_2(x_{2j-1}, x_{2j}). \tag{1.10}$$

Note that the functions from the Hilbert space are not defined pointwise, and therefore the Hilbert space does not reflect how the edges connect to each other. Particular values that a function attains at the vertices (forming a set of measure zero) do not play any role. In particular, we shall use

$$\int_\Gamma f(x)dx = \sum_{n=1}^{N} \int_{E_n} f(x)dx. \tag{1.11}$$

Even if the endpoints belonging to the same equivalence class V^m are identified, in the case of continuous on the edges functions it appears natural to introduce their values at the endpoints using the limits from inside the edges

$$u(x_j) = \lim_{x \to x_j} u(x). \tag{1.12}$$

Note that these limits may be different for x_j belonging to the same vertex V^m, so that the value pf the function at the vertex, $u(V^m)$, in general is not well-defined. It is well-defined only if all $u(x_j)$, $x_j \in V^m$ are equal, that is if u is continuous not only on the edges but at the vertex V^m as well. If the function is continuously differentiable on the edges, we introduce the **normal derivatives**

$$\partial_{\mathbf{n}} u(x_j) = \begin{cases} \lim_{x \to x_j} \frac{d}{dx} u(x), & x_j \text{ is the left endpoint,} \\ -\lim_{x \to x_j} \frac{d}{dx} u(x), & x_j \text{ is the right endpoint.} \end{cases} \tag{1.13}$$

The limits are taken from inside of the corresponding interval. The normal derivatives are independent of the direction in which the edge is parametrised and always point inside the interval. Note that in contrast to function values, it is wrong to speak about continuity of normal derivatives at a vertex as the normal derivatives are not defined inside the edges.

The introduced limiting values $u(x_j)$, $\partial_{\mathbf{n}} u(x_j)$ will be used for the vertex conditions.

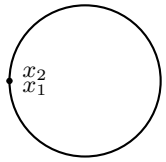

FIGURE 1.4. The circle graph $\Gamma_{(1.2)}$

Consider for example the circle graph $\Gamma_{(1.2)}$[1] formed by one interval $[x_1, x_2]$ with the endpoints identified. Then the normal derivatives are given by

$$\partial_{\mathbf{n}} u(x_1) = u'(x_1), \qquad \partial_{\mathbf{n}} u(x_2) = -u'(x_2).$$

Then the vertex conditions

$$\begin{cases} u(x_1) = u(x_2), \\ \partial_{\mathbf{n}} u(x_1) + \partial_{\mathbf{n}} u(x_2) = 0; \end{cases} \tag{1.14}$$

usually called standard (to be discussed below in Section 1.1.3) imply that

$$\begin{cases} u(x_1) = u(x_2), \\ u'(x_1) = u'(x_2); \end{cases}$$

i.e. that the function and its first derivative are continuous at the vertex.

1.1.2. Differential operators. The differential operator describes the dynamics of waves or particles travelling along the edges. One may consider different operators depending on the particular phenomena one would like to describe. In this book we shall limit our consideration to the Schrödinger operator, which is standard for quantum mechanical problems. Other differential operators can also be studied. Some developed ideas can be used but often serious modifications are necessary.

More precisely, we are going to consider the following three differential operators:

- the **Laplace** operator

$$\tau = -\frac{d^2}{dx^2}; \tag{1.15}$$

[1]Here and in what follows considering graphs on one, two, and three edges we shall refer to their classification presented in Fig. 6.7 below. It is natural to use the same classification for metric and discrete graphs, so that the metric graph $\Gamma_{(i.j)}$ corresponds to the discrete graph $G_{(i.j)}$. Remember that graphs with different enumerations of edges and vertices are considered to be equivalent.

- the **Schrödinger** operator

$$\tau_q = -\frac{d^2}{dx^2} + q(x). \tag{1.16}$$

The Schrödinger operator τ_q describes quantum particles moving under the influence of the electric potential q. The case where the electric potential vanishes corresponds to free motion and is described by the Laplace operator $\tau \equiv \tau_0$.

