Spectral analysis of Discrete Approximations of Quantum Graphs

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Abstract

The main purpose of this paper is to study a discrete approximation of metric quantum graphs and show that the spectra of the discrete Laplace and Schrödinger operators converge to that of their continuous counterparts as the resolution gets finer. We will also prove some topological spectral invariants of these models. The approach is similar to that used by P. Kurasov and M. Nowaczyk to analyze the inverse spectral problem of metric quantum graphs, and some of the notation and figures used here are adopted from these papers.

1 Preface

The theory of quantum graphs has applications in various branches of physics, notably quantum chemistry and nanotechnology. The notion of quantum graphs first appeared in the 1980-ies in works of B. Pavlov, N. Gerasimenko, P. Exner, P Seba and Y. Colin de Verdière. In recent years the spectral problem has been investigated by K. Naimark, A. Sobolev and M. Solomyak, the inverse spectral problem by B. Gutkin and U. Smilansky, the direct scattering problem by V. Kostrykin and R. Schrader and the inverse scattering problem by J. Boman, P. Kurasov and F. Stenberg. In this paper we will investigate discrete Laplace and Schrödinger operators as approximations of the corresponding differential operators. The main problem tackled could be viewed as a special case of a more general question, namely, whether given any Riemannian manifold it is possible to find a family of discrete nets whose (Laplacian) spectrum converges to that of the manifold in question.

For a discussion and some results on this more general problem we refer to [5]. What might be novel in this paper is the application of techniques from quantum scattering theory to combinatorial graphs, and to the extend needed we will in parallel present the same theory applied to metric graphs. During the work we found that our results on the convergence of the Laplacian spectrum have already been proven by X.W.C. Faber. However, with some extra assumptions made on regularity of the models we are able to present a substantially simpler proof. We begin by introducing the basic concepts and definitions used in the sequel, together with some elementary theorems. The spectral analysis of the discrete Laplace operator is then given a separate treatment, and in the last chapter we show how the main theorem can be generalized to discrete Schrödinger operators.

2 Definitions

2.1 Quantum Graphs

A quantum graph Γ consists of a collection of edges $\Delta_j = [x_{2j-1}, x_{2j}]$, which are copies of intervals of the real line. The set of edges is denoted $E(\Gamma)$, and the points x_{2j-1} and x_{2j} are said to be the endpoints of the edge Δ_j. We will only discuss compact graphs, where $E(\Gamma)$ is a finite set and all edges are copies of compact intervals[1]. We allow the endpoints to be 'glued together', which we technically express by introducing a vertex set $V(\Gamma)$ consisting of equivalence classes of the set of endpoints. All endpoints belonging to the same vertex are thus identified, and the number of points belonging to a vertex is called the valency of the vertex. We let N be the number of edges and M the number of vertices. The space $L^2(\Gamma)$ is defined by

$$L^2(\Gamma) = \oplus \sum_{j=1}^{N} L^2(\Delta_j) \tag{1}$$

and the differential expression for the Laplace operator L acting on $L^2(\Gamma)$ is simply

$$L = \oplus \sum_{j=1}^{N} (-\frac{d^2}{dx^2}). \tag{2}$$

[1] To ease the flow of the text we will repeatedly use the term 'continuous quantum graph' instead of 'finite compact metric graph'

The maximal domain of this operator is the space $\mathrm{Dom}_{max} = \oplus \sum_{j=1}^{N} W_2^2(\Delta_j)$ where $W_2^2(\Delta_j)$ denotes the Sobolev space

$$W_2^2(\Delta_j) = \{f \in L^2(\Delta_j) | f', f'' \in L^2(\Delta_j)\}. \tag{3}$$

However, the operator defined by the differential expression L with domain Dom_{max} is not self-adjoint, so in order to get a self-adjoint restriction of the maximal operator one introduces boundary conditions at the vertices. These conditions may be of several different kinds, but the most common are the so called Standard (Neumann, natural) boundary conditions. These impose the requirement that the functions be continuous at the vertices and that the sum of all normal derivatives be equal to zero. With standard boundary conditions any vertex of valency 2 becomes superfluous and may be removed, resulting in a so called 'clean' graph. Two edges connected by a vertex of valency 2 then merge into one edge, with the total length preserved. Having specified the boundary conditions, the Laplace operator is uniquely determined by the graph and one can show that it has a pure discrete spectrum. For a proof of this statement and a detailed exposition on different boundary conditions we refer to [3]. In recent years, extensive research has been done on quantum graphs and some of the spectral invariants found so far are stated in the following proposition:

Proposition 1 *For any compact metric quantum graph the following properties are determined by the spectrum of the Laplace operator (determined by standard boundary conditions at the vertices)*

- *The number of connected components*
- *The total length*
- *The Euler Characteristic* $\chi = M - N$

For proof, see [2].

2.2 The Discrete Quantum Graph

We have chosen to maintain the terminology used for continuous quantum graphs with the disadvantage that it might lead to some confusion regarding the use of the words 'vertex' and 'edge'. However, having pointed this out we hope that the reader will find the presentation accessible. The following definition is almost a replica of that of a continuous quantum graph.

Let Γ be a finite collection of finite sequences of consecutive integers, and let $V(\Gamma)$ be a set of equivalence classes of the the set of endpoints of these sequences. An endpoint is understood as the first or last element of a sequence. For reasons which will be apparent later we also require that every sequence consists of at least 3 elements. In accordance with the terminology of continuous graphs a sequence will be denoted 'edge' and a member of $V(\Gamma)$ will be denoted 'vertex', and as before we let N denote the number of edges and M the number of vertices. Further we introduce the symmetric relation $\sim$ denoted 'neighbour' defined as follows: Two points x_i and x_j are neighbours if they belong to the same edge and $\mid x_i - x_j \mid = 1$. We identify all elements belonging to the same vertex V_m, and all neighbours of the constituent points are inherited by the vertex. The valency of a vertex V_m is defined as the number of neighbours of the vertex (or equivalently the number of endpoints belonging to the vertex) and is denoted v_m, where m is an index identifying the vertex.

