Spectral Problems for some Finite and Infinite Quantum Graphs

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Abstract

We present an introduction into the theory of quantum graphs and prove the corresponding trace formula. It is proven that two non-isometric graphs can be isospectral. The distribution connected with the spectrum is computed for four quantum graphs and it is demonstrated how the Euler characteristic of a graph can be calculated from the spectrum. The limiting procedure when the length of an edge tends to zero is considered and it is shown that a single vertex can replace two vertices connected by a disappearing edge. The same procedure applied to direct spectral problems is considered.

Contents

1 Introduction

Quantum Graphs have been introduced to model the electron probability density distribution of a free π-electron in conjugated molecules such as naphthalene $C_{10}H_8$ and benzene C_6H_6. The model was first suggested by Ruedenberg and Scherr in 1953 [20] as an alternative to the, at that time prevailing LCAO[1] model for molecular orbitals. The model has been thoroughly studied since then but there are still open questions. Mathematically, a Quantum Graph consists of a geometric graph with a differential operator on the edges and certain boundary conditions at the vertices that guarantee the self-adjointness of the operator. The geometric graph consists of edges, considered as intervals of the real axis that are joined together at the vertices. The operator is usually the Schrödinger operator and that is where the name 'Quantum Graphs' comes from. Quantum graph problems are closely related to problems in other research areas, for example averaging in dynamical systems, light propagation in thin structures, antennas and more. A survey of various applications can be found in [8].

A natural problem for Quantum Graphs is to determine the spectrum of the operator, since the physical interpretation of this quantity is energy of an electron in the structure. Such problems will be called *direct problems*. The corresponding *inverse problem* is to recover the Quantum graph or some of its properties, from the spectrum of the operator. The inverse problem does in general not have a unique solution, which is clear from [5], and in the content of scattering in [12]. Other articles related to the inverse problem are for example [5, 10, 11, 14].

An overview of the theoretical results that are needed to understand our arguments will be presented along the text. The reader might want to use [1] for the theory of operators in Hilbert spaces, [2, 18] for spectral theory of operators and [21] for complex analysis.

1.1 Quantum Graphs as a model in quantum chemistry

Quantum graphs describe free electrons within thin structures. This section will show how to do that and is based on the article that Ruedenberg and Scherr [20] presented in 1952[2].

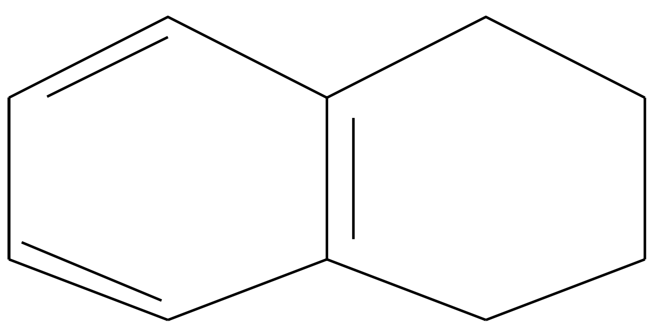

Figure 1: The molecular structure of Naphthalene.

[1] LCAO stands for linear combination of atomic orbits.
[2] This is the first article in a series of three [6, 17].

Consider an organic molecule with conjugated bonds; say for example the Naphthalene molecule $C_{10}H_8$ shown in figure 1. A *π-electron* is not strongly bounded to any specific atom and is free to move along the molecule structure or *Molecular skeleton*. The full Hamiltonian for such a system is rather complicated as the potential involves all nucleus and electrons. Under the assumption that only the studied electron move the time independent part is:

$$H\varphi(r) = \left[-\frac{\hbar}{2m}\Delta + \sum v_i(r_i - r) \right] \varphi(r), \tag{1}$$

where m is the electron mass and v_i are the potentials from the nearby electrons and protons. Even this simplified Hamiltonian is complicated enough to motivate the search for a simpler model and that is what Ruedenberg and Scherr did.