In our studies we are going to assume that the potential satisfy the following natural assumptions:

(1) the potential is real-valued

$$q(x) \in \mathbb{R}; \tag{1.17}$$

(2) the potential is absolutely integrable

$$q \in L_1(\Gamma),$$

and satisfies Faddeev condition

$$\int_\Gamma (1 + |x|) \cdot |q(x)| dx < \infty.$$

Faddeev condition holds automatically for any $q \in L_1$ if the graph Γ is compact.

In the introductory chapters, we are going to use slightly stronger assumptions on the potential. The reason is that without such assumptions the domain of the operator may depend on the potential, which makes presentation more involved. We postpone this discussion to Chapter 4 and assume here in addition to (1.17) that the potential is essentially bounded

$$q \in L_\infty(\Gamma). \tag{1.18}$$

The differential expressions (1.15) or (1.16) do not determine unique self-adjoint operators, since one needs to specify the operator domain. We are going to see that the freedom in selecting the domain is not very broad, and is limited to selecting different vertex conditions. One may define certain maximal and minimal operators so that the domain of any self-adjoint operator associated with the differential expression τ_q is always contained in the domain of the maximal operator, and includes the domain of the minimal one.

The **minimal** operator is defined on the domain $\mathrm{Dom}\,(L_q^{\min}) = C_0^\infty(\Gamma \setminus \mathbf{V})$ consisting of smooth (*i.e.* infinitely many times differentiable) functions with compact support separated from the vertices. This domain is dense in the Hilbert space $L_2(\Gamma)$, and the operator defined by the differential expression τ_q on this domain is symmetric, not self-adjoint.[2] (We shall prove the symmetry of $L_q^{\min}$ by integrating

[2]We remind that an operator is called **symmetric** if

$$\langle Au, v\rangle = \langle u, Av\rangle$$

holds for any $u, v \in \mathrm{Dom}\,(A)$. A densely defined symmetric operator is called **self-adjoint** if $\|\langle Au, v\rangle\| \le C \parallel u \parallel$ holds for a certain $C = C(v) \in \mathbb{R}_+$ and any $u \in \mathrm{Dom}\,(A)$ only if $v \in \mathrm{Dom}\,(A)$. Note that due to Riesz representation theorem the last inequality implies that there exists a certain $w \in \mathscr{H}$, such that $\langle Au, v\rangle = \langle u, w\rangle$ holds. In other words, a densely defined symmetric operator is self-adjoint if the domain of the adjoint operator A^* coincides with the domain of A, then the action of the adjoint operator necessarily coincides with the action of the original operator. We reserve the name **Hermitian** for symmetric and self-adjoint operators in a finite dimensional Hilbert space. For details see any course on the theory of (unbounded) self-adjoint operators in Hilbert spaces, for example [?BirSol, ?ReSi] or Volume 4, Chapter 7 of [?simon].

by parts in (1.23).) The **maximal** operator is defined on the domain of all functions from the Hilbert space $L_2(\Gamma)$ whose images (under the differential operator) are still in the Hilbert space:

$$\mathrm{Dom}\,(L_q^{\max}) = \{u \in L_2(\Gamma) : \tau_q u \in L_2(\Gamma)\}\,. \tag{1.19}$$

Since we assume here that $q \in L_\infty(\Gamma)$, the operator of multiplication by q is bounded, so $\tau_q u \in L_2(\Gamma)$ if and only if $-\frac{d^2}{dx^2}u \equiv -u'' \in L_2(\Gamma)$. We have proven that

$$\mathrm{Dom}\,(L_q^{\max}) = W_2^2(\Gamma \setminus \mathbf{V}), \tag{1.20}$$

since every function from this domain is mapped by τ_q into a function from the Hilbert space. We stress once more that formula (1.20) holds under the assumption that $q \in L_\infty(\Gamma)$. The maximal operator is not symmetric, but it is an extension of the minimal operator $L_q^{\min}$, since the differential expression τ_q is formally symmetric. Therefore any self-adjoint operator L_q associated with the differential expression τ_q satisfies:

$$\mathrm{Dom}\,(L_q^{\min}) \subset \mathrm{Dom}\,(L_q) \subset \mathrm{Dom}\,(L_q^{\max}). \tag{1.21}$$