In the absence of the usual topology, connectedness of a discrete graph is defined by use of the neighbour relation as follows: A path is defined as a sequence of points $\{x_1, x_2, .., x_n\}$ such that $x_k \sim x_{k+1}$ and a graph is said to be connected if there is a path between any two points of the graph. We stress that since we have identified all points belonging to the same vertex any complex valued function defined on Γ must attain the same value at all these points. The latter restriction is in accordance with the continuity condition on continuous graphs. The purpose of identifying each point with an integer is to be able to get analytic expressions for the eigenfunctions of the Laplace operator. The requirement that every edge should consist of at least 3 points enables us to treat each edge separately, however, since we are mainly interested in the behaviour as the number of points goes to infinity that restriction should be seen as just a precaution.

2.3 The Laplace Operator

For scaling purposes we modify the graph Γ by multiplying each integer point with a positive real number h which we call step length, and the graph derived in this way will be denoted Γ_h. All operators mentioned in this section are acting on $l_2(\Gamma_h)$. The Laplace operator we are going to analyze is the usual one, anyhow we will first give a brief motivation to our choice. We take as starting point the ordinary Laplace operator as it is defined on continuous edges, that is $L = -\frac{d^2}{dx^2}$. As a natural analog to the first order differential operator we define

$$D\Psi(nh) = \frac{\Psi((n+1)h) - \Psi(nh)}{(n+1)h - nh} = \frac{\Psi((n+1)h) - \Psi(nh)}{h} \tag{4}$$

Consequently we get

$$-D^2\Psi(nh) = -\frac{\Psi((n+2)h) - 2\Psi((n+1)h) + \Psi(nh)}{h^2} \tag{5}$$

However, there's no reason to prefer right derivatives before left derivatives, so in order to obtain a symmetric expression we define

$$L\Psi(nh) = -\frac{\Psi((n+1)h) - 2\Psi(nh) + \Psi((n-1)h)}{h^2} \tag{6}$$

The above formula is obviously only valid for points not belonging to any vertex. On continuous quantum graphs one introduces boundary conditions at the vertices in order to get a self-adjoint restriction of the maximal operator. For the discrete graph there is no need for a self-adjoint restriction, instead we seek a generalization of the Laplace operator defined on the whole graph, thats is, including the vertices. Formula (6) suggests a natural generalization:

$$L\Psi(x) = \frac{1}{h^2} \sum_{y \sim x} (\Psi(x) - \Psi(y)). \tag{7}$$

With the above operator we see that points on edges could equally well be considered as a vertices of valency 2, similar to the situation with standard boundary conditions on continuous graphs.

There is a very simple argument showing that the Laplace operator is positive on the graph we have constructed:

Lemma 1 *The Laplace operator is non-negative on* Γ_h.

PROOF[2]. Let f be an eigenfunction of L on $l_2(\Gamma_h)$ with eigenvalue $E < 0$. Since Γ_h is finite, there are points a and b on Γ_h such that $\Re f(a)$ is maximal and and $\Re f(b)$ is minimal. By looking at formula (7) it is obvious that $\Re Lf(a) = E\Re f(a)$ is non-negative, so $\Re f(a)$ must be non-positive since E is negative. On the other hand, $\Re Lf(b)$ is necessarily negative so $\Re f(b)$ must be non-negative. By arguing in the same way with the imaginary part of f we must conclude that f is identically equal to zero, and we have a contradiction. $\square$

2.4 The Laplacian Matrix

Some of the elementary properties of the Laplace operator can be found by looking at the corresponding Laplacian Matrix. Obviously, the model we have just defined could be seen as a special case of an ordinary combinatorial graph with weighted edges. Thus, we now consider all points of Γ_h as vertices belonging to a vertex set V and we let E be the set of all unordered pairs $\{x, y\}$ such that $x \sim y$. The set E is called the edge set. Note carefully that the notions 'vertex' and 'edge' have different meanings in this context. Further, let $m = |V|$ and $n = |E|$. We enumerate all the vertices with and index ranging from 1 to n, and we let $v(x_i)$ denote the valency of x_i. The Laplace operator will now be represented by the $n \times n$ matrix L, called Laplacian matrix, defined by $(L)_{ii} = v(x_i)/h^2$, $(L)_{ij} = -1/h^2$ if $x_i \sim x_j$ and zero otherwise. L is a real symmetric $n \times n$ matrix, hence it has exactly n eigenvalues (counting multiplicity) all of which are real. In order to be able to identify Γ_h as a net of a continuous quantum graph we extend the notion of geometric length to the former as follows

$$\mathcal{L}(\Gamma_h) = h|E(\Gamma_h)|. \tag{8}$$

Given this definition, Γ_h will in fact share many of the spectral invariants of continuous quantum graphs. Parts of the proof depend on the following lemma

Lemma 2 *Given a non-weighted combinatorial graph without loops and multiple edges[3] with the Laplace eigenvalues $\{\lambda_i\}$ (where the index i counts the*

[2]This theorem could also be proved by deriving the quadratic form corresponding to L. We refer to for example [8]

[3]Of course, this requirement does not imply that the graph cannot *model* a continuous graph with loops and multiple edges.