The main simplification in their article is to disregard all directions but the one along the molecular skeleton. This was well motivated since the energies of the states that is associated to the other directions are extremely large. Consider the cuboid in figure 2. The eigenvalues will be

$$\lambda_{n,m,p} = k\left[\left(\frac{m}{l}\right)^2 + \left(\frac{n}{\epsilon}\right)^2 + \left(\frac{p}{\epsilon}\right)^2 \right], \tag{2}$$

where m, n and p are non-negative integers. It is clear that λ associated to $n, p \neq 0$ when ϵ is small can be neglected. This assures that $-\Delta$ can be replaced by $-\frac{d^2}{dx^2}$ in (1).

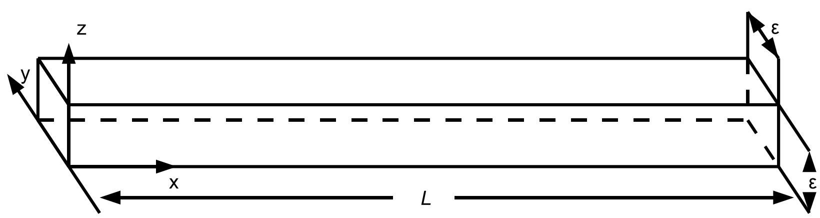

Figure 2: The potential along a molecular skeleton has roughly the form of a cuboid.

A point where two or more edges of the skeleton join together is called a *branching point*. The number edges that end in a branching point is called the *valency* or *degree* of the branching point. To define $-\frac{d^2}{dx^2}$ on the graph as a self-adjoint operator we need to introduce boundary conditions on all branching points. Ruedenberg and Scherr assumed that the functions from the domain of the operator have to be continuous, and argued that a *conservation condition* must be satisfied at each branching point. The conservation condition is that the sum of the normal derivatives just outside the branching point is zero for any function in the domain of the operator.

2 Mathematical Theory

This section will give an overview of the most important mathematical concepts used in connection with quantum graphs.

2.1 Operators in Hilbert Spaces

Since we would like to use the framework of quantum mechanics, only self-adjoint operators in a Hilbert space $\mathscr{H}$, will be considered. The corresponding scalar product will be denoted by $(\cdot,\cdot)$. The operators that will be used are generally not bounded. The *domain* of an operator T, will be denoted by $D(T)$ and the *range* by $R(T)$. A linear operator A is called *self-adjoint* if and only if

1. A is symmetric, i.e $(f, Ag) = (Af, g)$ for all $f, g \in D(A)$.

2. $R(A - \lambda I) = \mathscr{H}$ for any non-real $\lambda \in \mathbb{C} \setminus \mathbb{R}$.

In the case of a bounded operator it is easier to use the following definition: A linear bounded operator, A, is self-adjoint if $(f, Ag) = (Af, g)$ for all $f, g \in \mathscr{H}$. Such operators are also called *Hermitian*.

An operator T is an *extension* of an operator S (or $S \subset T$) if $D(S) \subset D(T)$ and $Tf = Sf$ for each $f \in D(S)$. On the other hand, an operator, T, can be *restricted*, to T_1 ($T_1 \subset T$) if , $D(T_1) \subset D(T)$ and $T_1 f = Tf$ for any $f \in D(T_1)$.

2.2 Metric graphs

A metric graph Γ is an ordered pair (V, E) where $E = \{E_1, E_2, ..., E_N\}$, is a set of edges and $V = \{V_1, V_2, ..., V_M\}$ is a set of vertices. Every edge E_n, is associated with an interval $\Delta_n = [x_{2n-1}, x_{2n}] \subset \mathbb{R}$ with the length $d_n = |x_{2n} - x_{2n-1}|$. Each vertex is an equivalence class in the set of all endpoints, $\{x_n\}_{n=1}^{N}$. Points from the same equivalence class are identical.

The *Euler Characteristic* of a graph with N edges and M vertices is defined as

$$\chi(\Gamma) = M - N. \tag{3}$$

A graph is a *tree* if $\chi = 1$. The relation $V_i \sim V_j$ denotes that there exists an edge E_n connecting V_i and V_j. Information on how vertices are connected to each other in a graph can be represented by a *vertex connectivity matrix* C, of dimension MxM, which is defined by

$$C_{ij} = \begin{cases} 1, & \text{if } V_i \sim V_j; \\ 0, & \text{otherwise.} \end{cases} \tag{4}$$

A *compact graph* is a graph that consists of a finite number of compact intervals. By a connected graph we mean a graph where any two vertices may be joined by a continuous path. All graphs that will be considered in this paper are connected. The *volume* ot the total lenght $\mathscr{L}$ of a metric graph is the sum of the lengths of the edges that it is formed of. The *distance* between two points in a connected graph is the length of the shortest path between them. The diameter of a graph is the largest distance between two points in the graph. A graph is decorated if it has at least one node with valency 2. To add a node on an edge is called decoration. Observe that decoration does not change the graph as a metric space.