Our task is to specify the domain of the self-adjoint operator L_q. To solve such a problem it is standard to use von Neumann extension theory for symmetric operators which characterizes all possible extensions, but our goal is to describe those extensions that correspond to the graph Γ. Note that neither the minimal nor the maximal operator respect how different edges are connected to each other - each of these operators can be written as an orthogonal sum of operators in $L_2(E_n)$:

$$L_q^{\min}(\Gamma) = \bigoplus_{n=1}^{N} L_q^{\min}(E_n), \qquad L_q^{\max}(\Gamma) = \bigoplus_{n=1}^{N} L_q^{\max}(E_n), \tag{1.22}$$

where to define $L_q^{\max/\min}(E_n)$ we consider each edge E_n as a graph formed by one edge. Thus selecting the domain of L_q one has to respect the topological structure. Therefore we prefer to use a constructive approach to describe the self-adjoint extensions.[3]

To understand whether an operator is symmetric or not it is useful to calculate the boundary form, which vanishes if the operator is symmetric. Let us calculate

[3]Another possibility would be to use the theory of boundary triples, since the minimal operator has finite deficiency indices (equal to the number of endpoints). In fact differential operators on metric graphs is an area where the theory of boundary triples can be applied.

the boundary form for the maximal operator:[4]

$$
\begin{aligned}
&\langle L_q^{\max} u, v\rangle - \langle u, L_q^{\max} v\rangle \\
&= \sum_{n=1}^{N} \left\{ \int_{E_n} \overline{\left[-\frac{d^2}{dx^2} + q(x)\right] u(x)} \cdot v(x) dx \right. \\
&\qquad \left. - \int_{E_n} \overline{u(x)} \cdot \left[-\frac{d^2}{dx^2} + q(x)\right] v(x) dx \right\} \qquad (1.23) \\
&= \sum_{x_j \in \mathbf{V}} \left\{ \overline{\partial_{\mathbf{n}} u(x_j)} \cdot v(x_j) - \overline{u(x_j)} \cdot \partial_{\mathbf{n}} v(x_j) \right\},
\end{aligned}
$$

where we used notations (1.12) and (1.13). The limits are taken as x approaches the endpoint x_j from inside the edge. The limits in (1.23) exist since the functions u and v belong to the Sobolev space $W_2^2(E_n)$. In formula (1.23), one should ignore the right endpoints in the case of semi-infinite edges. We see that the boundary form does not necessarily vanish if no further conditions on the functions are introduced.

The minimal operator $L_q^{\min}$ is symmetric, since it is given by the same differential expression on the domain $\operatorname{Dom}(L_q^{\min}) = C_0^\infty(\Gamma \setminus \mathbf{V}) \subset W_2^2(\Gamma \setminus \mathbf{V}) = \operatorname{Dom}(L_q^{\max})$, and the values $u(x_j), \partial u(x_j)$ are equal to zero:

$$\langle L_q^{\min} u, v\rangle = \langle u, L_q^{\min} v\rangle.$$

The differential operator τ_q can be made self-adjoint by restricting the maximal operator using certain vertex conditions described below: in the following subsection we give an example of such conditions, while the most general case is discussed in Chapter 2.

1.1.3. Standard vertex conditions. The vertex conditions are needed in order to make the differential operator self-adjoint, but their role is not limited to this. These conditions should relate only the values $u(x_j), \partial u(x_j)$ associated with the same vertex. These conditions should also be irreducible so that the vertex cannot be divided into two or more smaller vertices (in which case the vertex conditions would connect the values belonging to each of the smaller vertices separately). Then the vertex conditions would correctly reflect how different edges in Γ are connected to each other.

The set of all appropriate vertex conditions is well-understood and will be described in Chapter 2. We start with describing here the most natural conditions to be called **standard vertex conditions** imposed at each vertex V^m

$$
\begin{cases}
x_i, x_j \in V^m \Rightarrow u(x_i) = u(x_j) & - \textbf{continuity} \text{ condition}, \\
\displaystyle\sum_{x_j \in V^m} \partial_{\mathbf{n}} u(x_j) = 0 & - \textbf{Kirchhoff} \text{ condition}.
\end{cases} \qquad (1.24)
$$

For every m formula (1.24) gives d^m independent conditions on the function u, where d^m is the valence of the vertex V^m. These two conditions together are sometimes called **Kirchhoff, Neumann, natural**, or **free** in the literature, but we

[4]Here we use the convention from mathematical physics that the scalar product in a Hilbert space is linear in the second argument and anti-linear in the first one: $\langle \alpha u, \beta v\rangle = \overline{\alpha}\beta\langle u, v\rangle,\ \alpha, \beta \in \mathbb{C}$.

prefer to reserve the name Kirchhoff for the balans condition on the derivatives alone.