multiplicity of the eigenvalues) and the edge set E we have that

$$|E| = \frac{1}{2}\sum_{i=1}^{n}\lambda_i. \tag{9}$$

PROOF. We use the well known fact that the trace of a symmetric matrix equals the sum of its eigenvalues, and we get with our assumptions:

$$\sum_{i=1}^{n}\lambda_i = TrL = \sum_{i=1}^{n} v(x_i) = 2|E|. \tag{10}$$

□

If the graph is constructed in the way described in section (2.2) we have that $M - N = m - n$, and in analogy with Proposition (1) we get:

Theorem 1 *The following properties of Γ_h are determined by the Laplace eigenvalues $\{\lambda_i\}$ (where the index i counts the multiplicity of the eigenvalues)*

- *The number of connected components is equal to the spectral multiplicity of the zero eigenvalue*
- *The total length is equal to* $\frac{h^3}{2}\sum_{i=1}^{n}\lambda_i$
- *The Euler Characteristic χ = M-N is equal to* $\sum_{i=1}^{n}(1 - \frac{h^2}{2}\lambda_i)$

PROOF. The first part is well known, and a proof can be found for example in [8]. The second and third part follows from the definitions and Lemma 2 □

As we will show further on, the discrete graphs as we have defined them will indeed serve as models for continuous quantum graphs in the way described in the beginning paragraph. One might therefore ask whether the spectral invariants also carry over to the continuous graphs in a natural way. It appears though that such a connection in the case of the total length and the Euler characteristic is far fetched. One reason to believe that is that for continuous graphs, only the asymptotic behaviour of the spectrum is important, which clearly is not the case for discrete graphs.

3 The Eigenfunctions of the Discrete Laplace Operator: Scattering Matrix Approach

The purpose of this section is to obtain the secular equation determining the spectrum of the Laplace operator using a method first developed by B. Gutkin and U. Smilansky. The word 'edge' will now have the meaning it was given in section 2.2. The starting point for our analysis are the solutions to the equation

$$L\Psi = E\Psi. \tag{11}$$

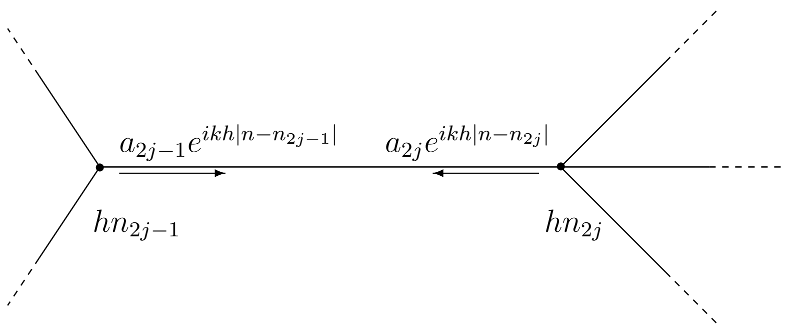
Considering only internal points on the edges, equation (11) gives rise to difference equation having the general solution

$$\Psi(hn) = ae^{ikhn} + be^{-ikhn}. \tag{12}$$

The eigenvalue E is given by

$$E = \frac{2 - 2\cos(kh)}{h^2}. \tag{13}$$

Equation (12) with hn replaced by the continuous variable x is of course also a solution to the differential equation $-\frac{d^2}{dx^2}\Psi = E\Psi$, with the difference being that in this case $E = k^2$. Limiting our discussion to an edge, indexed j, with starting point n_{2j-1} and endpoint n_{2j}, we will choose $\{e^{ikh|n-n_{2j-1}|}, e^{ikh|n-n_{2j}|}\}$ and $\{e^{-ikh|n-n_{2j-1}|}, e^{-ikh|n-n_{2j}|}\}$ as bases for the space of eigenfunctions. Physically, one may interpret this as a base of 'incoming waves' or 'outgoing waves'. Expressing $\Psi(nh)$ in these two bases:



$$\Psi(nh) = a_{2j-1}e^{ikh|n-n_{2j-1}|} + a_{2j}e^{ikh|n-n_{2j}|} = b_{2j-1}e^{-ikh|n-n_{2j-1}|} + b_{2j}e^{-ikh|n-n_{2j}|}, \tag{14}$$

we see that whenever k is not an integer multiple of π/h the equations (14) are only satisfied when[4]

$$b_{2j-1} = e^{ikh|n_{2j}-n_{2j-1}|}a_{2j}, \qquad b_{2j} = e^{ikh|n_{2j}-n_{2j-1}|}a_{2j-1}. \tag{15}$$

All the equations can be put together in matrix notation using the following definitions:

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_{2N} \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_{2N} \end{pmatrix}, \tag{16}$$

$$m_j = |n_{2j} - n_{2j-1}|, \qquad \epsilon_h^j = \begin{pmatrix} 0 & e^{ikhm_j} \\ e^{ikhm_j} & 0 \end{pmatrix}. \tag{17}$$

We may now write equations (15) simply as

$$\mathbf{b} = \mathcal{E}_h \mathbf{a}, \tag{18}$$

where we have introduced the edge scattering matrix $\mathcal{E}_h$ defined by

$$\mathcal{E}_h = \left(\begin{array}{c|c|c} \epsilon_h^1 & 0 & \cdots \\ \hline 0 & \epsilon_h^2 & \cdots \\ \hline \vdots & \vdots & \ddots \end{array}\right). \tag{19}$$

