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On the ground state of quantum graphs: δ-conditions and potentials

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Abstract

Quantum graphs consists of differential operators acting on metric graphs with matching conditions at its vertices. One of their main properties that are studied is their eigenvalues which can be described by their quadratic form. Using the quadratic form, quantum graphs with δ-interaction at its vertices are investigated. By looking at how changes in the metric graph and the matching conditions affect the quadratic form a number of useful tools for analysing the ground state energy are formulated. They are then used to show a sharp lower bound on the ground state energy for the Laplace operator on such graphs, and to find the graph with the lowest ground state energy. Similar methods are then used to find a non-sharp upper bound. The results are then generalized from the Laplacian to the Shrödinger operator with standard conditions, where the upper bound turn out to be part of a more general theorem.

Acknowledgements

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Contents

Introduction

The study of quantum graphs originates from physics and chemistry, and even though the study is purely mathematical, it is motivated mainly by physics. The first person to study systems similar to quantum graphs was the double Nobel laureate Linus Paul who studied free electrons in molecules during the 1930s. To study quantum graphs is to study differential operators on networks or metric graphs with certain conditions at its vertices. The main aspects studied are usually the eigenfunctions and the eigenvalues of the operator, which have clear physical interpretations.

The most common operator to study is different variants of the (magnetic) Schrödinger operator, defined using the differential expression

$$\left(i\frac{d}{dx} + a(x)\right)^2 + q(x).$$

The Schrödinger operator describes the motion of a free particle, for example an electron, influenced by a magnetic potential $a(x)$ and an electric potential $q(x)$.

One physical interpretation of a quantum graph is thus as an approximation of a two or three dimensional system using a graph, where the matching conditions corresponds to different kind of behavior at certain points.

In this thesis a special kind of quantum graph with so called δ-interaction at its vertices is studied. The goal is to find lower and upper bounds for the lowest eigenvalue of them, the so called ground state energy.

Chapter 1

Quantum graphs

In this chapter quantum graphs are introduced, and some of their properties are examined. Focus is on explaining the basic concepts and ideas as well as introducing some of the questions that will be investigated later on. A more complete description of quantum graphs containing more background theory can be found in [3] or [8].

1.1 The definition of quantum graphs

A quantum graph consists of three things:

- a metric graph,
- a self-adjoint differential operator acting on the metric graph,
- matching conditions at the vertices of the metric graph.

The metric graph of a quantum graph will sometimes be referred to the underlying graph of the quantum graph, and the operator as the associated operator of the quantum graph. This chapter introduces these three components together with some of the basic properties of quantum graphs. The main focus is on the Laplace operator acting on a specific class of graphs with so called δ-conditions, as well as on the Schrödinger operator.

1.1.1 The metric graph

In discrete mathematics a graph is just a set of vertices that are connected in a certain way. How they connect is usually described by a set of pairs containing every two vertices that are connected, meaning that the edges are just reduced to pairs of end points. A metric graph can be described as a combinatorial graph where the edges have been assigned a specific length or weight. Here another definition than the combinatorial one, namely one where where the graphs are constructed by gluing intervals together, will be used as it shifts the focus towards the edges.

Consider a set of N intervals $E = \{e_n\}_{n=1}^{\infty}$, where each edge e_i is defined as

$$e_i = \begin{cases} [x_{2i-1}, x_{2i}] : & i \in [0, N_C] \\ [x_{2i-1}, \infty) : & i \in [N_C + 1, N], \end{cases}$$

and where N_C is the number of compact edges of finite length in E. Let V be the set of all end points of the edges in E. The intervals can then be combined into a metric graph by dividing V into subsets V_m such that

$$V_m \cap V_n = \emptyset \text{ for } m \neq n, \text{ and } V = \bigcup_i V_i.$$

Each V_m then corresponds to the vertices of the graph. Metric graphs can thus be viewed as a number of closed intervals, who's endpoints have been identified with each other in a certain way. This construction is much more useful than the combinatorial one, as it emphasises that the graph consists of intervals, connected in a certain way. We give a formal definition of a metric graph.

Definition. A set of N closed or semi-infinite intervals E together with a partition of the set of their endpoints V into equivalence classes is called a **metric graph**. The intervals in E are called **edges** of the graph, and the equivalence classes of V are called the **vertices** of the graph. The end points belonging to the same vertex are identified.

Note that the graph does not need to be realisable in the plane or $\mathbb{R}^n$ at all. The definition does not limit the number of edges to a finite number, but only graphs with a finite number of edges will be studied in this thesis.

Each edge $e_m = [x_{2m-1}, x_{2m}]$ of a metric graph Γ has a length l_m defined as $l_m = x_{2m} - x_{2m-1}$. The length of the whole graph is denoted by $\mathcal{L}(\Gamma)$ and is

defined as the sum of the lengths of the individual edges of Γ. The length can only be defined for graphs where each edge is of finite length.

A metric graph is said to be **connected** if there exists a path connecting any two points on the graph. The spectrum of a disconnected graph is simply the sum of the spectrum of the disconnected components, so they can be studied separately. All graphs will thus be assumed to be connected. Graphs with edges of infinite length lack some important properties, which makes many of the interesting questions about quantum graphs trivial. All graphs will thus also be assumed to be of finite length.

As a metric graph consists of intervals it is possible to define functions on the interior of the edges. The biggest space of functions on a metric graph Γ that will be considered is the Hilbert space $L^2(\Gamma)$. It is defined as the sum of the individual L^2-spaces that can be defined on the interior of the edges e_n. Formally it is defined as

$$L^2(\Gamma) = \bigoplus_{e_n \in \Gamma} L^2(e_n \setminus V).$$

The scalar product in the space will be defined as the sum of the scalar products on the separate edges by:

$$\langle f, g \rangle = \int_\Gamma f(x)\overline{g(x)}dx = \sum_{e_n \in \Gamma} \int_{e_n} f(x)\overline{g(x)}dx.$$

The values of the functions at the endpoints of the edges is a little trickier question as two endpoints that belongs to the same vertices are considered as the same point of the graph. To expand the functions to the end points of the interval the following definition will be used:

$$f(x_j) = \lim_{x \to x_j} f(x)$$

if x_j is an endpoint and where the limits is the one sided limit taken from the inside of the interval. In most cases the problem of the value of functions at the endpoints will disappear as the functions will be assumed to be continuous at the vertices. If the function is continuous at a vertex v, the notation $f(v)$ will be used to denote the value of the function at all endpoints belonging to v. With the extension of the functions to the endpoints, the derivative of any function from $L^2(\Gamma)$ can be defined on every edge and thus on the whole graph. Instead of the usual derivative of the function, the **normal derivatives** will be used at the endpoints. They are defined as

$$\partial u(x_i) = \begin{cases} \lim\limits_{x \to x_j} \frac{d}{dx} u(x) & \text{if } x_j = x_{2m+1}, \text{ i.e. } x_j \text{ is the left end point,} \\ -\lim\limits_{x \to x_j} \frac{d}{dx} u(x) & \text{if } x_j = x_{2m}, \text{ i.e. } x_j \text{ is the right end point.} \end{cases}$$

Normal derivatives are thus the same as the usual derivative, but with a possibly different sign at the endpoints of an interval. The virtue of this definition will be made clearer later on as it makes the formulation of matching conditions easier. The normal derivative in the left endpoints is also called the outgoing derivative.

1.1.2 The differential operator

As a metric graph can be viewed as a number of intervals glued together, it is possible to define a differential operator on the graph by defining it on the interior of every edge separately, and adding conditions at the vertices. Recall that a self-adjoint operator L is an operator on a vector space with an inner product (e.g. the Hilbert space $L^2(\Gamma)$) that is its own adjoint. A more thorough description of self adjoint operators can be found in Appendix A.

The operators that are mainly studied for quantum graphs are the ones that can be defined using the following formal expressions:

- The Laplacian L_0 defined as

$$L_0 = -\frac{d^2}{dx^2}.$$

- The Schrödinger operator L_q defined as

$$L_q = -\frac{d^2}{dx^2} + q(x),$$

  where $q(x)$ is called the electric potential.

- The magnetic Schrödinger operator $L_{q,a}$ defined as

$$L_{q,a} = \left(i\frac{d}{dx} + a(x)\right)^2 + q(x),$$

  where $q(x)$ is called the electric potential and $a(x)$ the magnetic potential.

The magnetic Schrödinger operator describes the movement of a quantum particle influenced by a magnetic potential $a(x)$ and an electric potential $q(x)$.

Clearly the first two operators are special cases of the last one. Putting $a(x) \equiv 0$ gives

$$L_{q,a=0} = L_q,$$

and putting $q(x) \equiv 0$ as well gives

$$L_{q=0,a=0} = L_{q=0} = L_0$$

which motivates denoting the Laplace operator with L_0. Arbitrary self-adjoint operators will be denoted by L without subscript.

In the text, we will not go into any details about the magnetic Schrödinger operator, but focus on the first two. The magnetic Schrödinger operator are only introduced for the completeness of the theory, and the potential $a(x)$ will usually be assumed to be identically equal to zero.

The electric potential $q(x)$ is assumed to be real valued and in $L^2(\Gamma)$, and to vanish sufficiently fast on infinite edges in the sense that

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

In Chapter 3, the δ-distribution will also be used as a potential.

The formal expressions above can be defined on different dense subsets of the Hilbert space L^2, and thus becoming different operators. Two very important operators are the **minimal** and the **maximal** operators defined using the Schrödinger differential expression. The minimal operator is defined on $C_0(\Gamma \setminus V)$ which is the set of all continuous functions with compact support on each edge (i.e. that are zero in all vertices). The maximal operator is defined on Sobolev space $W_2^2(\Gamma \setminus V))$ which is the set of all L^2-functions with their second derivative in L^2 as well. This is basically the biggest subset of L^2 that is mapped into L^2 by the Schrödinger operator. Both of these domains are dense in the set $L^2(\Gamma)$ and all interesting operators are defined on some domain in between the domains of these two. The minimal and maximal operator are studied in more detail in Appendix A.

1.1.3 Matching condition

The matching conditions describe the connection of the functions at the vertices. From a physical point of view this can be interpreted as different kinds of behavior of a quantum particle (recall that the Schrödinger operator

describes particles). The matching conditions also are important in order to make the operators self adjoint.

Some of the most studied kinds of conditions are the following:

- **Dirichlet-conditions**, requiring that all functions fulfills

$$\begin{cases} \psi \text{ is continuous at } v \\ \psi(v) = 0 \end{cases}$$

  at every vertex $v \in V$. Note that the first condition is implied by the second one. It is included just to emphasis the similarity between this and the next condition.

- **Neumann-conditions** or **standard conditions**, requiring that all functions fulfills

$$\begin{cases} \psi \text{ is continuous at } v \\ \sum\limits_{x_k \in V} \partial\psi(x_k) = 0 \end{cases}$$

  at every vertex $v \in V$.