For degree one vertices, these conditions are reduced to just one Neumann condition as follows

$$\partial u(x_j) = 0,\ x_j \in V^m,\ \ d^m = 1. \tag{1.25}$$

This fact explains why standard vertex conditions are often called Neumann.

In the case of two intervals joined together, the standard vertex conditions imply that the function and its extended derivative are continuous at this vertex. The vertex can be removed in this case and two intervals may be substituted by one with the length equal to the sum of the lengths of the two original intervals. This property explains why standard conditions are sometimes called free. Any other condition at such vertex corresponds to a certain point interaction or separates the two intervals.

We have just described so-called standard vertex conditions. These conditions are often chosen when it is not known which particular properties of the vertex are required from the model.

1.1.4. Definition of the operator. In this subsection, we are going to sum up our discussions and define the standard Schrödinger operator under the stronger assumption (1.18) on the potential.

Definition 1.2. *The* **standard Schrödinger operator** L_q^{st} *is defined by the differential expression (1.15) on the domain of functions from the Sobolev space* $W_2^2(\Gamma \setminus \mathbf{V})$ *satisfying the standard vertex conditions (1.24) at all vertices.*

The standard Schrödinger and Laplace operators are defined similarly. In what follows we shall often use the simplified notation L_q for the operator with standard vertex conditions. This is motivated by the fact that the standard operators are uniquely determined by the metric graphs and the differential expressions. Moreover, the standard Laplacian is determined by the metric graph alone.

The standard operators are self-adjoint. This fact will be proved in the following chapter, but already now we can see that these operators are symmetric. Consider the boundary form given by (1.23), and rearrange the summation as follows

$$\begin{aligned} &\langle L_q^{\mathrm{st}} u, v\rangle - \langle u, L_q^{\mathrm{st}} v\rangle \\ = &\sum_{m=1}^{M} \left\{ \underbrace{\left(\sum_{x_j \in V^m} \overline{\partial_{\mathbf{n}} u(x_j)} \right)}_{=0} v(V^m) - \overline{u(V^m)} \underbrace{\left(\sum_{x_j \in V^m} \partial_{\mathbf{n}} v(x_j) \right)}_{=0} \right\} = 0. \end{aligned}$$

Note that the values $u(V^m), v(V^m)$ are well-defined, since the functions satisfying the standard vertex conditions are continuous even at the vertices. The sum of the extended normal derivatives over each particular vertex is zero due to the Kirchhoff condition in (1.24), hence the boundary form is zero implying that the operator is symmetric.

In what follows we are going to call by **quantum graph** any Schrödinger operator on a metric graph refereeing to its spectrum as the **spectrum of the quantum graph**. The standard Laplacians is uniquely determined by the metric graph, therefore we are going to refer to its spectrum as the **spectrum of the**

metric graph. Few chapters below will be devoted to the spectral analysis of metric graphs.

1.2. Elementary examples

In this section we are going to look at few examples of quantum graphs and calculate their spectra. A function $f \in L_2(\Gamma)$ is an eigenfunction of the operator L_q^{st} if and only if it satisfies the eigenfunction equation

$$-\frac{d^2}{dx^2}\psi(x) + q(x)\psi(x) = \lambda\psi(x) \tag{1.26}$$

on every edge and vertex conditions at every vertex, in our case standard vertex conditions (1.24). Here, λ is the spectral parameter. Generalised eigenfunctions corresponding to the continuous spectrum are not necessarily from $L_2(\Gamma)$ but satisfy the same differential equation and vertex conditions. We are going to discuss spectral properties of quantum graphs in more detail later on, but consider elementary examples here. In all these examples the potentials will be identically equal to zero, hence we are going to look at spectral properties of metric graphs.

The ring graph. Consider the ring graph $\Gamma_{(1.2)}$ depicted in Fig. 1.4. The corresponding standard Laplacian L has purely discrete spectrum and we are going to calculate it. It is clear that only the length of the interval is importanrt hence let us identify the edge with the interval $[x_1, x_2] = [-\ell_1/2, \ell_1/2]$, ℓ_1 is the length of the ring.