So far we have only treated the edges. For each vertex V_m, we introduce new vectors $\mathbf{a^m}$ and $\mathbf{b^m}$ containing the amplitudes of the waves going out from the vertex and the waves approaching the vertex respectively:

$$\mathbf{a^m} = \begin{pmatrix} a_{l_1} \\ a_{l_2} \\ \vdots \\ a_{l_{v_m}} \end{pmatrix}, \qquad \mathbf{b^m} = \begin{pmatrix} b_{l_1} \\ b_{l_2} \\ \vdots \\ b_{l_{v_m}} \end{pmatrix}. \tag{20}$$

We now seek the matrix $\sigma_{\mathbf{h}}^{\mathbf{m}}$, called vertex scattering matrix, such that

$$\mathbf{a^m} = \sigma_{\mathbf{h}}^{\mathbf{m}} \mathbf{b^m}. \tag{21}$$

[4] The remaining values $k = n\pi/h$ correspond to the zero eigenvalue and for some graphs the maximum eigenvalue. However, we may exclude these from further consideration since the first can be treated separately and the second will not be important for our later results

The calculations are straightforward but we demonstrate them for the sake of clarity. Let $a_+ = \sum_{j=1}^{v_m} a_{l_j}$ and $b_+ = \sum_{j=1}^{v_m} b_{l_j}$. With the ansatz given by formula (12) we must have that

$$a_{l_j} + b_{l_j} = a_{l_i} + b_{l_i} \tag{22}$$

in order for the function to be uniquely defined at the vertex. Furthermore, we have the eigenvalue equation at the vertex:

$$(2 - 2\cos(kh))(a_{l_j} + b_{l_j}) = v_m(a_{l_j} + b_{l_j}) - (a_+ e^{ikh} + b_+ e^{-ikh}). \tag{23}$$

By symmetry considerations we see that $\sigma_{\mathbf{h}}^{\mathbf{m}}$ should have the following appearance:

$$\sigma_{\mathbf{h}}^{\mathbf{m}} = \begin{pmatrix} r & t & t & \dots \\ t & r & t & \dots \\ t & t & r & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}. \tag{24}$$

The coefficients r and t (which are dependent on m) are called reflection- and transmission coefficients respectively. The equations (22) immediately yield

$$r = t - 1, \tag{25}$$

thus the eigenvalue equation (23) becomes:

$$(2 - 2\cos(kh))tb_+ = v_m t b_+ - (t - 1 + (v_m - 1)t))b_+ e^{ikh} - b_+ e^{-ikh}, \tag{26}$$

which yields

$$t = \frac{2i\sin(kh)}{v_m(e^{ikh} - 1) + 2 - 2\cos(kh)}, \tag{27}$$

and one can show that the vertex scattering matrix so defined is unitary. The amplitudes of the outgoing waves may now be expressed in terms of the amplitudes of the incoming waves as demonstrated below:

$$\begin{pmatrix} \mathbf{a}^1 \\ \mathbf{a}^2 \\ \vdots \\ \mathbf{a}^M \end{pmatrix} = \Sigma_h \begin{pmatrix} \mathbf{b}^1 \\ \mathbf{b}^2 \\ \vdots \\ \mathbf{b}^M \end{pmatrix}, \quad \text{where } \Sigma_h = \left(\begin{array}{c|c|c} \sigma_h^1 & 0 & \dots \\ \hline 0 & \sigma_h^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array}\right). \tag{28}$$

If necessary, the basis vectors are renumbered so that equation (28) is satisfied. By virtue of the above calculations and definitions we conclude that every eigenfunction of the Laplace operator corresponds to a vector in $\mathbb{R}^{2N}$ which satisfies the following equation:

$$\mathbf{a} = U_h \mathbf{a}, \qquad \text{where} \qquad U_h(k) = \Sigma_h(k)\mathcal{E}_h(k). \tag{29}$$

Conversely, for any vector satisfying equation (29) there corresponds an eigenfunction. However, we stress that the number of distinct vectors corresponding to a certain eigenvalue might not coincide with the spectral multiplicity of the eigenvalue in question, see [2]. Finally we are in position to express the secular equation leading to the spectrum of L:

$$f_h(k) = \det(U_h(k) - I) = 0. \tag{30}$$

We first point out some immediate observations about the solutions to equation (30).

Lemma 3 *If k is a zero of $f_h(k)$ then so is $k + 2n\pi/h$ for all $n \in \mathbb{Z}$.*

Lemma 4 *If k is a zero of $f_h(k)$ then so is $-k$.*

Lemma 5 *The zeros of $f_h(k)$ are real numbers.*

PROOF. Lemma 3 follows from inspection. Lemma 4 amounts to taking the conjugate value of all entries in the scattering matrix. To prove Lemma 5 we recollect our earlier observations that the eigenvalue E must be a positive real number. This is only fulfilled when k is real, since $\cos(k)$ has to be a real number less than 1, see (13). □
From Lemma (3) and (4) we see that the zeros are placed symmetrically around the point $\frac{\pi}{h}$, and since the formula for the eigenvalue (13) is also symmetric around the same point we need only find the zeros in the interval $[0, \frac{\pi}{h}]$, which are finitely many as we would expect. Further, if we let λ_i denote the eigenvalue corresponding to the zero k_i then in the interval $[0, \frac{\pi}{h}]$ we have that $k_i < k_j \Rightarrow \lambda_i < \lambda_j$.

4 The Scattering Matrix Approach applied to Continuous Graphs

The scattering matrix method was originally developed for the analysis of continuous graphs, and a detailed treatment can be found for example in [1].

Since the procedure is almost identical to the one presented in the previous section we will here only present an outline and point out where the two cases differ. The subscript c will be used to indicate that we are now dealing with continuous graphs.