- **δ-conditions** describing δ-interaction in the vertices. This is defined as

$$\begin{cases} \psi \text{ is continuous at } v \\ \sum\limits_{x_k \in v} \partial\psi(x_k) = \alpha_v \psi(v) \end{cases}$$

  at every vertex $v \in V$.

These are just a few of all possible matching conditions that makes the operator self-adjoint. All possible matching conditions have been described in many different ways, for example in [3] and [8].

1.1.4 Summary

The description of a quantum graph as a triplet of a metric graph, a differential expression and matching conditions is very useful as it emphasize the different aspects of a quantum graphs. As seen above, these three parts are not independent. The matching conditions are defined at the vertices of the metric graph, and the operator is defined on the metric graph using

the matching conditions. For these reasons there are many different ways to describe properties of quantum graphs, useful in different situations. When one of the things change, so must the others. Usually it is not necessary to go into the details of this. For example, we will later look at a graph and what happens when one vertex is split in two. This creates a new graph, so a new operator must be defined on it. There is however no ambiguity in how to translate the old operator to the new graph, so this will not be commented on. The matching conditions can however be chosen in many different ways, so they will be discussed in detail.

1.2 The spectrum

The three parts introduced above constitutes a quantum graph. There are of course many questions that can be asked about them, but the main thing investigated is the spectrum of the graphs, which is the collection of eigenvalues of the operator acting on the underlying metric graph. Many questions can be asked about the spectrum. The most basic one is how to determine it, but also inverse problems and methods for estimating the spectrum have been studied by many authors, for example in [1], [10] and [3].

As we will see later on, finding the spectrum of a graph can be very hard, and an analytic solution to the equations describing the spectrum can often not be found. This makes the question of estimates and bounds on the eigenvalues relevant.

The main question that will be dealt with here is "how does the graph influence the eigenvalue?" and how that can be used to create upper and lower bounds for the first eigenvalue.

1.2.1 The eigenvalues of a quantum graph

The spectrum of a quantum graph is the collection of eigenvalues of the differential operator acting on the metric graph. The eigenvalues of an operator L is the real values of λ for which there exists a function u that fulfills the eigenvalue equation

$$Lu = \lambda u.$$

If the graph has no infinite edge, as is always assumed here, then the spectrum is purely discrete and grows towards infinity. The spectrum of all operators

studied here is also bounded from below. This makes it possible to index the eigenvalues as $\{\lambda_n\}_{n=0}^{\infty}$ such that $\lambda_n \leq \lambda_{n+1}$. With this indexing, which always will be used, the eigenvalues fulfils the Weyl asymptotics

$$\frac{\lambda_n}{n^2} \to \frac{\pi^2}{\mathcal{L}(\Gamma)^2} \text{ as } n \to \infty.$$

Each eigenvalue λ_n has an associated eigenfunction u_n which is the function that fulfills the equation

$$Lu = \lambda_n u.$$

As is known for self-adjoint operators, their eigenfunctions can be chosen orthogonal, and spans the whole Hilbert space. It is possible that there exists m orthogonal functions for which λ is an eigenvalue. We then say that λ has multiplicity m. If the i:th eigenvalue has multiplicity m, then the eigenvalues will be indexed such that

$$\lambda_i = \lambda_{i+1} = ... = \lambda_{i+m-1}$$

meaning that the eigenvalues are counted as many times as their multiplicity.

For the Laplace operator the eigenvalue equation becomes

$$-u'' = \lambda u,$$

which has the solution

$$u(x) = A\sin(\sqrt{\lambda}x) + B\cos(\sqrt{\lambda}x).$$

As $\sqrt{\lambda}$ occurs in every solution to the eigenvalue equation it is convenient to introduce the variable k which is defined by $k^2 = \lambda$. k will through out the text be used as the square root of λ with out explicitly defining it as such every time. By the square root, or $\sqrt{\cdot}$, we will always mean the square root with the branch cut along the positive real axis. This means that k will always be in the closed upper half-plane.

For $\lambda = 0$ another possible solution is

$$u(x) = Ax + B.$$

This solution does rarely fulfil any of the matching conditions studied here, so it will usually not be important.

1.2.2 The ground state energy

The physical interpretation of the eigenvalues is as the possible energy levels of the system described by the differential operator. From that point of view the lowest eigenvalue λ_0 corresponds to the lowest possible energy state of the system, which makes it interesting to examine. For this reason the first eigenvalue is called the **ground state** or the **ground state energy** of the system. The main goal of the following chapters is to determine an upper and lower bound for the ground state energy of quantum graphs with δ-conditions and quantum graphs with the Schrödinger operator.

1.2.3 Graphs with δ-conditions

An important part of this thesis is quantum graphs consisting of the Laplace operator acting on finite graphs with δ-conditions. Recall that a graph with δ-conditions is a graph that at every vertex $v_i \in V$ has the conditions

$$\begin{cases} u \text{ is continuous at } v \\ \sum_{x_k \in v} \partial u(x_k) = \alpha_v u(v) \end{cases}$$

for some $\alpha_i \in \mathbb{R}$. α_i will always be used to denote the constant in the conditions at the vertex v_i, and we define

$$\alpha(\Gamma) = \alpha = \sum_i \alpha_i.$$

The α_i of a quantum graphs are usually called the strengths of the graphs. For simplicity, all requirements of the graphs studied in this thesis are collected in the following definition.

Definition. A quantum graph consisting of a connected metric graph of finite length and with a finite number of edges, the Laplace operators, and δ-conditions is called a δ**-graph**.

An observation that will be useful later on is that for δ-graphs where $\alpha_i \neq 0$ for any i, the constant function can not be an eigenfunction, as it does not fulfill the vertex conditions at the vertices where $\alpha_i \neq 0$. By adding vertices to the interior of the edges, it is thus possible to ensure that there always will be two vertices where the function attains different values.

1.2.4 The spectrum of commuting operators

There are some standard techniques for calculating the eigenvalues of a differential operator without having to do all the calculations. One of the most useful of those is a theorem that states that the eigenfunctions of two commuting operators can be chosen to be equal. A more complete discussion of this theorem, together with its proof, can be found in [9].

Proposition 1. *Let A and B be two self-adjoint operators with*

$$AB = BA$$

such that the domain of AB and BA are the same. Then the eigenfunctions of A and B can be chosen to be equal.

An example of how this theorem can be used is when $A = -\frac{d^2}{dx^2}$ (the Laplacian), and $B : f(x) \mapsto f(-x)$. We can then see that $B^2 = I$ where I is the identity. If u is an eigenfunction to B, then $Bu = \lambda u$, and thus is $u = Iu = B^2u = B\lambda u = \lambda^2 u$. This shows that $\lambda = \pm 1$, so the eigenfunctions of B must be even or odd, so it follows that the eigenfunctions of A can be chosen to be even or odd. As the eigenfunctions of the Laplacian are $u(x) = A\sin(kx) + B\cos(kx)$, it follows that the eigenfunctions can be chosen to be either $A\sin(kx)$ or $B\cos(kx)$. Dealing with these functions separately makes the equations much simpler to work with.

It is worth noticing that this is only possible to do when there exists such an operator, which usually happens when the graph has some kind of mirror or rotational symmetry. It will for example be used in a following example of a quantum graph in the form of a loop.

1.2.5 Examples

To illustrate the concepts introduced in this chapter, some examples of quantum graphs will be introduced, and using the techniques presented above their spectra will be calculated or described. The three graphs here are chosen with care as they all illustrates important aspects of the spectrum of quantum graphs. Some of these results will also be useful in the following chapters.

The interval

The simplest possible δ-graph is the interval with $\alpha_1 = 0$ and $\alpha_2 = \alpha$, illustrated in Figure 1.1.

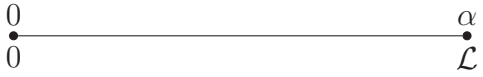


Figure 1.1: The interval with δ-conditions with the strengths in each point indicated (above), together with its parametrization (below).

The solutions of the eigenvalue equation are of the form

$$u(x) = A\sin(kx) + B\cos(kx),$$

or

$$u(x) = Cx + D.$$

For the linear functions the vertex conditions is

$$u'(0) = C = 0 \text{ and } u'(\mathcal{L}) = u(\mathcal{L}),$$

which gives

$$\begin{cases} u(x) = 0, \\ D\mathcal{L} = 0. \end{cases}$$

This gives that $C = D = 0$, so the linear function is not a solution.

For the other solution, we get

$$u'(x) = Ak\cos(kx) - Bk\sin(kx).$$

At the left endpoint we have the condition

$$u'(0) = 0 \cdot u(0) = 0,$$

which implies that $u'(0) = A = 0$, so the function is just a cosine function. In the right endpoint the function must fulfil

$$-u'(\mathcal{L}) = \alpha u(\mathcal{L}),$$

which translates into

$$Bk\sin(k\mathcal{L}) = \alpha B\cos(k\mathcal{L}).$$

Rewriting it a little gives

$$k\tan(k\mathcal{L}) = \alpha.$$

This equation not does have an analytic solution in the general case. We can however draw some conclusions about the eigenvalues by considering the function $k\tan(k\mathcal{L})$. The equation does not have any complex solutions for $\alpha_v > 0$, and for $\alpha_v < 0$ it has two purely imaginary, where the second one is just minus the first one, so both gives the same eigenvalues. We are however only interested in solutions in the upper half-plane, due to the branch cut, so only one imaginary solution (corresponding to a negative eigenvalue) exists. The function behaves very similar to the tangent function, and drawing it on the real axis for some $\mathcal{L}$ gives the graph in Figure 1.2.

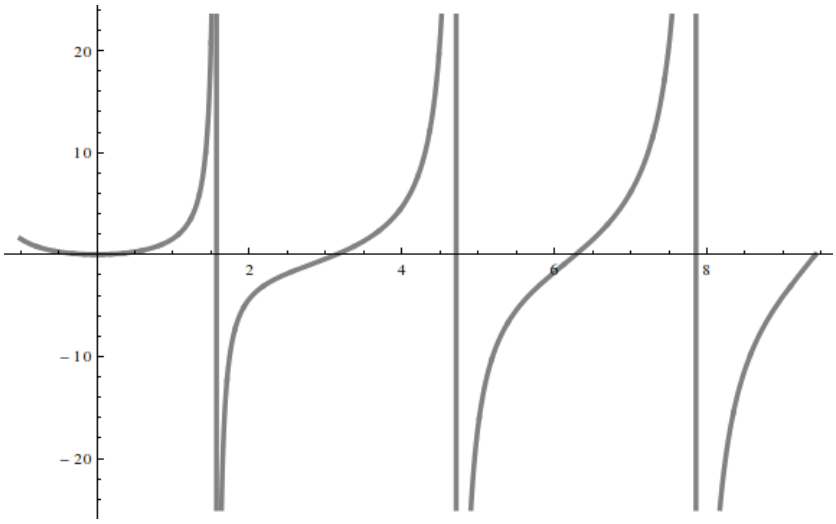


Figure 1.2: $k\tan(k)$ plotted from -1 to 3π. Note that the function assume each value exactly once between every singularity (indicated by the vertical lines).