The differential equation (1.26) takes the form

$$-\psi'' = k^2\psi \tag{1.27}$$

and the standard vertex conditions (1.24) are

$$\begin{cases} \psi(-\ell_1/2) = \psi(\ell_1/2), \\ \psi'(-\ell_1/2) = \psi'(\ell_1/2). \end{cases}$$

Consider first the case $\lambda = 0$, then the general solution to the differential equation is given by

$$\psi(x) = Ax + B.$$

Substitution into the vertex conditions gives unique (up to a multiplier) eigenfunction

$$\psi_1(x) = 1.$$

Assume that $\lambda \neq 0$ then any solution to the differential equation (1.27) can be written as

$$\psi(x) = c_1 \cos kx + c_2 \sin kx, \quad c_1, c_2 \in \mathbb{C}. \tag{1.28}$$

Substituting (1.28) into the vertex conditions we get the homogeneous linear system

$$\begin{cases} \cos k\ell_1/2 \cdot c_1 - \sin k\ell_1/2 \cdot c_2 = \cos k\ell_1/2 \cdot c_1 + \sin k\ell_1/2 \cdot c_2, \\ k \sin k\ell_1/2 \cdot c_1 + k \cos k\ell_1/2 \cdot c_2 = -k \sin k\ell_1/2 \cdot c_1 + k \cos k\ell_1/2 \cdot c_2, \end{cases}$$

$$\Rightarrow \begin{cases} \sin k\ell_1/2 \cdot c_2 = 0, \\ \\ \sin k\ell_1/2 \cdot c_1 = 0. \end{cases}$$

The eigenvalues $\left(\frac{2\pi}{\ell_1}\right)^2 n^2, n = 1, 2, 3, \dots$, have multiplicity 2 with the eigenfunctions

$$\psi_n^{\mathrm{e}}(x) = \cos\left(\frac{2\pi}{\ell_1} nx\right), \quad \psi_n^{\mathrm{o}}(x) = \sin\left(\frac{2\pi}{\ell_1} nx\right).$$

The eigenfunctions can be divided into even and odd ones due to the fact the operator is invariant under the change of variables $x \mapsto -x$. The appearance of multiple eigenvalues distinguishes this operator from any Schrödinger operator on a finite interval. Of course the eigenvalues satisfy Weyl's asymptotic law (see (4.14) below).

The lasso graph. Next consider the non-compact lasso graph Γ formed by a ring and one semi-infinite interval attached to it. This graph can be defined as a union of two intervals $[x_1, x_2]$ and $[x_3, \infty)$ with the endpoints x_1, x_2, and x_3 identified, *i.e.* the graph has one vertex $V^1 = \{x_1, x_2, x_3\}$.

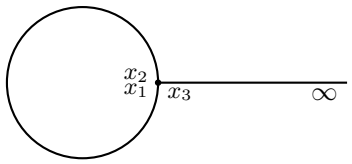

FIGURE 1.5. Non-compact lasso graph

Consider the standard Laplace operator L defined on the functions from $W_2^2(\Gamma \setminus V^1)$ and satisfying standard vertex conditions at the vertex V^1.

The spectrum of L is formed by the branch $[0, \infty)$ of absolutely continuous spectrum and an infinite sequence of (embedded) eigenvalues λ_n tending to $+\infty$. The generalised eigenfunctions corresponding to the absolutely continuous spectrum are solutions to the differential equation (1.27) satisfying the vertex conditions that are bounded linear functionals but do not belong to the domain of the operator or even to the Hilbert space. These functions are given by a combination of incoming and outgoing waves on the semi-infinite edges.[5]

For the sake of convenience, let us choose the parametrization of the edges so that

$$E_1 = [x_1, x_2] = [-\ell_1/2, \ell_1/2], \quad E_2 = [x_3, \infty) = [0, \infty).$$

The operator is invariant under the change of variables

$$J : x \mapsto \begin{cases} -x, & x \in E_1, \\ x, & x \in E_2. \end{cases}$$

This change of variables preserves all points on the semi-infinite interval and reflects the finite interval. Even and odd eigenfunctions can be calculated separately. The eigenfunctions including generalised eigenfunctions corresponding to the absolutely continuous spectrum are solutions to (1.27) on every edge satisfying the standard vertex conditions at the vertex.