Let Γ_c be a finite compact metric graph with an edge set $E = \{\Delta_j\}$, where $\Delta_j = [x_{2j-1}, x_{2j}]$. On every edge, the general solution to the eigenvalue equation

$$L\Psi = E\Psi \tag{31}$$

is given by

$$\Psi(x) = ae^{ikx} + be^{-ikx}, \tag{32}$$

where $E = k^2$. We choose $\{e^{ik|x-x_{2j-1}|}, e^{ik|x-x_{2j}|}\}$ and $\{e^{-ik|x-x_{2j-1}|}, e^{-ik|x-x_{2j}|}\}$ as bases for the space of eigenfunctions and write

$$\Psi(x) = a_{2j-1}e^{ik|x-x_{2j-1}|} + a_{2j}e^{ik|x-x_{2j}|} = b_{2j-1}e^{-ik|x-x_{2j-1}|} + b_{2j}e^{-ik|x-x_{2j}|}. \tag{33}$$

For all k different from zero we obtain

$$b_{2j-1} = e^{ik|x_{2j}-x_{2j-1}|}a_{2j}, \qquad b_{2j} = e^{ik|x_{2j}-x_{2j-1}|}a_{2j-1}. \tag{34}$$

Further we define

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_{2N} \end{pmatrix}, \qquad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_{2N} \end{pmatrix}, \tag{35}$$

$$d_j = |x_{2j} - x_{2j-1}|, \qquad \epsilon_c^j = \begin{pmatrix} 0 & e^{ikd_j} \\ e^{ikd_j} & 0 \end{pmatrix}, \tag{36}$$

$$\mathcal{E}_c = \left(\begin{array}{c|c|c} \epsilon_c^1 & 0 & \dots \\ \hline 0 & \epsilon_c^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array}\right), \tag{37}$$

after which we may write

$$\mathbf{b} = \mathcal{E}_c\mathbf{a}. \tag{38}$$

For each vertex V_j we define the vectors $\mathbf{a^m}$ and $\mathbf{b^m}$ in just the same way as in the previous section, but as we will see the vertex scattering matrix

$\sigma^{\mathbf{m}}$ will be different for continuous graphs. The continuity condition at the vertex yields the equations

$$a_{l_j} + b_{l_j} = a_{l_i} + b_{l_i} \tag{39}$$

just as for discrete graphs. The cruisal point is that equation (23) is now replaced by the condition that all normal derivatives be equal to zero:

$$\sum_{x_j \in V_m} \partial_n \Psi(x_j) = 0 \Longleftrightarrow \sum_{x_j \in V_m} (a_j - b_j) = 0. \tag{40}$$

Using the same ansatz for the vertex scattering matrix:

$$\sigma_{\mathbf{c}}^{\mathbf{m}} = \begin{pmatrix} r & t & t & \dots \\ t & r & t & \dots \\ t & t & r & \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{41}$$

we obtain

$$r = t - 1 \tag{42}$$

as before, but now

$$t = 2/v_m \tag{43}$$

One important observation one should make is that for the continuous graph, the scattering matrix is not dependent on the energy. Finally we introduce the following definitions:

$$\Sigma_c = \left(\begin{array}{c|c|c} \sigma_c^1 & 0 & \dots \\ \hline 0 & \sigma_c^2 & \dots \\ \hline \vdots & \vdots & \ddots \end{array} \right), \tag{44}$$

$$U_c(k) = \Sigma_c(k)\mathcal{E}_c(k), \tag{45}$$

$$f_c(k) = \det(U_c(k) - I) = 0. \tag{46}$$

5 Discrete Models of Quantum Graphs

We will now demonstrate how the discrete graph Γ_h can be used to model a continuous quantum graph. We remind the reader that the subscripts h and

c indicate whether we are talking about the discrete graph with step length h or the continuous graph. Let Γ_c be a finite compact metric graph with an edge set $E(\Gamma_c)$ and a vertex set $V(\Gamma_c)$. If the lengths of the edges have a basic length[5] δ we let the step length h be equal to δ/p for some integer p. We then replace each edge E_j in $E(\Gamma_c)$ with a sequence of m_j+1 points such that $m_j h$ equals d_j. We denote the discrete graph constructed in this way Γ_h and the corresponding scattering matrices $\mathcal{E}_h$ and Σ_h. By the construction it is obvious that $\mathcal{L}(\Gamma_c) = \mathcal{L}(\Gamma_h)$. In the absence of a basic length we could pick an arbitrary small number h and let m_j be equal to the integer part of d_j/h, though strictly speaking, the discrete graph obtained in this way could no longer be considered as a net of Γ_c. We will now investigate what happens as we let h tend to zero.

Lemma 6 *Let Γ_c be a finite compact metric graph with edge-scattering matrix $\mathcal{E}_c$ and vertex-scattering matrix Σ_c and let Γ_h be a discrete model of Γ_c with edge-scattering matrix $\mathcal{E}_h$ and vertex-scattering matrix Σ_h. Then we have*

$$\mathcal{E}_h \to \mathcal{E}_c \qquad as \qquad h \to 0 \tag{47}$$

(with equality for graphs where the edges have a basic length), and

$$\Sigma_h \to \Sigma_c \qquad as \qquad h \to 0. \tag{48}$$

PROOF. The lemma follows from the fact that $m_j h \to d_j$ as $h \to 0$ and that

$$t = \frac{2i\sin(kh)}{v_m(e^{ikh}-1)+2-2\cos(kh)} \to \frac{2}{v_m} \qquad \text{as} \qquad h \to 0. \tag{49}$$