This shows that the solutions are bounded by the singularities of the function $\tan(k\mathcal{L})$. From the branch cut it follows that all negative solutions are irrelevant. On the imaginary axis the function behaves a little differently, which are shown in the graph in Figure 1.3 below.

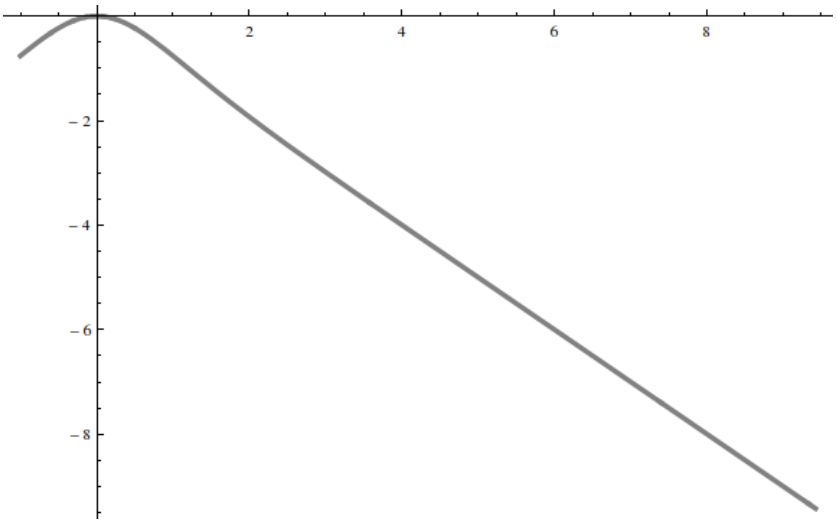


Figure 1.3: $k\tan(k)$ plotted from $-i$ to $3\pi i$. The function assume each negative value once on the upper axis.

This shows that if $\alpha > 0$, then there are no negative eigenvalues, but if $\alpha < 0$ there will always be one. This means that for $\alpha > 0$ and $n > 0$,

$$\left(\frac{\pi}{2\mathcal{L}}(n-1)\right)^2 \leq \lambda_n \leq \left(\frac{\pi}{2\mathcal{L}}n\right)^2 \tag{1.1}$$

which shows that λ_n in fact fulfils the Weyl asymptotic introduced earlier. What happens when α reduces is that the lowest eigenvalue becomes smaller and smaller without bound, and every other eigenvalue will converges to their lower bound as can be seen in (1.1).

The star graph

An example of a graph where most of the eigenvalues can be calculated explicitly is the symmetric star graph which is a common name for graphs consisting of any finite number of edges of the same length joined together at one vertex as shown in Figure 1.4.

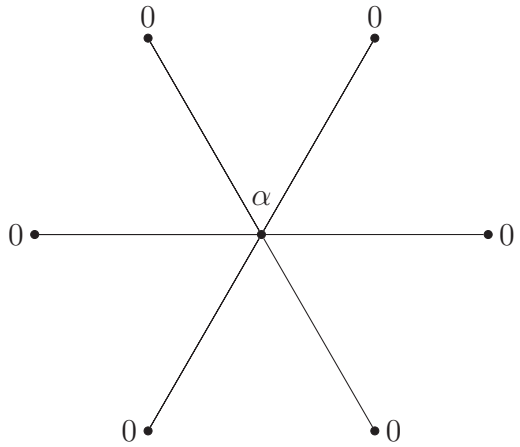


Figure 1.4: The symmetric star graph with δ-conditions. The strengths in each vertex are indicated.

We solve the eigenvalue problem for a star graph with m edges. Parametrise the graph such that each edges ends at the middle vertex. The linear function can not be a solution here either, as the conditions at the outer vertices then would require it to be constant, which does not fulfil the conditions in the middle vertex. If the edges are indexed from 1 to m, then the function on the i:th edge is given by $u_i(x) = A_i \sin(kx) + B_i \cos(kx)$.

The condition at the outer vertex of an arbitrary edge then gives:

$$u'(x) = A_i = 0.$$

In the middle vertex the conditions then becomes:

$$\begin{cases} u_i(\frac{\mathcal{L}}{m}) = u_j(\frac{\mathcal{L}}{m}) \\ \sum_{i=1}^{m} B_i k \sin(\frac{\mathcal{L}}{m}k) = \alpha B_i \cos(\frac{\mathcal{L}}{m}k) \end{cases}.$$

The first condition is either fulfilled if $B_i = B_j$ for all i, j, or if the function is zero in the middle. If the function is zero in the middle vertex, the system if reduced to

$$\begin{cases} u_i(x) = B_i \cos(kx) \\ \sum_{i=1}^{m} B_i \sin(\frac{\mathcal{L}}{m}) = 0. \end{cases}$$

This has the solutions

$$k = \frac{m\pi}{2\mathcal{L}} + \frac{n\pi}{\mathcal{L}}m, \quad n \in \mathbb{N}.$$

where each eigenvalue have $m-1$ as the constants B_i can be chosen in $m-1$ independent ways. Note that these eigenvalues does not depend on α in any way.

On the other hand, if

$$k \neq \frac{m\pi}{2\mathcal{L}} + \frac{n\pi}{\mathcal{L}}m, \quad n \in \mathbb{N},$$

then $B_i = B_j$ must hold. This gives

$$km\sin(\frac{\mathcal{L}}{m}k) = \alpha\cos(\frac{\mathcal{L}}{m}k)$$

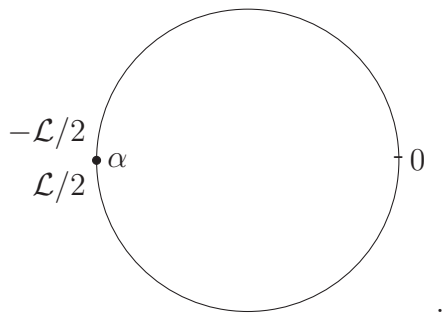
which is the same equation as

$$km\tan(\frac{\mathcal{L}}{m}k) = \alpha.$$

The eigenvalues of the star graph are thus described by the solutions to the equation above, as well as the singularities of the function $m\tan(\frac{L}{m}k)$.

The loop graph

The loop graph is a graph consisting of a single loop. Its spectrum can be calculated directly, but it is much easier to use Proposition 1. We parametrize the graph as shown in Figure 1.2.5.



This parametrization creates a very useful reflection symmetry of the graph. Let S be the operator which takes $u(x)$ to $u(-x)$ on the loop. Then

$$SL_0 = L_0S$$

since

$$LSu(x) = -\frac{\partial^2}{\partial x^2}u(-x) = -(-1)^2u''(-x) = -u''(-x) = SLu(x).$$

From the definition of their domain, it is easy to see that they coincide. Proposition 1 then states that their eigenfunctions can be chosen to coincide. As $S^2u(x) = u(x)$, $S^2 = I$, so the eigenvalues of S must be 1 or -1.

By definition, the only functions that fulfills $u(-x) = \pm u(x)$ are even or odd functions. We know from earlier that the eigenfunctions of L_0 are $A\sin(kx)+B\cos(kx)$. The constant function can not be a solution here either due to the vertex conditins. For them to be even or odd A or B must be zero. This gives that the eigenfunctions of S, and thus the eigenfunctions of L_0, can be chosen as $A\sin(kx)$ and $B\cos(kx)$. It is thus possible to calculate the spectrum of the loop graph by looking at even and odd solutions separately.

If the function is even, then it is symmetric around zero. As it is defined on a circle it must also be symmetric around the point $\frac{\mathcal{L}}{2}$. As $\sin(0) = 0$, we get the following:

$$A\sin(\frac{\mathcal{L}}{2}k) = 0 \quad \Leftrightarrow \quad k = \frac{2\pi}{\mathcal{L}}n \quad n \in \mathbb{N}.$$

Furthermore, the function must fulfill

$$2Ak\sin(kL/2) = \alpha A\cos(\frac{\mathcal{L}}{2}k) \quad \Leftrightarrow \quad k\tan(kL/2) = \frac{\alpha}{2}. \tag{1.2}$$

This is again very similar to the solutions to the interval.

For $u(x) = B\cos(kx)$ we instead get that

$$\begin{cases} -B\sin(0) = 0 \\ -2B\sin(\frac{\mathcal{L}}{2}k) = 0 \end{cases}$$

This have the solution

$$k = \frac{\mathcal{L}}{2}\pi n.$$

The spectrum of the loop graph is thus given by the solutions to Equation 1.2 and by $k = \frac{\mathcal{L}}{2}\pi n$. It is easy to see that these two interlace. It is interesting to once again note how some of the eigenvalues depends on α while some does not, and how the ones that increase with alpha are bounded by the one unaffected of it.

1.3 The quadratic form and the Rayleigh quotient

A very useful tool for analysing the spectrum of a quantum graph is the quadratic form and the Rayleigh quotient. In this section some properties of the quadratic form are introduced and examined, together with the basic concept of the Rayleigh quotient.

For every operator L on a graph Γ, a quadratic form can be defined by

$$\langle Lu(x), u(x)\rangle_\gamma = \int_\Gamma Lu(x)\cdot\overline{u(x)}dx.$$

The subscript indicates in what space the quadratic form is from, and will be dropped whenever there is no risk of ambiguity.

Interpreting the integral in the quadratic form formally it is possible to write the quadratic form of the Schrödinger operator as

$$\begin{aligned}
\langle L_q u, u\rangle_\Gamma &= \int_\Gamma(-u''(x)+q(x)u(x))\overline{u(x)}dx\\
&= -\int_\Gamma u''(x)\overline{u(x)}dx+\int_\Gamma q(x)|u(x)|^2dx\\
&= \int_\Gamma|u'|^2dx+\sum_i\left[u_i'(x_{2i-1})\overline{u_i(x_{2i-1})}-u_i'(x_{2i})\overline{u_i(x_{2i})}\right]+\int_\Gamma q(x)|u(x)|^2dx\\
&= \int_\Gamma|u'|^2dx+\sum_i\left[\partial u_i(x_{2i-1})\overline{u_i(x_{2i-1})}+\partial u_i(x_{2i})\overline{u_i(x_{2i})}\right]+\int_\Gamma q(x)|u(x)|^2dx.\\
&= \langle L_0u(x),u(x)\rangle+\langle q(x)u(x),u(x)\rangle
\end{aligned}$$

This gives a way to extend the domain of the quadratic form as the intersection of the domain of $\langle L_0u(x),u(x)\rangle$ and $\langle q(x)u(x),u(x)\rangle$. The expression

$$\langle L_0u(x),u(x)\rangle=\int_\Gamma|u'|^2dx+\sum_i\left[\partial u_i(x_{2i-1})\overline{u_i(x_{2i-1})}+\partial u_i(x_{2i})\overline{u_i(x_{2i})}\right]$$

is clearly defined for all functions with a derivative in L^2 that are continuous over the vertices, in other words it is defined for all $u\in W_2^1(\Gamma)$, where

$$W_2^1(\Gamma)=\{u\in L_2(\Gamma\setminus V)|u \text{ is continuous on } \Gamma\}.$$

The second quadratic form

$$\langle q(x)u(x),u(x)\rangle=\int_\Gamma q(x)|u(x)|^2$$

is defined for all functions in L^2 (which contains W_2^1) when q is nice. If the potential is not nice, the domain can be smaller.