The odd eigenfunctions satisfying $Ju = -u$ are necessarily equal to zero on the semi-infinite interval. On the loop these functions are given by

$$\psi = c \sin kx.$$

[5]For example the Dirichlet Laplacian on $[0, \infty)$ has generalised eigenfunctions given by regular at the origin solutions of (1.27) $\psi = \sin kx$, $k \in \mathbf{R}_+$.

Substitution into the vertex conditions gives:

$$\begin{cases} c\sin k\ell_1/2 = c\sin k(-\ell_1)/2 = u(x_3) = 0; \\ kc\cos k\ell_1/2 - kc\cos k(-\ell_1)/2 + u'(x_3) = kc\cos k\ell_1/2 - kc\cos k(-\ell_1)/2 + 0 = 0. \end{cases}$$

The second condition is satisfied for any k, while the first condition gives us the quantization rule:

$$\sin k\ell_1/2 = 0 \Rightarrow k = \frac{2\pi}{\ell_1}n,\ n = 1, 2, \dots$$

The corresponding eigenvalues are

$$\left(\frac{2\pi}{\ell_1}\right)^2 n^2, \quad n = 1, 2, 3, \dots .$$

The even eigenfunctions are scattered waves ψ and we use the usual representation with the reflection coefficient R

$$\psi(x) = \begin{cases} c\cos kx, & x \in E_1, \\ \exp(-ikx) + R(k)\exp(ikx), & x \in E_2. \end{cases} \tag{1.29}$$

The component ψ_{E_2} is written as a sum of the incoming wave $\exp(-ikx)$ with the unit amplitude and of the outgoing wave $\exp(ikx)$ with the amplitude R in order to remind the scattering theory for the one-dimensional Schrödinger equation, where this representation holds asymptotically for large x [?ReSi]. The coefficient R is then called the reflection coefficient. Substitution into the vertex conditions gives the 2×2 linear system

$$\begin{cases} c\cos k\ell/2 = 1 + R \\ 2ck\sin k\ell/2 + ik(-1 + R) = 0 \end{cases} \Rightarrow \begin{pmatrix} \cos k\ell/2 & -1 \\ 2\sin k\ell/2 & i \end{pmatrix} \begin{pmatrix} c \\ R \end{pmatrix} = \begin{pmatrix} 1 \\ i \end{pmatrix}.$$

Solving the system we get the reflection coefficient

$$R(k) = \frac{\cos k\ell/2 + 2i\sin k\ell/2}{\cos k\ell/2 - 2i\sin k\ell/2}. \tag{1.30}$$

The reflection coefficient has modulus one on the real axis $k \in \mathbb{R}$. The singularities are situated at the points where $\tan k\ell/2 = i/2$. These points are different from k_n calculated earlier.

It follows that the discrete spectrum of the operator on a graph cannot always be determined from the corresponding scattering coefficient, which is the case for the Schrödinger operator in $\mathbf{R}^n$. In our example, the discrete spectrum eigenfunctions and the scattered waves belong to different subspaces in the Hilbert space $L_2(\Gamma)$, *i.e.* the eigenfunctions possess different symmetries, hence it is not surprising that the singularities of the scattering coefficient do not coincide with the discrete spectrum. One may think that this phenomena occurs just due to the symmetry of the graph Γ. In my opinion, the symmetry just facilitates occurrence of this phenomena, but is not necessary. The reason that the discrete spectrum eigenfunctions are not *seen* from the scattering coefficient is that they are vanishing at the vertex V^1.

Figure eight graph and isoscattering. Using symmetries of metric graphs, one may construct interesting examples of isospectral and isoscattering graphs. Two quantum graphs are called **isoscattering** if the corresponding scattering matrices[6] are equal. Of course the isoscattering property depends heavily on the potential.

[6]If you are not familiar with the definition of the stationary scattering matrix, consult Section 2.3 (where the vertex scattering matrix is introduced).