2.3 The Schrödinger Equation

Eigenfunctions to the Schrödinger operator H, describe probability densities for electrons. The corresponding eigenvalues are just the energies of the states.

$$H = \oplus \sum_{k=1}^{N} \Big(-\frac{d^2}{dx^2} + q(x) \Big), \tag{5}$$

where $q(x)$ is a real valued potential on the graph. As a first step, we may neglect the potential q and consider the *Laplace operator*

$$L \equiv \oplus \sum_{k=1}^{N} \Big(-\frac{d^2}{dx^2} \Big). \tag{6}$$

In what follows we are going to discuss this differential operator on the Hilbert space $\mathscr{H}$:

$$\mathscr{H} \equiv L^2(\Gamma) = \oplus_{n=1}^{N} L^2(\Delta_n) = \oplus_{n=1}^{N} L^2[x_{2j-1}, x_{2j}], \tag{7}$$

where L^2 denotes the space of square integrable functions.

2.4 Boundary conditions and eigenvalues.

With our new notation, we formulate the *natural boundary conditions*, the ones that Ruedenberg and Scherr found, as:

$$\left\{ \begin{array}{ll} f(x_j) = f(x_k), \quad x_j, x_k \in V_m, & \\ \sum_{x_j \in V_m} \partial_n f(x_j) = 0, & \end{array} \right. \quad m = 1, 2, ..., M. \tag{8}$$

Where ∂_n are normal derivatives, which we define as

$$\partial_n f(x_j) = \left\{ \begin{array}{rl} f'(x_j), & \text{if } x_j \text{ is the left endpoint;} \\ -f'(x_j), & \text{if } x_j \text{ is the right end point.} \end{array} \right. \tag{9}$$

Let us denote by $L(\Gamma)$ the Laplace operator (6) defined on the set of functions from the Sobolev space $W_2^2(\Gamma \setminus V)$ satisfying boundary conditions (8). Observe that such operator is uniquely defined by the geometric graph Γ. In quantum mechanics it is only possible to measure eigenvalues of operators, and this is meaningful only if the operators have real eigenvalues. Symmetric operators, T, have this property. If $\varphi \in D(T)$, then the symmetric property $(T\varphi, \varphi) = (\varphi, T\varphi)$ assures this since:

$$\begin{array}{rcl} (T\varphi, \varphi) & = & \lambda(\varphi, \varphi), \\ (\varphi, T\varphi) & = & \overline{\lambda}(\varphi, \varphi). \end{array} \tag{10}$$

Thus $\lambda = \overline{\lambda}$, and hence $\mathrm{Im}(\lambda) = 0$. Our operator $L(\Gamma)$ is symmetric when the standard boundary conditions are imposed. Take $\varphi, \phi \in D(L)$ then:

$$(L\varphi, \phi) = \sum_{n=1}^{N} \int_{\Delta_n} -\varphi''(x)\overline{\phi(x)} dx. \tag{11}$$

Performing partial integration twice yields:

$$= \underbrace{\sum_{n=1}^{N} [\varphi(x)\overline{\phi'(x)}]_{x_{2n-1}}^{x_{2n}}}_{(*)} - \sum_{n=1}^{N} [\varphi'(x)\overline{\phi(x)}]_{x_{2n-1}}^{x_{2n}} + (\varphi, L\phi). \tag{12}$$

The term $(*)$ is a sum over all edges, we write it as a sum over all vertices:

$$(*) = \sum_{m=1}^{M} \sum_{x_j \in V_m} \partial_n \varphi(x_j) \overline{\phi'(x_j)}. \tag{13}$$

The boundary conditions give that $\varphi(x_j) = \varphi(x_k)$ for all $x_j, x_j \in V_m$, so for any $x_l \in V_m$ we further have

$$(*) = \sum_{m=1}^{M} \left(\varphi(x_l) \sum_{x_j \in V_m} \partial_n \overline{\phi'(x_j)} \right) = 0, \tag{14}$$

by virtue of the standard boundary conditions (8), the other sum in (12) can be proved to be zero in the same way. The operator $L(\Gamma)$ is also self-adjoint, we refer to [15] for a proof.