As will be shown later on, the function that minimizes the quadratic form is the first eigenfunctions. Expanding the domain could thus make this property untrue, if doing so adds an function whit a smaller value in the form, but as it turns out, any function from W_2^1 that minimizes the quadratic form must also be from W_2^2.

The domain of the quadratic form on a graph Γ is denoted by $\mathrm{dom}_Q(\Gamma)$. We make a formal definition of the quadratic form.

Definition. The **quadratic form** of the Schrödinger operator L_q is defined as

$$\langle L_0 u(x), u(x)\rangle + \langle q(x)u(x), u(x)\rangle$$

where L_0 is the Laplacian with standard conditions. The form is defined on the intersection of the domain of the two forms, which is $W_2^1(\Gamma)$ and the subset of $W_2^1(\Gamma)$ where $\langle q(x)u(x), u(x)\rangle$ is defined. This means that

$$dom_Q(L_q) = \{u \in W_2^1 || \langle q(x)u(x), u(x)\rangle| < \infty\}.$$

Using that the quadratic form is defined on some subset of $W_2^1(\Gamma)$ makes it possible to reconstruct the operator from the form. This means that the quadratic form uniquely determines the operator, so if two operators have the same quadratic form they actually are the same operators.

From now on the quadratic form will be used to define the Schrödinger operator, not the other way around, as it makes it easier to study the eigenvalues and the similarities between different operators. The Schrödinger operator $L_q = -\frac{d^2}{dx^2} + q$ will always be assumed to denote the operator defined by the quadratic form of

$$\langle L_0 u, u\rangle + \langle qu, u\rangle$$

where L_0 is the Laplacian with standard conditions. This means that the boundary terms disappear, making the quadratic form

$$\int_\gamma |u'(x)|^2 dx + \int_\Gamma q(x)|u(x)|^2 dx.$$

We start our analysis of the quadratic form with two basic theorems concerning δ-graphs.

Lemma 1.1. *The quadratic form of the Laplace operator on a δ-graph is given by*

$$\langle Lu, u\rangle = \int_\Gamma |u'|^2 dx + \sum_{v\in V} \alpha_v |u(v)|^2$$

where V is the set of vertices of Γ.

Proof. Let e_i denote the edges and V the set of vertices of Γ. Then

$$\begin{aligned}
\langle Lu, u\rangle_\Gamma &= \int_\Gamma -u''(x)\overline{u(x)}dx \\
&= \int_\Gamma |u'|^2 dx + \sum_i u_i'(x_{2i-1})\overline{u_i(x_{2i-1})} - u_i'(x_{2i})\overline{u_i(x_{2i})} \\
&= \int_\Gamma |u'|^2 dx + \sum_i \partial u_i(x_{2i-1})\overline{u_i(x_{2i-1})} + \partial u_i(x_{2i})\overline{u_i(x_{2i})} \\
&= \int_\Gamma |u'|^2 dx + \sum_{v\in V} [\overline{u_i(v)} \underbrace{\sum_{x_k\in v} \partial u(x_k)}_{=\alpha_v u(v)}] \\
&= \int_\Gamma |u'|^2 dx + \sum_{v\in V} \alpha_v |u(v)|^2.
\end{aligned}$$

The last step is possible as the function $u(x)$ is continuous over the vertices. □

Another useful theorem that follows directly from the definition of the quadratic form is the following regarding how the domain depends on the δ-conditions.

Lemma 1.2. *Let L and $\widehat{L}$ be two Laplace operators acting on the same metric graph Γ with different δ-conditions. Then the domain of the quadratic forms of L and $\widehat{L}$ coincide.*

Proof. The result follows directly from that there are no requirement on the potential or the value of the derivative at certain point in the definition of the domain of quadratic form. □

Using the quadratic form of an operator L, it is possible to define the Rayleigh quotient of a quantum graph.

Definition. The **Rayleigh quotient** $R(u)$ of a quantum graph is the normed quadratic form defined as

$$R(u) = \frac{\langle Lu, u\rangle}{\langle u, u\rangle}$$

for every function $u(x) \neq 0$ in the domain of the quadratic form.

The Rayleigh quotient has the curious property that it is minimized by the first eigenfunction, and that its minimal value is the first eigenvalue. This, together with a generalization to all eigenvalues is described in Theorem 1.1 below.

Theorem 1.1. *The first eigenvalue of a self-adjoint operator L is given by the minimum value of the Rayleigh quotient on the domain of the quadratic form. Further more,*

$$\lambda_n(L) = \min_{u \perp u_i, i<n} \frac{\langle Lu, u\rangle}{\langle u, u\rangle} \quad \textit{for } u \neq 0,$$

where u_i denotes the i:th eigenfunction. The function from the domain of the quadratic form that minimizes the expression above is the n:th eigenfunction.

Proof. Recall that the eigenvalues of a self-adjoint operator on a graph is bounded from below, and that they are indexed such that $\lambda_n \leq \lambda_{n+1}$.

Every function in the domain of a self-adjoint operator can be expressed as a linear combination of its eigenvalues. So if $\{u_n\}_{n=0}^{\infty}$ denotes the eigenfunctions of a self-adjoint operator L, then any function u in its domain can be expressed as

$$u = \sum_{n=0}^{\infty} \langle u, u_n\rangle \, u_n.$$

The Rayleigh quotient for a function u can thus be expanded as follows.

$$\begin{aligned}
\frac{\langle Lu, u\rangle}{\langle u, u\rangle} &= \frac{\left\langle \sum_n L \langle u, u_i\rangle \, u_i, u \right\rangle}{\langle u, u\rangle} \\
&= \frac{\left\langle \sum_n \lambda_i \langle u, u_i\rangle \, u_i, u \right\rangle}{\langle u, u\rangle} \\
&= \frac{\sum_n \lambda_n \langle u, u_i\rangle \langle u_i, u\rangle}{\langle u, u\rangle} \\
&\geq \lambda_0 \frac{\sum_n |\langle u, u_i\rangle|^2}{\sum_n |\langle u, u_i\rangle|^2} \\
&= \lambda_0
\end{aligned}$$

This shows that the minimal value of the Rayleigh quotient is λ_0. The inequality becomes an equality if and only if $\langle u, u_i \rangle = 0$ for all $i \neq 0$, which shows that if a function u minimizes the quadratic form then u must be the first eigenfunction.

This proves the first statement of the theorem. To see the result for λ_n, assume that we are only looking at functions orthogonal to the first $n-1$ eigenfunctions. This means that $\langle u, u_i \rangle = 0$ for $i < n$. Using the calculations above we see that

$$\begin{aligned}
\frac{\langle Lu, u \rangle}{\langle u, u \rangle} &= \frac{\left\langle \sum_{i=n}^{\infty} L \langle u, u_i \rangle u_i, u \right\rangle}{\langle u, u \rangle} \\
&= \frac{\sum_{i=n}^{\infty} \lambda_i |\langle u, u_i \rangle|^2}{\sum_{n} |\langle u, u_i \rangle|^2} \\
&\geq \lambda_n \frac{\sum_{i=n}^{\infty} |\langle u, u_i \rangle|^2}{\sum_{n} |\langle u, u_i \rangle|^2} \\
&= \lambda_n
\end{aligned}$$

and

$$\lambda_n = \frac{\langle Lu_n, u_n \rangle}{\langle u_n, u_n \rangle} \leq \frac{\langle Lu, u \rangle}{\langle u, u \rangle}.$$

for all functions u orthogonal to the first $n-1$ eigenfunctions of L. In other words

$$\lambda_n = \frac{\langle Lu_n, u_n \rangle}{\langle u_n, u_n \rangle} \leq \frac{\langle Lu, u \rangle}{\langle u, u \rangle}.$$

This concludes the proof. □

This theorem means that it it possible to look at the quadratic form and how it changes to determine how different changes of the quantum graph effect its spectrum.

The denominator of the quadratic form is the square of the norm of the function, so for functions of norm 1 the Rayleigh quotient simply becomes the quadratic form. An equivalent to finding the function that minimizes the Rayleigh quotient is thus to find the function with norm 1 that minimizes the quadratic form.

Chapter 2

Estimates on the ground state energy

A natural question to ask is if there exist a lower and an upper bound for the ground state energy of a quantum graph, and if so, what they are. In this chapter we examine how different parameters influence the ground state energy in order to find bounds for it subject to some natural constraints of the graph.

A related question to ask is what graph has the lowest or highest eigenvalue. This question goes hand in hand with the previous one, and it is possible that the two can be answered at the same time.

This chapter only deals with the Laplacian with δ-conditions. The results will be generalized to the Schrödinger operator in Chapter 3. Many of the results presented will be given for all eigenvalues, and some of the other results can be generalized to all λ_n by following analogous arguments.

2.1 The length, the strengths and the eigenvalues of a graph

In this chapter a lower and an upper bound for the ground state energy will be proven. There is, however, no general smallest or highest ground state energy for δ-graphs, so the bounds can only be formulated in terms of some characteristics of the graph.

From the previous chapter we know that the eigenvalues of the star graph can be made sufficiently small as long as the total lengths of the graph is made sufficiently large. One might wonder if this is a special property of the star graph (and the other graphs in the examples) or not. From the Weyl asymptotics it follows that

$$\lambda_n \sim \left(\frac{\pi}{\mathcal{L}} n\right)^2,$$

which tells us how the length of the graph affect the larger eigenvalues, but nothing about the smaller one. One can thus ask if it is always true that the eigenvalues become smaller if the graph is scaled with some factor greater than one.

From the quadratic form it can be easily seen that if a function $u(x)$ with norm 1 minimizes the quadratic form for some graph Γ, then the function $\hat{u}(x) = \frac{1}{\sqrt{t}} u(\frac{x}{t})$ minimizes the quadratic form of the graph Γ_t, created from Γ by scaling it with a factor t. The factor $\frac{1}{\sqrt{t}}$ is necessary in order to make the norm of $\hat{u}(x)$ equal to 1.