Since the Laplace operator on a metric graph is uniquely determined by the metric graph, one speaks about isoscattering graphs if the scattering matrices for the two Laplacians coincide. The first example of isoscattering graphs was constructed in [?KuSt], and is presented in Fig. 1.8. It is assumed that the following relations between the lengths of the graphs hold:

$$\begin{aligned} &\ell_1 = \ell_2 = \ell'_1 + \ell'_3 = \ell'_2 + \ell'_4; \\ &\ell'_1 = \ell'_2. \end{aligned} \tag{1.31}$$

It is remarkable that these two graphs have different topological structure. This counterexample shows that the scattering matrix does not determine the number of cycles in the graph or its size, since the lengths $\ell'_1 = \ell'_2$ can be chosen arbitrarily.

PROBLEM 1. *Prove that $\lambda_1 = 0$ is an eigenvalue for the standard Laplacian on any compact finite graph. What is the multiplicity of this eigenvalue?*

PROBLEM 2. *Calculate the spectrum of the standard Laplacian of the compact star graph formed by three intervals of length* 1*, shown in Fig. 1.6.*

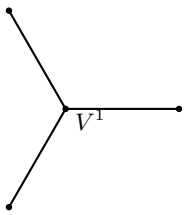

FIGURE 1.6. Compact star graph $\Gamma_{(3.2)}$

PROBLEM 3. *Calculate the spectrum of the standard Laplacian on the figure eight graph $\Gamma_{(2.4)}$ shown in Fig. 1.7, assuming that*

(a) the lengths of the loops are equal $\ell_1 = \ell_2 = \pi$,
(b) the lengths ℓ_1 and ℓ_2 are arbitrary.

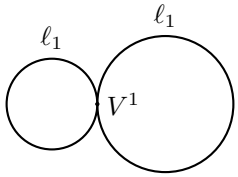

FIGURE 1.7. Figure eight graph $\Gamma_{(2.4)}$

PROBLEM 4. *Consider any compact metric graph and the standard Laplacian on it. What happens to the spectrum if one doubles the lengths of all edges?*

PROBLEM 5 (Kurasov-Stenberg). [?KuSt] *Consider the two graphs Γ and Γ' presented in Fig. 1.8. Prove that the scattering matrices for the Laplace operators on the graphs Γ and Γ' are equal under the assumption that*

$$\begin{aligned} &\ell_1 = \ell_2 = \ell'_1 + \ell'_3 = \ell'_2 + \ell'_4; \\ &\ell'_1 = \ell'_2;\ \ell'_3 = \ell'_4. \end{aligned}$$

Calculate the scattering matrix for the graph Γ. *Calculate the spectra of the Laplacians on* Γ *and* Γ'

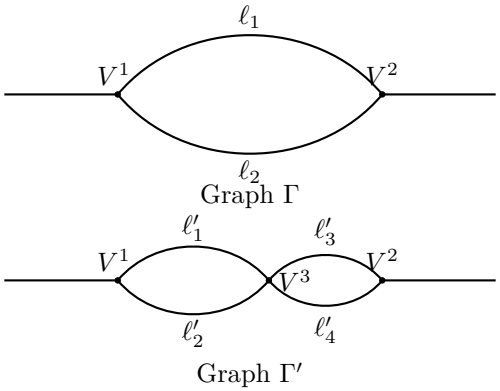

FIGURE 1.8. Two topologically different graphs having the same scattering matrix

Isospectral graphs. Two operators are called **isospectral** if they have the same spectrum. We present here one example of isospectral graphs developed by B. Gutkin and U. Smilansky in [?GuSm]. This example grew up from the famous counterexample to M. Kac' question 'Can one hear the shape of a drum?' formulated in 1966. The counterexample constructed by C. Gordon, D.L. Webb, and S. Wolpert [?GoWeWo] may be modified in order to simulate metric graphs. As the counterexample provided two drums having precisely the same Laplacian spectrum, the two obtained metric graphs isospectral. The two isospectral graphs (trees) presented first in [?GuSm] are shown in the Figure 1.9.