2.5 The Trace Formula

The Trace formula relates the geometry of a graph to the spectrum of the corresponding Laplacian and has proved to be very fruitful. It was first derived by J.-P. Roth [19] using the heat kernel approach. This section is, however, based on a paper by M. Nowaczyk and P. Kurasov [11] in which another approach is used. The idea of the proof is to first solve the direct problem or to determine the eigenvalues to an arbitrary compact quantum graph. The notation from the previous section is used. A function, φ is an eigenfunction of $L(\Gamma)$ if and only if

$$L(\Gamma)\varphi = \lambda\varphi, \tag{15}$$

or expanded

$$-\varphi'' = \lambda\varphi, \quad \text{on every edge} \tag{16}$$

and satisfy

$$\begin{cases} \sum_{x_i \in V_m} \partial_n \varphi(x_i) = 0, \\ \varphi(x_i) = \varphi(x_j),\ x_j, x_i \in V_m, \end{cases} \quad m = 1, ..., M. \tag{17}$$

The differential equation (16) can easily be calculated and the solution on each edge is

$$\varphi_n = Ae^{ikx} + Be^{-ikx}, \tag{18}$$

where $k = \sqrt{\lambda}$. Two other representations of (18) are useful. One as *incoming waves* and one as *outgoing waves*, see Figure 3. To get the basis of incoming waves, set

$$A = a_{2j-1}e^{-ikx_{2j-1}}, \quad B = a_{2j}e^{ikx_{2j}}, \tag{19}$$

then

$$\varphi_n = a_{2j-1}e^{ik(x-x_{2j-1})} + a_{2j}e^{ik(x_{2j}-x)} \tag{20}$$

so

$$\varphi_n = a_{2j-1}e^{ik|x-x_{2j-1}|} + a_{2j}e^{ik|x-x_{2j}|}. \tag{21}$$

In the basis of outgoing waves, the function is:

$$\varphi_n = b_{2j}e^{-ik|x-x2j|} + b_{2j-1}e^{-ik|x-x_{2j-1}|}. \tag{22}$$

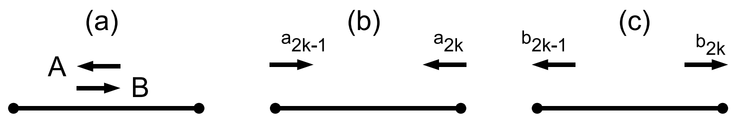

Figure 3: Three different bases describe the eigenfunctions on an edge.

The relation between the coefficients in the two representations on an edges, E_n, of length d_n is:

$$\begin{pmatrix} b_{2n-1} \\ b_{2n} \end{pmatrix} = \underbrace{\begin{pmatrix} 0 & e^{ikd_n} \\ e^{ikd_n} & 0 \end{pmatrix}}_{S_e^n} \begin{pmatrix} a_{2j-1} \\ a_{2j} \end{pmatrix}. \tag{23}$$

To express this for all edges on Γ, let

$$\mathbf{a} = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{pmatrix}, \tag{24}$$

and then

$$\mathbf{b} = \underbrace{\begin{pmatrix} S_e^1 & 0 & \cdots \\ 0 & S_e^2 & \\ \vdots & & \ddots \end{pmatrix}}_{S_E} \mathbf{a}. \tag{25}$$

The matrix S_E has the dimension $2N$x$2N$, is block-diagonal and invertible.

The standard boundary conditions (8) give another condition between the amplitudes.

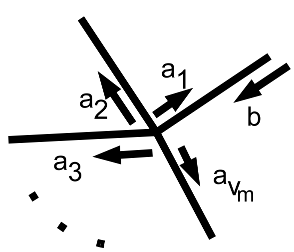

Figure 4: scattering at a vertex.