Parametrising each edge E_n^t of a graph with δ-conditions from 0 to $\mathcal{L}(E_i)$, and plugging $\hat{u}(x)$ into the quadratic form gives

$$\begin{aligned}
\langle L_0\hat{u}(x), \hat{u}(x)\rangle_{\Gamma_t} &= \sum_{n=1}^{N} \int_{E_n} |\hat{u}'(x)|^2 dx + \sum_v \alpha \hat{u}(v)^2 \\
&= \sum_{n=1}^{N} \int_0^{\mathcal{L}(E_n^t)} |\hat{u}'(x)|^2 dx + \sum_v \alpha \hat{u}(v)^2 \\
&= \{s = \frac{x}{t}\} \\
&= \sum_{n=1}^{N} \int_0^{\mathcal{L}(E_n)} t \cdot |\hat{u}'(st)|^2 ds + \sum_v \alpha \hat{u}(v)^2 \\
&= \sum_{n=1}^{N} \int_0^{\mathcal{L}(E_n)} t \cdot \frac{1}{t^3} |u'(s)|^2 ds + \sum_v \alpha \hat{u}(v)^2 \\
&= \sum_{n=1}^{N} \int_0^{\mathcal{L}(E_n)} t \cdot \frac{1}{t^3} |u'(s)|^2 ds + \frac{1}{t} \sum_v \alpha \hat{u}(v)^2 \\
&= \frac{1}{t} \cdot \left(\frac{1}{t} \sum_{n=1}^{N} \int_0^{\mathcal{L}(E_n)} |u'(s)|^2 ds + \sum_v \alpha u(v)^2 \right)
\end{aligned}$$

where $\mathcal{L}(E_n)$ denotes the length of the n:th edge of Γ, and $\mathcal{L}(E_n^t)$ the length

of E_n^t.

The last step follows as

$$\hat{u}'(st) = \frac{1}{\sqrt{t}} \cdot \frac{1}{t} u'(s)$$

and

$$\hat{u}(v) = \frac{1}{\sqrt{t}} u(v) \quad \text{for all vertices } v.$$

This is very similar to the quadratic form of the graph Γ (the unscaled one), and it shows that the eigenvalues has a tendency to scale in some way with the length of the graph. Letting t go to infinity pushes the value of the quadratic form for all functions with a given norm, and thus the eigenvalues, towards zero. Letting t go to zero will instead make the form go towards $\pm\infty$. This shows that when looking for a bound of the spectrum it is necessary to do so subject to a given total length of the metric graph, as it is always possible to make the eigenvalues larger or smaller by simply scaling the metric graph.

It also follows that if a graph is scaled with t, and the strength α with $\frac{1}{t}$, then the value of the quadratic form for a function on Γ, and its corresponding function on Γ_t, will scale with $\frac{1}{t^2}$ in the sense that

$$\lambda_n(\Gamma_t) = \frac{1}{t^2} \lambda_n(\Gamma).$$

In the examples earlier, the eigenvalues all depended positively on the strengths of the δ-conditions. Looking at the conditions at the vertices it is not obvious that this will always be the case, but looking at the quadratic form it is possible to formulate the following simple relation between the strengths and the eigenvalues.

Lemma 2.1. *The eigenvalues of a δ-graph depends positively (in fact non-negatively) on each strength α_v at the vertices of the graph.*

Proof. As can be seen directly from the quadratic form in Theorem 1.1, increasing any α_v increases the value of the Rayleigh quotient for all functions. This proves the statement. □

Based on this lemma one might suggest that another good constraint is the sum of the strengths, $\sum_i \alpha_i$. This idea, however, does not work properly if some α_v are negative. The argument is simple: let $u(x)$ be the first eigenfunction of the δ-graph Γ. Then it minimizes the quadratic form

$$\langle \mathcal{L}\psi, \psi \rangle_\Gamma = \int_\Gamma |\psi'|^2 dx + \sum_{v \in V} \alpha_v |\psi(v)|^2.$$

From earlier it is known that there always exist two points where the eigenfunctions attain different values. It, thus, follows that there must be two points v_1 and v_2 that can be viewed as vertices, provided that not all $\alpha_i = 0$, such that $u(v_1) < u(v_2)$. If both are positive, then decreasing α_2 and increasing α_1 such that their sum is constant would make it possible to make the quadratic form arbitrarily negative without changing the sum of the strength. If $u(v_1)$ is smaller than zero, the same process is possible by decreasing α_1 and increasing α_2.

A better version of the constraint is that the sums of the absolute values should be equal to a given number. The sum of the absolute values of individual strengths will from now on be denoted by $|\alpha|$.

The dependence of the eigenvalues on the strengths is different from the dependence on the length. When the parameters α_v increase on a given graph, the eigenvalues do increase. They do not however go to infinity, but converges to some value from below. The eigenvalues of a quantum graph are thus bounded subject to the underlying metric graph and the strength. This is shown and dealt with in details in [3].

2.2 A lower bound on the ground state energy

There are many possible approaches to the question of which δ-graph has the lowest eigenvalues, and what those values are. In this section the Rayleigh quotient is used to analyse how different changes in the matching condition and in the metric graph effect the spectrum of δ-graphs.

2.2.1 How changes in the quantum graph affect the eigenvalues

One of the most apparent property of a graph is how the edges connect, and a fundamental question is how this affect the eigenvalues. A higher connectivity does, on one hand, force more conditions on the values of the

eigenfunction at the vertices due to the continuity criteria, but can on the other hand it allow more freedom as the functions can be chosen such that the derivatives cancel each other out. For example, in a vertex of degree two the value of ingoing and outgoing derivatives must be equal, but if we add another edge then the values of two of the derivatives can be chosen independent of each other. The domain of the quadratic form does however tell different story. As stated in Theorem 1.2 the domain of the quadratic form does not depend on the values of the derivative at a specific point. This gives the following very useful theorem.

Theorem 2.1. *Let v be a vertex of the δ-graph Γ with the vertex condition*

$$\begin{cases} \psi \text{ is continuous at } v \\ \sum_{x_k \in v} \partial\psi(x_k) = \alpha_v \psi(v) \end{cases}$$

and let $\widehat{\Gamma}$ be the graph obtained from Γ by separating the vertex v into two vertices v' and v'' and endowing them with vertex conditions

$$\begin{cases} \psi \text{ is continuous at } v' \\ \sum_{x_k \in v'} \partial\psi(x_k) = \alpha_{v'} \psi(v') \end{cases} \quad \text{and} \quad \begin{cases} \psi \text{ is continuous at } v'' \\ \sum_{x_k \in v''} \partial\psi(x_k) = \alpha_{v''} \psi(v'') \end{cases}$$

such that $\alpha_{v'} + \alpha_{v''} = \alpha_v$. Then

$$\lambda_0(\widehat{\Gamma}) \leq \lambda_0(\Gamma).$$

Proof. Expressing $\lambda_0(\Gamma)$ and $\lambda_0(\widehat{\Gamma})$ using the Rayleigh quotient gives:

$$\lambda_0(\Gamma) = \left(\min_{\substack{||u||=1 \\ u \in \mathrm{dom}_Q(\Gamma)}} \langle Lu, u \rangle \right) \quad \text{and} \quad \lambda_0(\widehat{\Gamma}) = \left(\min_{\substack{||u||=1 \\ u \in \mathrm{dom}_Q(\Gamma')}} \langle Lu, u \rangle \right).$$

Any $u \in \mathrm{dom}_Q(\Gamma)$ can be identified with a function $\hat{u}$ in $\mathrm{dom}_Q(\widehat{\Gamma})$ with $R(u) = \hat{R}(\hat{u})$ and $||u|| = ||\hat{u}||$. Either $\hat{u}$ is the function minimizing $\hat{R}$, or there exists some function where $\hat{R}$ is even smaller. This gives that

$$\lambda_0(\widehat{\Gamma}) \leq \lambda_0(\Gamma).$$

□

This result can be generalized with an analogous argument to all eigenvalues of the graphs Γ and $\hat{\Gamma}$.

The theorem basically states that for any quantum graph, the graph created from it by cutting it in its vertices or edges (as a vertex with $\alpha_v = 0$ can be placed anywhere), and splitting the strengths between the new vertices, has a lower ground state energy.

Another interesting question is how the distribution of the strengths over the graph affect the ground state energy. Looking at the Rayleigh quotient it becomes reasonable to assume that concentrating the strengths to one point would decrease the eigenvalues as it makes it possible to "escape" the region where a trial function is large, by choosing another function with a low value at that point. This argument is quite hard to formalize, but a similar result can be obtained by a simpler argument. We start with a lemma.

Lemma 2.2. *In every δ-graph Γ where all α_i has the same sign, there is a vertex v' such that changing the δ-conditions of Γ such that $\alpha_{v'} = \sum_{v\in\Gamma} \alpha_v = \alpha$ at v', and putting standard conditions ($\alpha_v = 0$) at all other vertices, gives a new quantum graph $\widehat{\Gamma}$ with*

$$\lambda_0(\widehat{\Gamma}) \leq \lambda_0(\Gamma).$$

Proof. Assume that all $\alpha_i > 0$, and let $u \in \mathrm{dom}_Q(\Gamma)$ be the function that minimizes the Rayleigh quotient of Γ. Then u is the first eigenfunction of Γ, corresponding to the eigenvalue λ_0. Let v' be the vertex where $|u(x)|$ attains the smallest value and $\widehat{\Gamma}$ be the graph created from Γ by putting $\alpha_v = 0$ for all $v \neq v'$ and $\alpha_{v'} = \alpha$. By Lemma 1.2 $\mathrm{dom}_Q(\Gamma) = \mathrm{dom}_Q(\widehat{\Gamma})$, so $u \in \mathrm{dom}_Q(\Gamma')$. Together with Lemma 1.1 this gives that

$$\langle Lu, u\rangle_\Gamma = \int_\Gamma |u'|^2 dx + \sum_{v\in V} \alpha_v |u(v)|^2 \geq \int_\Gamma |u'|^2 dx + \alpha |u(v')|^2 = \langle \mathcal{L}u, u\rangle_{\widehat{\Gamma}}.$$

From this it follows directly that

$$\lambda_0(\widehat{\Gamma}) = \min_{||\psi||=1, \psi\in \mathrm{dom}_Q(\Gamma)} \frac{\langle L\psi, \psi\rangle_{\widehat{\Gamma}}}{\langle \psi, \psi\rangle} \leq \frac{\langle Lu, u\rangle_{\widehat{\Gamma}}}{\langle u, u\rangle} \leq \frac{\langle Lu, u\rangle_\Gamma}{\langle u, u\rangle} = \lambda_0(\Gamma).$$

The results for negative strengths follows by a similar inequality by choosing the vertex where the function assumes its highest values instead. □

This result can be generalized to δ-graphs where the signs of the strength different, by first changing all the signs to negative ones, which reduces the eigenvalues, and then applying the theorem.