□

To prove that the Laplace eigenvalues of the discrete graphs converge to the Laplace eigenvalues of the corresponding continuous graph is now a straightforward matter. We let λ_i^h denote the i:th Laplace eigenvalue of Γ_h and let λ_i^c denote the i:th Laplace eigenvalue of Γ_c (counting from below with multiplicity). We may now state our main theorem:

Theorem 2 *For a finite compact metric quantum graph Γ_c with a discrete model Γ_h we have that*

$$\lambda_i^h \to \lambda_i^c \qquad as \qquad h \to 0 \tag{50}$$

[5] A number δ such that $d_j = n_j\delta$, where $\{d_j\}$ are the lengths of the edges and $\{n_j\}$ are integers.

where $\{\lambda_i^h\}$ *and* $\{\lambda_i^c\}$ *are the Laplace eigenvalues of* Γ_h *and* Γ_c *respectively (counting from below with multiplicity).*

PROOF. After inspection one verifies that $t = t(h,k)$ has removable singularities at the points $2\pi n/h$, $n \in \mathbb{Z}$, so it can be treated as an entire analytic function with respect to k. Thus $f_h(k)$ can also be considered as an entire analytic function. By Lemma (6) we get that $f_h(k)$ converges uniformly to $f_c(k)$ on any compact set. Let k_c be any zero of $f_c(k)$ and take a positive number r that is smaller than the distance to any neighbouring zero. There is always such a number since the set of zeros of an analytic functions has no finite point of accumulation. We now consider the contour integral of $f_h'(k)/f_h(k)$ and $f_c'(k)/f_c(k)$ around the circle centered at k_c with radius r. Since $f_h(k)$ converges uniformly to $f_c(k)$ on any compact interval, it is clear that for h small enough $f_h(k)$ and $f_c(k)$ will have the same number of zeros inside this circle. We let ρ denote the spectral multiplicity of the zero eigenvalue, which by Proposition (1) and Theorem (1) we know is the same on Γ_c and Γ_h. Theorem (2) is thus fulfilled for $i \leqslant \rho$. Further we let

$$0 < k_{\rho+1}^h \leqslant k_{\rho+2}^h \leqslant \dots \qquad 0 < k_{\rho+1}^c \leqslant k_{\rho+2}^c \leqslant \dots \tag{51}$$

denote the zeros of $f_h(k)$ and $f_c(k)$ on the positive real axis, where we have taken into account the algebraic multiplicity. We have proved that for $i > \rho$, $k_i^h \to k_i^c$ as $h \to 0$ and from this we obtain

$$\lambda_i^h = \frac{2 - 2\cos(k_i^h h)}{h^2} \to (k_i^c)^2 = \lambda_i^c \qquad \text{as } h \to 0. \tag{52}$$

for $i > \rho$ and the theorem is proven. □

So far we have not said anything about the nature of the convergence of the eigenvalues. Empirical data suggests that the eigenvalues of the discrete nets with equal step length increases monotonically to the eigenvalues of the continuous graph, a conjecture also stated in [4]. We will now discuss how this conjecture relates to the zeros of the analytic functions used in the proof of Theorem 2, and the lemma stated below provides some information in that direction.

Lemma 7 *If* k_i^h *increases monotonically to* k_i^c *as* $h \to 0$*, then* λ_i^h *increases monotonically to* λ_i^c *as* $h \to 0$*.*

PROOF. By the combined use of Lemma (3) and Lemma (4) we see that the zeros of f_h are situated symmetrically around the point $\frac{\pi}{h}$. Since $E = (2 - 2\cos(kh))/h^2$ is also symmetric around the same point we are justified in considering only the zeros smaller than $\frac{\pi}{h}$. Consider two different step lengths h_1 and h_2 such that $h_2 < h_1$ or equivalently $h_2 = \alpha h_1$ where $\alpha < 1$. Let k_1 and k_2 be the i:th zero of f_{h_1} and f_{h_2} respectively and suppose that $k_2 = \beta k_1$ where $\beta > 1$. We may assume that both $h_1 k_1$ and $h_2 k_2$ are less than π, and we make the following series of estimates:

$$\lambda_i^{h_2} = \frac{2 - 2\cos(\beta k_1 \alpha h_1)}{(\alpha h_1)^2} > \frac{2 - 2\cos(k_1 \alpha h_1)}{(\alpha h_1)^2} > \frac{2 - 2\cos(k_1 h_1)}{(h_1)^2} = \lambda_i^{h_1} \quad (53)$$

where we have used the fact that $(2-2\cos(\xi))/\xi^2$ is decreasing in the interval $0 < \xi < \pi$. The inequality $(2 - 2\cos(hk))/h^2 < k^2$ shows that the series of eigenvalues is bounded by λ_i^c, which concludes the proof of the lemma. □
The significance of Lemma 7 lies in the fact that, again, empirical data suggest that the zeros of f_h do increase monotonically to their limits.

6 Discrete Schrödinger Operators

The apparatus developed for the analysis of the Laplacian spectra is well suited also for the study of the stationary one-dimensional Schrödinger operator, the difference being that the edge-scattering matrices will be more complicated. Explicit solutions of the Schrödinger equation are in general impossible to obtain so we will only be concerned with generalizing the spectral convergence theorem to also include these operators.