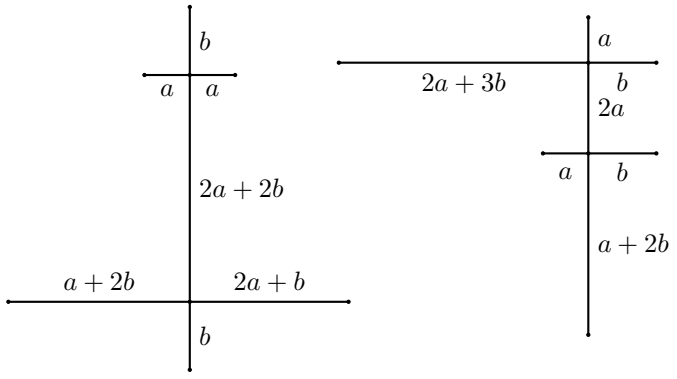

FIGURE 1.9. Gutkin-Smilansky isospectral graphs

PROBLEM 6 (Gutkin-Smilansky [?GuSm]). *The spectra of the Laplacians on the graphs presented in Fig. 1.9 are given by zeroes of the following two functions*

[?GuSm]
(1.32)

$$\begin{aligned} Z_I(k) &= \tan(2(a+b)k) \\ &+ \frac{2\tan ak + 2\tan bk + \tan(2a+b)k + \tan(a+2b)k}{1-(2\tan ak+\tan bk)\,(\tan bk+\tan(2a+b)k+\tan(a+2b)k)}, \end{aligned}$$

$$\begin{aligned} Z_{II}(k) &= \tan 2ak \\ &+ \frac{2\tan ak + 2\tan bk + \tan(a+2b)k + \tan(2a+3b)k}{1-(\tan ak+\tan bk+\tan(a+2b)k)\,(\tan ak+\tan bk+\tan(2a+3b)k)}. \end{aligned}$$

Show that the zeroes of the two functions $Z_I(k)$ and $Z_{II}(k)$ coincide.

PROBLEM 7 (Parzanchevski-Band [?PaBa]). *Consider the Laplace operator defined on the graphs depicted in Fig. 1.10. Dirichlet and Neumann conditions*[7] *(indicated by letters D and N) are introduced at different degree one vertices and standard vertex conditions at all internal vertices. Prove that the corresponding operators are isospespectral assuming the indicated lengths of the edges.*

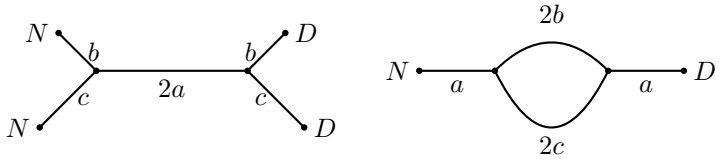

FIGURE 1.10. Parzanchevski-Band graphs

PROBLEM 8 (Kurasov-Muller). *The two graphs depicted in Fig. 5.3 are equilateral, i.e. all edge lengths are equal. Calculate graphs spectra and show that they are isospectral.*

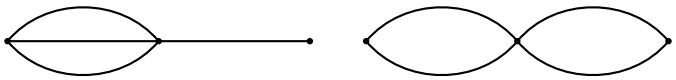

FIGURE 1.11. Kurasov-Muller graphs

There is no general understanding how isospectral graphs may be constructed. It is clear that the edge lengths of such graphs have to be rationally dependent (as will be shown in Section 10.3) and it is believed that symmetry arguments should play an important role in classification of isospectral families. Gutkin-Smilansly and Parzanchevski-Band examples appear reducing large graphs with symmetries to certain fundamental domains. The last example (Kurasov-Muller) [?KuMu4] can be constructed by cutting in two different ways one of the vertices in the watermelon graph $\mathbf{W}_4$.

[7]The Dirichlet and Neumann conditions at degree one vertices are $u(x_j)=0, x_j=V^m$ and $\partial_{\mathbf{n}}\psi(x_j)=0, x_j=V^m$ respectively.

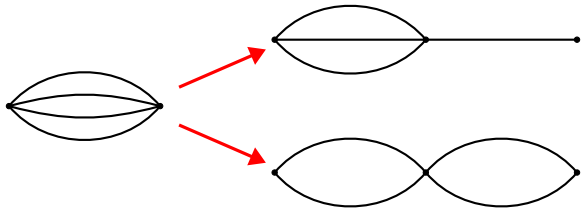

FIGURE 1.12. The watermelon graph $\mathbf{W}_4$ and its two cuts