Theorem 2.2. *Every δ-graph Γ has a vertex v' such that changing the δ-conditions of Γ such that $\alpha_{v'} = -\sum_{v\in\Gamma} |\alpha_v|$ at v', and putting standard conditions ($\alpha_v = 0$) at all other vertices, gives a new quantum graph $\widehat{\Gamma}$ with*

$$\lambda_0(\widehat{\Gamma}) \leq \lambda_0(\Gamma).$$

Proof. From Lemma 2.1 it is known that the eigenvalues depends positively on each α_i. Changing the matching condition of Γ by multiplying each positive α_i with -1 would thus reduce the eigenvalues. From Lemma 2.2 it is known that the graph created by moving all strengths into a certain vertex reduces the values of all eigenvalues further. This proves the theorem. □

The usefulness of this theorem is apparent as the condition in vertices with $\alpha_i = 0$ is much easier to deal with. Consolidating all strengths at one point also makes the dependence of the strength much more apparent.

The double cover of a graph

From any δ-graph Γ it is possible to construct a certain "double cover" defined in the following way.

Definition. Let Γ be a δ-graph. The graph Γ^2 created from Γ by

- for each edge between two vertices of a given length, adding another edge between the same two vertices of the same length, and
- changing the matching conditions by doubling the strengths in every vertex,

is called the **double cover** of Γ.

An example of a graph and its double cover can be seen in figure 2.1 below.

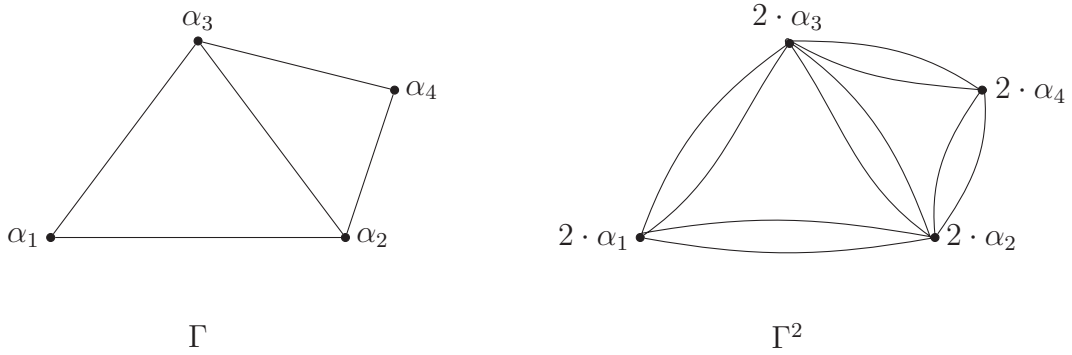


Figure 2.1: An example of Γ and Γ^2, with the strengths in each vertex indicated.

This operation might appear strange, but it will prove to be useful later on due to the similarities of the eigenvalues of the loop graph and the interval. An important property of the double cover of a graph is that the degree of all vertices is even, as the number of connected edges is doubled. This makes it much easier to cut the graph into a useful shape using Theorem 2.1. As the total length of the double cover is twice that of the graph, a reasonable guess is that the double cover has lower eigenvalues than the original graph.

The idea of using the double cover originates from an article by Kurasov and Naboko [10], where graph graphs are cut using so called Eulerian path. A **Eulerian path** on a graph is a path that visit every edge of the graph exactly once, and starts and ends at the same vertex. It is a widely known theorem (by Euler) that a graph has has an Eulerian path if and only if the degree of all vertices is even. Such graphs can thus be cut into loops by cutting each vertex such that only edges connected in the Eulerian path are connected in the graph. In order for this to work, it must be shown that the double cover in fact has a lower eigenvalues than the original graph.

This is formulated and proved in the next theorem.

Theorem 2.3. *For any δ-graph Γ and its associated double cover Γ^2,*

$$\lambda_n(\Gamma^2) \leq \lambda_n(\Gamma).$$

Proof. Let u_n be the n:th eigenfunction of Γ. Let u_n^2 denote the extension of u_n to Γ^2 by letting it assume the same values on the corresponding points on the added edges. Clearly u_n^2 satisfies the eigenvalue equation $-\frac{d^2}{dx^2}f = \lambda_n f$ and the vertex conditions in every vertex of Γ^2 (as the number of incoming

functions have been doubled, the sum of the derivatives will be twice as big which is captured in that the strengths have double value). This means that $\lambda_n(\Gamma)$ is an eigenvalue to the Laplacian on Γ^2 as well, so all eigenfunctions and all eigenvalues of Γ are also eigenfunctions and eigenvalues of Γ^2. This proves that $\lambda_n(\Gamma^2) \leq \lambda_n(\Gamma)$. □

In this section a number of theorems that estimate the eigenvalues of δ-graph from below have been proved. None of the theorems gives however a lower bound for all graphs. In the next section such an estimate will be proved by combining these results.

2.3 A general theorem for a lower bound.

The main goal of this thesis is to find general bounds for the ground state energy. In this section the previous results of this thesis are used to prove a universal bound for the eigenvalues by combining them in a certain way.

The idea is to start with an arbitrary graph, and estimate the lowest eigenvalue from below using the theorems from the previous section until the ground state of the interval is reached. In short the graph will be transformed into its double cover and then cut into a loop graph using an Eulerian cycle. It is then shown that the first eigenvalues of the loop graph coincide with the first eigenvalue of the interval if all strengths are moved to one point.

Theorem 2.4. *The lowest eigenvalue of a δ-graph with total length $\mathcal{L}$ and with the sum of the absolute values of the strengths equal to $|\alpha|$ is bounded from below by the lowest eigenvalue of the interval with the same length and with all strengths equal to $-|\alpha|$ concentrated to one endpoint. Further more, the eigenvalue of this graph is given by the square of the purely imaginary solution to the equation*

$$k\tan(k\mathcal{L}) = -|\alpha|.$$

Proof. We make the following definitions.

- Let Γ be any δ-graph of length $\mathcal{L}$.

- Let S be some δ-graph defined on the loop with the length $2\mathcal{L}$, and with the same strengths as Γ distributed in a way specified later.

- Let S_0 be the δ-graph defined from S putting all strengths but one equal to zero, and the strength in one vertex to $-|\alpha|$.

- Let $I_{|\alpha|}$ be the δ-graph of length $\mathcal{L}$ defined on the interval, with the strengths 0 and $-|\alpha|$ in the endpoints.

The result then follows from the following sequence of inequalities:

$$\lambda_0(I) \underset{(d)}{=} \lambda_0(S_0) \underset{(c)}{\leq} \lambda_0(S) \underset{(b)}{\leq} \lambda_0\left((\Gamma)^2\right) \underset{(a)}{\leq} \lambda_0(\Gamma)$$

Inequality (a) follows directly from Theorem 2.3.

Inequality (b) follows by the following reasoning. All the vertices of $(\Gamma)^2$ have of even degree. Therefore there must exist an Eulerian cycle on the underlying graph. Using such an Eulerian cycle, a loop graph S can be obtained by a sequence of cuts in the vertices of the graphs in a manner specified in Theorem 2.1. By the theorem each such cut reduces or preserves each eigenvalue.

Inequality (c) follows directly from Theorem 2.2 and the fact that if $\alpha_v = 0$ and the degree of v is 2 then the vertex conditions does not imply any extra restrictions on the domain and may be removed without affecting the spectrum.

For equality (d), recall the results from the example where the first eigenvalue of the loop graph were shown to be given by the equation

$$k\tan(k\frac{\mathcal{L}}{2}) = \alpha/2,$$

and that the first eigenvalue of the quantum graph on the interval $I_{|\alpha|}$, is given by the square of the smallest solution to

$$k\tan(\mathcal{L}k) = \alpha.$$

It follows that the first eigenvalues of the interval and the loop coincide as length and the strengths of the loop is twice those for the interval. In other words, $\lambda_0(I_{|\alpha|}) = \lambda_0(S_0)$, which proves the equality (d). □

The strength of this proof is that it uses geometric ideas, and for any graph an estimate can be calculated quite quickly. For any specific graph a better

estimate can then be achieved if some of the steps of the proof can be skipped. For example, if all the strengths are positive, then it is not necessary to change them to negative one, which is stated in the the following corollary.

Corollary 2.1. *The lowest eigenvalue of a δ-graph with total length $\mathcal{L}$ and with* only non-negative strengths *summing to α, is bounded from below by the lowest eigenvalue of the interval with the same length and with all strengths equal to $-|\alpha|$ concentrated to one endpoint. Further more, the eigenvalue of this graph is given by the square of the smallest solution to the equation*

$$k\tan(k\mathcal{L}) = \alpha.$$

Proof. This can be proved with the same argument as Theorem 2.4. As all strengths are positive, Lemma 2.2 instead of Theorem 2.2 can be used, which gives the that the loop with with the strength α at one vertex has a lower ground state energy than Γ. The first eigenvalue of this loop graph is given by the equation

$$k\tan(kL) = \alpha.$$

This completes the proof. □

The difference between this corollary and Theorem 2.4, is that this proof uses Lemma 2.2 instead of Theorem 2.2 which is possible as $\alpha_i > 0$ at all vertices.

If the the degree of all vertices is even then another step of the proof can be skipped, giving another corollary.

Corollary 2.2. *The lowest eigenvalue of a δ-graph* where all vertices have even degree *with total length $\mathcal{L}$ and with the sum of the absolute values of the strengths equal to $|\alpha|$ is bounded from below by the lowest eigenvalue of the interval with the same length and with all strengths equal to $-|\alpha|$ concentrated to one endpoint. Further more, the eigenvalue of this graph is given by the square of the purely imaginary solution to the equation*

$$k\tan\left(k\frac{\mathcal{L}}{2}\right) = -\frac{|\alpha|}{2}.$$

Proof. The result can be proved in a completely similar way as Theorem 2.4, but skipping the doubling of the edges. The resulting loop graph is thus of the same length, giving the result. □

The two corollaries can of course be combined into a result for even graphs with only positive strengths.

2.4 An upper bound on the ground state energy

Using the quadratic form it also possible to calculate an upper bound for λ_0 on any specific graph. As the lowest eigenvalue is given by the function that minimizes the Rayleigh quotient, such an estimate can easily be calculated by just plugging in any function with norm 1 into it. This bound would of course only be an approximation from above on the specific eigenvalue as in general the chosen function will not be the real eigenfunction.