We begin by studying the stationary Schrödinger differential equation on a compact interval $[x_{2j-1}, x_{2j}]$

$$-\frac{d^2}{dx^2}\Psi(x) + q(x)\Psi = k^2\Psi(x) \qquad x \in [x_{2j-1}, x_{2j}]. \quad (54)$$

We will assume that the potential $q(x)$ is sufficiently smooth[6] and that it is identically zero in a neighbourhood of x_{2j-1} and x_{2j} respectively. With no boundary conditions specified the equation has a solution for every k, thus

[6]Throughout this section we will assume that $q(x)$ has continuous derivatives of order up to at least 2 in order to insure that Ψ has continuous derivatives of order up to 4.

given any positive number k^2 and some Cauchy data at a certain point we obtain a unique solution. In the intervals where the potential vanishes the solution to the eigenvalue equation is, as before, given by the general formula $\Psi(x) = ae^{ikx} + be^{-ikx}$. We are interested in two specific solutions $f_+(k,x)$ and $f_-(k,x)$ characterized by the following initial data: $f_+(k,x) = e^{ikx}$ to the right of the potential, $f_-(k,x) = e^{-ikx}$ to the left of the potential. It is in general impossible to solve the equations exactly, we will merely observe that for some numbers $\{\alpha_+, \alpha_-, \beta_+, \beta_-\}$ we have that $f_+(k,x) = \alpha_+ e^{ikx} + \beta_+ e^{-ikx}$ to the left of the potential and $f_-(k,x) = \alpha_- e^{-ikx} + \beta_- e^{ikx}$ to the right of the potential. The numbers $\{t_+ = 1/\alpha_+, t_- = 1/\alpha_-\}$ are called the left and right transmission coefficients and $\{r_+ = \beta_+/\alpha_+, r_- = \beta_-/\alpha_-\}$ are called the left and right reflection coefficients, and these are in general dependent on k. With the notation used in Section (4) we have for a continuous graph

$$\begin{pmatrix} a_{2j-1} \\ a_{2j} \end{pmatrix} = \begin{pmatrix} r_+ & t_- e^{-ikd_j} \\ t_+ e^{-ikd_j} & r_- \end{pmatrix} \begin{pmatrix} b_{2j-1} \\ b_{2j} \end{pmatrix}. \tag{55}$$

One can show that the matrix above is unitary, and by inverting it we get the following generalization of the edge-scattering matrix:

$$\epsilon^j = \begin{pmatrix} r_+ & t_+ e^{ikd_j} \\ t_- e^{ikd_j} & r_- \end{pmatrix}. \tag{56}$$

In order to define the discrete Schrödinger operator we must first introduce some notation. We let Δ denote an edge on a continuous graph and we let Δ_h be the corresponding discretized edge with step-length h. Without loss of generality we may take the left endpoint equal to 0, and we suppose $\Delta = [0, b]$. We will use the notation $u^{(h)}$ when we speak about a function defined on Δ_h, and for any function u defined on Δ we write $\{u\}_h$ to denote the function on Δ_h which satisfies $\{u\}_h(hn) = u(hn)$. Whenever the symbol $\|\cdot\|$ is used on a function (vector) it should be understood as the supremum norm. The discrete Schrödinger operator is defined by the correspondence

$$-\frac{d^2}{dx^2} + q(x) \longrightarrow L + \{q\}_h. \tag{57}$$

The reflection- and transmission coefficients for the discrete Schrödinger operator are defined in just the same way as for the differential operator, and we assume that h is small enough so that there are sufficiently many points on Δ_h to the left and right of the potential for the definition to make sense.

It is evident that if we can show that these coefficients converges to those of the Schrödinger differential operator as h tends to zero, then without any changes the proof of Theorem 2 will also show the convergence of the Schrödinger spectrum for this class of potentials.

We introduce the following slightly modified operators acting on $L_2(\Delta)$ and $l_2(\Delta_h)$ respectively:

$$S = -\frac{d^2}{dx^2} + q(x) - k^2 \tag{58}$$

$$S_h = L + \{q\}_h - \frac{2 - 2\cos(kh)}{h^2} \tag{59}$$

where $q(x)$ is a sufficiently smooth function that vanishes in a neighbourhood of the endpoints. Further we introduce the boundary operators

$$\gamma u = \begin{bmatrix} u(0) \\ u'(0) \end{bmatrix}, \qquad \gamma_h u^{(h)} = \begin{bmatrix} u(0) \\ \frac{u(h)-u(0)}{h} \end{bmatrix} \tag{60}$$

and the boundary values

$$\phi = \begin{bmatrix} 1 \\ -ik \end{bmatrix}, \qquad \phi_h = \begin{bmatrix} 1 \\ \frac{e^{-ih}-1}{h} \end{bmatrix}. \tag{61}$$

As before we let f_- denote the solution to the equation $Su = 0$ satisfying the boundary condition $\gamma u = \phi$, and we let $f_-^{(h)}$ denote the function satisfying $S_h u^{(h)} = 0$ and $\gamma_h u^{(h)} = \phi_h$, and we now wish to make an estimate of $\|\{f_-\}_h - f_-^{(h)}\|$. With the aid of the following Taylor expansions

$$u(x+h) = u(x) + hu'(x) + \frac{1}{2}h^2u''(x) + \frac{1}{6}h^3u'''(x) + \frac{1}{24}h^4u^{(4)}(\xi_1) \tag{62}$$

$$u(x-h) = u(x) - hu'(x) + \frac{1}{2}h^2u''(x) - \frac{1}{6}h^3u'''(x) + \frac{1}{24}h^4u^{(4)}(\xi_2) \tag{63}$$

and the inequality

$$\|k^2 - \frac{2 - 2\cos(kh)}{h^2}\| < M_1h^2 \tag{64}$$

we see that for any function with bounded derivatives up to order 4 we have that

$$\left\|\frac{u(x+h) - 2u(x) + u(x-h)}{h^2} - u''(x)\right\| < M_2h^2 \tag{65}$$

and hence

$$\|S_h\{u\}_h - \{Su\}_h\| < M_3 h^2. \tag{66}$$

Thus, in particular

$$\|S_h[\{f_-\}_h - f_-^{(h)}]\| = \|S_h\{f_-\}_h\| = \|S_h\{f_-\}_h - \{Sf_-\}_h\| < Mh^2. \tag{67}$$