Consider an arbitrary vertex, V_m like the one shown in figure 4 with valency v_m. Let there be an outgoing wave, $a_p e^{ik(x-x_{2p-1})}$ on each edge E_p but only one incoming wave, $e^{-ik(x-x_1)}$ on edge E_1. The symmetries in the problem suggests that all outgoing waves on the edges $E_1, E_2, ..., E_{v_m}$ are equal since no consideration to ordering or angle between edges et cetera is taken. We make the following Ansatz:

$$\underbrace{\begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_{v_m} \end{pmatrix}}_{\mathbf{a}^m} = \underbrace{\begin{pmatrix} r & t & \cdots & t \\ t & r & & \\ \vdots & & \ddots & \\ t & & & r \end{pmatrix}}_{S_v^m} \underbrace{\begin{pmatrix} b \\ 0 \\ \vdots \\ 0 \end{pmatrix}}_{\mathbf{b}^m}, \tag{26}$$

and for simplicity, we set $b = 1$. The standard boundary conditions give the following relation:

$$\left\{ \begin{array}{l} 1 + r = t \\ (v_m - 1)t + r - 1 = 0. \end{array} \right. \tag{27}$$

This yields

$$\left\{ \begin{array}{l} t = 2/v_m, \\ r = (2 - v_m)/v_m. \end{array} \right. \tag{28}$$

Let $\mathbf{a}^m$ denote the vector of the amplitudes of the incoming waves and $\mathbf{b}^m$ the corresponding vector of the outgoing waves. If we let S_v^m be the matrix that describes the relation between these; then

$$\mathbf{a}^m = S_v^m \mathbf{b}^m, \quad (S_v^m)_{jk} = \left\{ \begin{array}{ll} 2/v_m, & j \neq k; \\ (2 - v_m)/v_m, & j = k, \end{array} \right. \tag{29}$$

where $1 \leq j, k \leq v$.

Let S_V be a matrix that holds all S_v^m, $m = 1, ..., M$ in the following way:

$$\left(\begin{array}{c} \mathbf{a}^1 \\ \mathbf{a}^2 \\ \vdots \\ \mathbf{a}^M \end{array} \right) = \underbrace{\left(\begin{array}{ccc} S_v^1 & 0 & \cdots \\ 0 & S_v^2 & \\ \vdots & & \ddots \end{array} \right)}_{S_V} \left(\begin{array}{c} \mathbf{b}^1 \\ \mathbf{b}^2 \\ \vdots \\ \mathbf{b}^M \end{array} \right). \tag{30}$$

Theorem I: *S_V is unitary.*

Proof: A matrix, A, is unitary if $A^* = A^{-1}$. This condition transforms to $S_V = S_V^{-1}$ since the matrix is both real and symmetric. We will therefore verify that the equality $S_V S_V = I$ holds. S_V is defined by it's diagonal blocks $S_v^1, S_v^2, ..., S_v^M$ so it is enough to verify that $(S_v^k)^2 = I$ for $1 \leq k \leq M$. Let $S_{v,i}$ be the row (or column) i in any S_v. From (28) follows that

$$< S_{v,i}, S_{v,j} >= \left\{ \begin{array}{ll} (v-1)t^2 + r^2 = 1, & i = j, \\ (v-2)t^2 + 2rt = 0, & i \neq j. \end{array} \right. \tag{31}$$

Thus $S_v S_v = I$ and $S_V^{-1} = S_V^*$. $\square$

From (25) and (30) follows that

$$\mathbf{a} = S_V S_E \mathbf{a} \tag{32}$$

is satisfied for every vector $\mathbf{a}$ that represents an eigenfuction to $L(\Gamma)$[3]. We define the total scattering matrix, $S(k)$, as

$$S(k) \equiv S_V S_E(k). \tag{33}$$

Non-trivial solutions to (32), i.e. eigenvectors $\mathbf{a}$ with eigenvalues 1 to $S(k)$ can be found, only for such k:s that

$$f(k) \equiv \det(S(k) - I) = 0. \tag{34}$$

[3]Observe that S_E and S_V are, in general, block diagonal in different bases.

Denote the *spectral multiplicity* of an eigenvalue λ to $L(\Gamma)$, by m_s, and let m_a denote the *algebraic multiplicity* i.e. the dimension of the linear space of solutions to (34). M. Nowaczyk and P. Kurasov [11] has shown that $E = 0$ has spectral multiplicity 1 and algebraic multiplicity $N - M + 2$. The algebraic and spectral multiplicities are equal for other eigenvalues.