Every domain of a the quadratic form of any δ-graph contains a constant function as it is infinitely differentiable and integrable on every compact graph. The constant function also attains the same values at every point, so it is also continuous everywhere. The constant function with norm 1 on any graph of length $\mathcal{L}$ is

$$u(x) = \frac{1}{\sqrt{\mathcal{L}}}.$$

Plugging this into any quadratic form gives an upper estimate on λ_0 of the graph, and can be calculated as:

$$\left\langle L\frac{1}{\sqrt{\mathcal{L}}}, \frac{1}{\sqrt{\mathcal{L}}} \right\rangle = \frac{1}{\mathcal{L}}\langle L1, 1\rangle = \frac{1}{\mathcal{L}}\left(\int_\Gamma |\frac{d}{dx}1|^2 dx + \sum_i \alpha_i \cdot 1\right) = \frac{1}{\mathcal{L}}\sum_i \alpha_i. \quad (2.1)$$

This means that λ_0 can be bounded from above by what can be interpreted as the average potential. As this can be done on any graph, the sum of the potentials times the normalization constant $\frac{1}{\mathcal{L}}$ will always be an upper bound of the ground state energy. This estimate is neat in its simplicity, but the proof does not tell us if this estimate is sharp, and what kind of distribution of the potential would give an eigenvalue close to it. Looking at the vertex conditions at any vertex with $\alpha_i \neq 0$ shows that the constant function does not fulfill the equation, so the estimate is not sharp (except when the strengths sums to 0, but this is an already known result). This estimate might thus appear very weak, but in Chapter 3 we will show that it is in fact part of a more general result.

We summarize the result in a theorem.

Theorem 2.5. *The eigenvalues of a δ-graph Γ of length $\mathcal{L}$ is bounded from above by*

$$\lambda_0(\Gamma) \leq \frac{1}{\mathcal{L}}\sum_i \alpha_i.$$

Proof. The result follows directly from that the domain of every quadratic form associated to a δ-graph contains a constant function, and (2.1). □

An interesting question is then how close the ground state energy be pushed towards this upper bound. Looking at the quadratic form there are reasons to believe that λ_0 increases when the strength are evenly distributed over the graph, as it makes it impossible to "escape" the strengths by choosing a function with a low value at the vertices with a high strength, and the other way around. We try to capture this by looking at what the quadratic form converges towards when we distribute the potentials evenly across the graph. This can be done as a new vertex can be added anywhere on an edge. Let n denote the number of charges, and fix a function $u(x)$. The quadratic form is then given by

$$\int_\Gamma |u'(x)|^2 dx + \sum_{i=1}^{n} \frac{\alpha}{n} |u(\frac{i}{n}\mathcal{L})|^2 = \int_\Gamma |u'(x)|^2 dx + \frac{1}{\mathcal{L}} \sum_{i=1}^{n} \frac{\alpha}{n} \mathcal{L} |u(\frac{i}{n}\mathcal{L})|^2.$$

Letting n go to infinity we see that the sum turns into an Riemann sum, and thus

$$\begin{aligned}
\lim_{n\to\infty} \langle Lu, u\rangle_\Gamma &= \lim_{n\to\infty} \left(\int_\Gamma |u'(x)|^2 dx + \frac{1}{\mathcal{L}} \sum_{i=1}^{n} \frac{\alpha}{n} \mathcal{L} |u(\frac{i}{n}\mathcal{L})|^2 \right) \\
&= \int_\Gamma |u'(x)|^2 dx + \frac{1}{\mathcal{L}} \int_\Gamma \alpha |u(x)|^2 dx \\
&= \int_\Gamma |u'(x)|^2 dx + \frac{\alpha}{\mathcal{L}}
\end{aligned}$$

given that the norm of u is 1.

The function with norm 1 that minimizes this expression is clearly $u(x) = \frac{1}{\sqrt{\mathcal{L}}}$, which gives the value $\frac{\alpha}{\mathcal{L}}$, which is exactly what we were looking for.

As the quadratic form determines the operator, this shows a convergence of the operator to an operator with $\lambda_0 = \frac{\alpha}{\mathcal{L}}$ in some sense. Convergence of the quadratic form does however not necessarily imply convergence of the spectrum, so this question is still open, but it gives a hint of where to look.

Chapter 3

The Schrödinger operator

In this chapter the Schrödinger operator will be analysed. Focus is on the relation between the Laplacian with δ-conditions and the Schrödinger operator with standard conditions, and how the results from the previous chapter can be transferred to it. The starting point for this analysis is the quadratic form of the two operators, and the similarities between them.

3.1 The quadratic form of the Schrödinger operator

As seen in the earlier chapters, the quadratic forms is not only an invaluable tool for analysing how changes in the operator effect the eigenvalues, but also for finding similarities. Recall from Chapter 1 that the Schrödinger operator is given by the differential expression

$$L_q = -\frac{d^2}{dx^2} + q(x)$$

where $q(x)$ is a real function such that $q \in L_1(\Gamma)$. The Schrödinger operator is however defined using its quadratic form, which for continuous functions is given by

$$\begin{aligned} \langle L_0\psi, \psi\rangle &= \langle L_0\psi, \psi\rangle + \langle q\psi, \psi\rangle \\ &= \int_\Gamma |\psi'|^2 dx + \int_\Gamma q(x)|\psi(v)|^2. \end{aligned}$$

This looks very similar to the quadratic form of the Laplacian with δ-conditions, making one wonder whether there exists any potential $q(x)$ such that the quadratic forms coincide (making them the same operator).

3.2 The Schrödinger potential and δ-conditions.

The similarities between the quadratic form of the two operators makes it plausible to think that it might be possible to choose the potential of the Schrödinger operator such that the two forms coincide.

In the following section the generalized function $\delta_v(x)$, sometimes called the δ-distribution, will be very useful. We define it as the function $\delta_v(x)$ that fulfills the following two properties:

- $\int_I \delta_v(x)dx = 1$ if $v \in I$,
- $\int_I f(x)\delta_v(x) = f(v)$ for any interval I such that $v \in I$, and any function f that is continuous in v.

Note that $\delta(x)$ is not in L^1.

The potential $q(x) = \sum_i \alpha_i \delta_{v_i}(x)$ will from now on be called the δ-potential. Using the intuitive interpretation of δ-conditions as point potential, and the δ-distribution, the following theorem can be proved.

Theorem 3.1. *The Schrödinger operator with δ-potential supported on its vertices on a graph (defined using its quadratic form) coincides with the Laplace operator defined on the set of functions from $W_2^2(\Gamma \setminus V)$ satisfying δ-conditions at its vertices.*

Proof. Let e_i denote the edges and V the set of vertices of Γ. Now put $q(x) = \sum_i \alpha_{v_i} \delta_{v_i}(x)$. This gives that

$$\begin{aligned} \langle q(x)\psi, \psi \rangle &= \int_\Gamma \sum_i \alpha_i \delta_{v_i}(x)|\psi(x)|^2 dx \\ &= \sum_i \alpha_i \int_\Gamma \delta(v_i)|\psi(x)|^2 dx \\ &= \sum_i \alpha_i |\psi(v_i)|^2. \end{aligned}$$

The operator L_q is defined by the sum of the quadratic form of L_0 and $q(x)$. In other words,

$$\langle L_q\psi, \psi\rangle = \int_\Gamma |\psi'|^2 dx + \sum_i \alpha_i |\psi(v_i)|^2.$$

This is exactly the same as for the Laplacian with δ-conditions. As we know that the domain is not effected by conditions on the derivative at single points, the domains of these two forms are the same. □

A Schrödinger operator with a δ-potential can thus be regarded as a Laplace operator with δ-conditions.

This theorem states that the class of quantum graphs examined in the previous chapters can be viewed as a special case of the Schrödinger operator in the sense that they all correspond to a Schrödinger operator with the δ-potential. The δ-conditions being only a singular case of a potential to the Schrödinger operator begs the question if the earlier results for δ-graphs can be generalized to the Schrödinger operator in any meaningful way, and what conditions that must be put on $q(x)$ for it to hold. In the following sections this question will be investigated, and some useful generalizations will follow.

3.3 What results holds for the Schrödinger operator?

The first thing that was dealt with with graphs with δ-conditions was how the length and the potential influenced the eigenvalue. A similar argument about the length is possible for the Schrödinger operator, and looking at the quadratic form it is clear that if $q(x)$ increase on an interval, so will the value for the quadratic form for any function. A suitable analog of the criteria of fixing the sum of the absolute value of the α_i, is to fix

$$\int_\Gamma |q(x)|dx,$$

as it transforms into our earlier condition when $q(x)$ is equal to the δ-potential. With this established, it is possible to move on to ask which of the earlier theorems that can be generalized to the Schrödinger operator.

Some of the earlier results follows with the same methods. For example Lemma 2.1, stating that the eigenvalues depend positively on the potential,

can be seen in a completely analogous way. The other results require some more reformulation and will be dealt with one by one.

Theorem 2.1 shows that a graph can be cut such that the eigenvalues decreases. The idea there was to introduce new conditions at the new vertices such that the strengths adds together to the old strength. For the Schrödinger operator this makes no sense, instead the requirement is that the integral over the potential at the two new vertices remains the same.

Theorem 3.2. *Let v be a vertex of a quantum graph Γ with a Schrödinger operator L_q acting on it, and let $\widehat{\Gamma}_{\hat{q}}$ be the graph obtained from Γ by splitting v into two vertices v' and v'' and choosing $\hat{q}(x)$ such that:*

- $q(x) = \hat{q}(x)$ *for all x outside the vertex v,*
- $\int_{\hat{\Gamma}} |\hat{q}(x)|dx = \int_{\Gamma} |q(x)|dx$.

Then

$$\lambda_0(\widehat{\Gamma}_{\hat{q}}) \leq \lambda_0(\Gamma_q).$$

Proof. As the only difference between Γ_q and $\widehat{\Gamma}_{\hat{q}}$ is that the eigenfunction must not attain the same values in v' as in v''. It follows that $\mathrm{dom}_Q(\Gamma_q) \subset \mathrm{dom}_Q(\widehat{\Gamma}_{\hat{q}})$. Plugging this into the Rayleigh quotient gives:

$$\lambda_0(\hat{\Gamma}_q) = \left(\min_{\substack{||u|| = 1 \\ u \in \mathrm{dom}_Q(\widehat{\Gamma}_{\hat{q}})}} \langle Lu, u \rangle \right) \leq \left(\min_{\substack{||u|| = 1 \\ u \in \mathrm{dom}_Q(\Gamma_q)}} \langle Lu, u \rangle \right) = \lambda_0(\Gamma_q).$$

□

The next result about the Laplacian with δ-condition stated that there was always possible to move all the strength to a certain point so that the first eigenvalue decreased. An analogous argument is possible for the Schrödinger operator.