From this estimate we conclude that the function $\{f_-\}_h - f_-^{(h)}$ satisfies the equation $S_h u^{(h)} = \psi^{(h)}$ for some function $\psi^{(h)}$ with norm less than Mh^2. Further is it obvious that $\gamma_h[\{f_-\}_h - f_-^{(h)}] = 0$. We shall prove that the difference equation $S_h u^{(h)} = \psi^{(h)}$ with boundary condition $\gamma_h u^{(h)} = \phi_h$ is stable, which means that for some constants N_1 and N_2 not depending on h the solution fulfills the condition

$$\|u^{(h)}\| < N_1\|\psi^{(h)}\| + N_2\|\phi_h\|. \tag{68}$$

The proof, which is somewhat technical, is left to the appendix. Accepting this for the moment, we see that the stability condition immediately yields $\|\{f_-\}_h - f_-^{(h)}\| \to 0$ as $h \to 0$. The treatment of f_+ is analogous, and the convergence of the reflection- and transmission coefficients is thereby established. We have thus proved the following generalization of Theorem (2):

Theorem 3 *Let Γ_c be a finite compact metric graph and let $q(x)$ be a potential defined on Γ_c that vanishes in a neighbourhood of the vertices and has bounded derivatives of order up to at least 2. Given a discrete model Γ_h we have that*

$$\lambda_i^h \to \lambda_i^c \qquad \text{as} \qquad h \to 0 \tag{69}$$

where $\{\lambda_i^c\}$ are the eigenvalues of $L+q(x)$ on Γ_c and $\{\lambda_i^h\}$ are the eigenvalues of $L + \{q\}_h$ on Γ_h.

Appendix

A Stability of Schrödinger Difference Equations

The aim of this section is to show the stability of the difference equation

$$Lu^{(h)} + \{q\}_h u^{(h)} = \psi^{(h)} \tag{70}$$

on a grid with step length h extracted from the interval $[0,1]$. The number of points on the grid is thus equal to $1/h$. We will only consider the case where q is a real-valued bounded function defined on the interval $[0,1]$. To some extend we will follow the procedure presented in Chapter II of [6], the first step being to reduce the equation to the canonical form

$$\mathbf{y}_{n+1}^{(h)} = R_{h,n}\mathbf{y}_n^{(h)} + h\varrho_n^{(h)}, \tag{71}$$

where we have introduced the vectors

$$\mathbf{y}_n^{(h)} = \begin{pmatrix} u^{(h)}(hn) \\ \frac{u^{(h)}(h(n+1))-u^{(h)}(hn)}{h} \end{pmatrix}, \qquad \varrho_n = \begin{bmatrix} 0 \\ \psi^{(h)}(h(n+1)) \end{bmatrix}. \tag{72}$$

It is readily checked that the matrix $R_{h,n}$ is given by

$$R_{h,n} = \begin{bmatrix} 1 & h \\ -h\{q\}_h(h(n+1)) & 1-h^2\{q\}_h(h(n+1)) \end{bmatrix}. \tag{73}$$

Essential for the proof will be to show that the norm[7] of the matrix $\prod_{i=1}^{1/h} R_{h,i}$ is bounded by some constant N independent of h (we let the product symbol denote matrix multiplication from right to left). The spectral norm of $R_{h,n}$ is equal to the square-root of the largest eigenvalue λ_{max} of $R_{h,n}^\dagger R_{h,n}$ which, omitting the details, to the first approximation in h is given by

$$\lambda_{max} = 1 + h\sqrt{(\{q\}_h(h(n+1))-1)^2} + O(h^2). \tag{74}$$

The function inside the square-root is positive and bounded since $\{q\}_h$ is real and bounded, so it is evident that $\|R_{h,n}\|^2 < 1 + Ch$ for some constant C. Thus,

$$\|\prod_{i=1}^{1/h} R_{h,i}\| \leqslant \prod_{i=1}^{1/h} \|R_{h,i}\| \leqslant \sqrt{(1+Ch)}^{1/h} \to e^{C/2} \equiv N. \tag{75}$$

Rewriting equation (71) in the form

$$\mathbf{y}_n^{(h)} = (\prod_{i=1}^{n} R_{h,i})\mathbf{y}_0^{(h)} + h\left[(\prod_{i=1}^{n-1} R_{h,i})\varrho_0^{(h)} + (\prod_{i=1}^{n-2} R_{h,i})\varrho_1^{(h)} + \ldots + \varrho_{n-1}^{(h)}\right] \tag{76}$$

[7] In the case of matrices we use the $\|\cdot\|_2$ norm. Since we are only dealing with finite-dimensional spaces, for convenience we will employ a somewhat sloppy use of norms.

we obtain the inequality

$$\|\mathbf{y}_n^{(h)}\| \le N \left[\|\mathbf{y}_0^{(h)}\| + hn(\mathtt{max}_{j=0..n-1}\{\|\varrho_j^{(h)}\|\} \right]. \tag{77}$$

Hence, since $hn < 1$, we arrive at

$$\|u^{(h)}\| \le N\|\psi^{(h)}\| + N\|\phi_h\|, \tag{78}$$

which means that it is stable.

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