Theorem 3.3. *Every quantum graph Γ_q has a point v (that can be viewed as a vertex) such that putting $\hat{q}(x) = -\int_{\Gamma} |q(x)|dx \cdot \delta_v(x)$ produces a new quantum graph $\hat{\Gamma}_{\hat{q}}$ with*

$$\lambda_0(\hat{\Gamma}_{\hat{q}}) \leq \lambda_0(\Gamma_q).$$

Furthermore,

$$\int_\Gamma |q(x)|dx = \int_{\widehat{\Gamma}} |\hat{q}(x)|dx.$$

Proof. Let Γ_q be any quantum graph and $u(x)$ be its first eigenfunction. Then there is a point where $|u(x)|$ attains its highest value. That point can be regarded as a vertex, and we denote it by v. Now let $\widehat{\Gamma}_{\hat{q}}$ be the quantum graph created from Γ_q by putting $\hat{q}(x) = -\int_\Gamma |q(t)|dt \cdot \delta_v(x)$. The Rayleigh quotient then gives:

$$\begin{aligned}
\lambda_0(\widehat{\Gamma}) &= \int_\Gamma |u'|^2 dx + \int_{\widehat{\Gamma}} \hat{q}(x)|u(x)|^2 dx \\
&= \int_\Gamma |u'|^2 dx - \int_\Gamma |q(t)|dt \cdot \int_{\widehat{\Gamma}} \delta_v(x)|u(x)|^2 dx \\
&= \int_\Gamma |u'|^2 dx - \int_\Gamma |q(t)| \cdot |u(v)|^2 dt \\
&\leq \int_\Gamma |u'|^2 dx - \int_\Gamma |q(t)| \cdot |u(t)|^2 dt \\
&\leq \int_\Gamma |u'|^2 dx + \int_\Gamma q(t) \cdot |u(t)|^2 dt \\
&= \lambda_0(\Gamma).
\end{aligned}$$

□

This is a very important result as it shows that the ground state of a Schrödinger operator is bounded from below by a quantum graph with δ-conditions. It does not only show that the potential with the lowest ground state energy is a δ-potential, but also gives a valuable tool for generalizing theorems for δ-graphs to the Schrödinger operator.

3.4 A lower bound for the ground state of the Schrödinger operator.

In the previous section, some of the results from Chapter 2 was generalized to the Schrödinger operator. A very interesting result was that the eigenvalues of the Schrödinger operator can always be estimated from below by the Schrödinger operator with a δ-potential, and thus a δ-graph. This makes it very simple to prove a generalization of Theorem 2.4 for the Schrödinger operator.

Theorem 3.4. *The first eigenvalue of the quantum graph* Γ *given by the Schrödinger operator acting on a metric graph with standard conditions are bounded from below by the square of purely imaginary solution to*

$$k\tan(kL) = -\int_\Gamma |q(x)|dx$$

with equality when Γ *is the interval with a negative* δ*-potential supported at one endpoint.*

Proof. Theorem 3.3 states that the first eigenvalue of a quantum graph Γ_q can be estimated from below by the first eigenvalue of a graph $\widehat{\Gamma}_{\hat{q}}$, where $\hat{q}(x) = -\int_\Gamma |q(x)|dx \cdot \delta_v(x)$ for some vertex v of Γ. As $\widehat{\Gamma}$ can be regarded as a quantum graph with δ-conditions, Theorem 2.4 applies, giving that the eigenvalues of $\widehat{\Gamma}_{\hat{q}}$ is bounded from below by the square of the smallest non-negative solution to

$$k\tan(k\mathcal{L}) = -\int_\Gamma |q(x)|dx.$$

As $\lambda_0(\widehat{\Gamma}_{\hat{q}}) \leq \lambda_0(\Gamma_q)$, this is a lower bound for the original graph as well. □

The idea expressed in Theorem 3.3 that λ_0 of a quantum graph with the Schrödinger operator can be approximated from below by the ground state of a quantum graph with δ-conditions means that every lower bound for the graph δ-conditions applies to the Schrödinger operator. It is thus possible to directly generalize any lower bound for δ-graphs without proof, e.g. Corollary 2.1 and Corollary 2.3.

Corollary 3.1. *The lowest eigenvalue of the Schrödinger operator with standard conditions, where the potential* $q(x) \geq 0$ *are bounded from below by the square of the smallest non-negative solution to*

$$k\tan(k\mathcal{L}) = \int_\Gamma |q(x)|dx.$$

Corollary 3.2. *The lowest eigenvalue of the Schrödinger operator with standard conditions acting on a graph of even degree is bounded from below by the square of the smallest non-negative solution to*

$$k\tan\left(k\frac{\mathcal{L}}{2}\right) = -\frac{1}{2}\int_\Gamma |q(x)|dx.$$

3.5 A generalization of the upper bound

As seen in Chapter 2, the lowest eigenvalue of a graph with δ-conditions can be bounded from above by the sum of the strength times $\frac{1}{\mathcal{L}}$. An analogue theorem for the Schrödinger operator would be that λ_0 is bounded by $\frac{1}{\mathcal{L}}\int_\Gamma q(x)dx$, which in fact is true. This can be proved in a similar way by calculating the value of the quadratic form of the constant function. Recall that there was no δ-conditions that actually would give this eigenvalue.

Consider the Schrödinger equation with the Schrödinger operator L_{q_0} with the potential identicaly equal to some constant q_0:

$$-u''(x) + q_0 u(u) = \lambda u(x).$$

It is easily seen that $u(x) = 1/\mathcal{L}$ with the associated eigenvalue $\lambda = q_0/\mathcal{L}$ is a solution. The quadratic form of L_{q_0} is given by

$$\langle L_{q_0}u, u\rangle = \int_\Gamma |u'(x)|^2 dx + q_0 \int_\Gamma |u(x)|^2.$$

The constant solution minimizes both the first and the second integral as the constant function attains the same value in all points, it also fulfills all continuity criteria, so it is in the domain of the form. This shows that $u(x) = \frac{1}{\mathcal{L}}$ must be the first eigenfunction. Using this it is possible to generalize the earlier result to a sharp bound.

Theorem 3.5. *The lowest eigenvalue of a Schrödinger operator, defined using the quadratic form, is bounded from above by average value of the potential. In other words,*

$$\lambda_0(\Gamma) \leq \frac{1}{\mathcal{L}}\int_\Gamma q(x)dx$$

with equality when $q(x)$ is constant. The Schrödinger operator with constant potential thus has the highest ground state energy subject to the integral over the value of the potential.

Proof. The result follows from the following chain of inequalities.

$$\lambda_0(\Gamma_q) = \min_{||u||=1}\langle L_q u, u\rangle \leq \frac{1}{\mathcal{L}}\langle L_q 1, 1\rangle \underset{(a)}{\leq} \frac{1}{\mathcal{L}}\langle L_{q_0}1, 1\rangle \underset{(b)}{=} \frac{1}{\mathcal{L}}\lambda_0(\Gamma_{q_0}) = \frac{q_0}{\mathcal{L}}$$

Inequality (a) follows as

$$\begin{aligned}\langle L_q 1, 1\rangle &= \int_\Gamma q(x)dx \\ &\leq \int_\Gamma |q(x)|dx \\ &= \int_\Gamma q_0 dx \\ &= \langle L_{q_0} 1, 1\rangle.\end{aligned}$$

Inequality (b) follows as the constant function is the first eigenfunction of L_{q_0}, which was proved in the beginning of this section. □

A difference between this theorem and the one giving the lower bound is that the upper bound does not depend on the structure of the underlying graphs. The Schrödinger operator with a constant potential thus has the same λ_0 on all graphs of the same length. This is explained by a constant function being in the domain of all operators. Another, more interesting difference is that this upper bound is subject to the integral over the potential, not the integral over the absolute value of the potential. This means that it takes more information into account.

Summary

It Chapter 2 it was shown how certain of operations on quantum graphs with δ-conditions change their spectrum. Using this, a lower bound on the ground state energy of δ-graphs was derived by showing that for a fixed length and fixed sum of the strengths, the graph with the lowest eigenvalue is the interval with all strength in one endpoint. The value is described by the equation

$$k \tan(k\mathcal{L}) = -|\alpha|.$$

By using the simple fact that the domain of every operator of a quantum graph contains some kind of constant function, we got the result that

$$\lambda_0(\Gamma) \leq \frac{1}{\mathcal{L}} \sum_i \alpha_i.$$

If there exists a graph where there is equality is still an open problem.

In Chapter 3 these results was generalized to the Schrödinger operator with standard conditions, which showed how the strengths and the potential of the Schrödinger operator relates to each other. For the Schrödinger operator the upper bound also became strict.

Putting these findings together gives that the ground state of δ-graphs is bounded from above by a Schrödinger operator with standard conditions defined on the same metric graph, while the ground state of the Schrödinger operator with standard conditions is bounded from below by a δ-graph defined on the same metric graph.

There are however a few questions that were not completely answered. As the potential that maximizes the ground state energy for the Schrödinger operator is the constant, and the eigenvalues of a δ-graph is known to reduce when the strength are concentrated to one point, it becomes reasonable to think that the eigenvalue of a δ-graph can be made arbitrary close to

$$\frac{1}{\mathcal{L}} \sum_i \alpha_i.$$

by distributing the strengths over sufficiently many vertices scattered over the graph. If this is true, and what distribution the vertices should have, are some of the questions left unanswered by this thesis.

Another question that is not touched on at all in this thesis is graphs with other matching conditions. Even though most of the theorems are built on specific properties of δ-graph, the same ideas could probably be applied to other kinds of graphs as well, as well as to Schrödinger operators with other conditions.

Appendix A

Self adjoint operators

Let L be any operator defined on an dense subset $Dom(L)$ of a Hilbert space $\mathcal{H}$. If $\langle Lu, v\rangle$ is a bounded functional with respect to $u \in Dom(L)$, where v is some element in $\mathcal{H}$, then there exists an $f \in \mathcal{H}$ such that

$$\langle u, f_v\rangle .$$

That the functional is bounded means that

$$|\langle Lu, v\rangle| \leq C_v||u||$$

for all $u \in Dom(L)$.

The operator that takes v to f_v is called the adjoint of L and is denoted by L^*. The domain of the adjoint is all v for which the functional is bounded. If $Dom(L) = Dom(L^*)$ and $Lu = L^*u$ for all $u \in Dom(L)$, then L is said to be self-adjoint.

Self-adjoint operators corresponds in some way to self-adjoint matrices in the sense that many of the properties of the matrices can be transfered to them. One of the most important property is that for any self-adjoint operator L on an infinite (finite) Hilbert space, it is possible to choose the eigenvalues of L orthogonal such that they span the whole $\mathcal{H}$. This means that any $u \in \mathcal{H}$ can be expressed as

$$u = \sum_{n=0}^{\infty} \langle u, u_n\rangle$$

where $\{u_n\}_{n=0}^{\infty}$ is the sequence of orthogonal eigenfunctions of L.

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