Let u be a distribution that contain information about the spectrum in the following way:

$$u \equiv 2\delta(k) + \sum_{n=1}^{\infty} \left(\delta(k - k_n) + \delta(k + k_n)\right), \tag{35}$$

where k_n are the zeros to (34), i.e. k_n^2 are eigenvalues of $L(\Gamma)$. Since k_n are the zeros of $\det(S(k) - I)$, the integral

$$\frac{1}{2\pi i} \oint \frac{f'(z)}{f(z)} dz, \tag{36}$$

that equals the sum of the orders of the zeros to the function $f(z)$ within the contour of the integral, can be used to construct (35). The value of the distribution can then be calculated for any test function $\varphi \in C_0^\infty$, as

$$e[\varphi] = \lim_{\epsilon \to 0} \frac{1}{2\pi i} \int_{-\infty}^{\infty} \left(\frac{f'(k - i\epsilon)}{f(k - i\epsilon)} - \frac{f'(k + i\epsilon)}{f(k + i\epsilon)} \right) \varphi(k) dk - (N - M)\varphi(0) \tag{37}$$

where the term $-(N - M)\varphi(0)$ corrects that $k_0 = 0$ has algebraic multiplicity $N - M + 1$. We use a few identities, for example $\ln(f)' = f'/f$; Liouvilles theorem: $\frac{d}{dt}(\log|\det A|) = \mathrm{Tr}\left(\frac{d}{dt}A^{-1}\right)$; geometric sum expansions and, the matrix

$$D = \begin{pmatrix} d_1 & 0 & 0 & 0 \\ 0 & d_1 & 0 & 0 \\ 0 & 0 & d_2 & 0 \\ 0 & 0 & 0 & \ddots \end{pmatrix}, \tag{38}$$

which is introduced from the relation

$$\frac{d}{dk} S = S_V \frac{d}{dk} S_E = ikSD. \tag{39}$$

Finally, we get:

$$\begin{aligned} u &= \frac{1}{2\pi i} \mathrm{Tr}\left[(... + S^{-1}(k) + I + S(k) + ...)iD\right] - (N - M)\delta(k) && (40) \\ &= \frac{1}{2\pi i} \mathrm{Tr}\left[\left(\sum_{s=-\infty}^{\infty} S^k\right) iD\right] - (N - M)\delta(k). && (41) \end{aligned}$$

We will now show that (41) can be calculated using the set of all periodic orbits on the graph. Let:

- p be a *periodic orbit* i.e. an oriented and closed path on the graph.
- $\mathrm{prim}(p)$ be the *primitive periodic orbit* of p, i.e. the periodic orbit without any repetitions such that $p = g \cdot \mathrm{prim}(p)$ where $g \in \mathcal{N} \setminus \{0\}$. We call g the degree of p.

- $l(p)$ be the geometric length of a periodic orbit.
- $T(p)$ be the set of all scattering coefficients along the orbit p.
- P be the set of all periodic orbits for a graph, Γ.
- P_m^n be a subset of P, consisting of all periodic orbits of discrete length n, that start in a certain vertex and goes into the interval $\Delta_{[\frac{m+1}{2}]}$, where the subscript $[x]$ denotes the integer part of x.

The first term from (41) is when

- $s = 0$, then

$$\frac{1}{2\pi i}\mathrm{Tr}(IiD) = \frac{1}{2\pi}\sum_{n=1}^{2N} d_n = \frac{\mathscr{L}}{2\pi}. \tag{42}$$

- When $s > 0$, let e be an orthonormal basis for the incoming waves. $e = \{e_1 = [1, 0, ...]^T, e_2 = [0, 1, 0, ...]^T, ...e_N = [0, ..., 0, 1]^T\}$ then

$$\begin{aligned} \frac{1}{2\pi i}\mathrm{Tr}(S^s iD) &= \frac{1}{2\pi}\sum_{n=1}^{2N} < S^s De_n, e_n > & (43)\\ &= \frac{1}{2\pi}\sum_{n=1}^{2N} d_{[\frac{n+1}{2}]} < S^s e_n, e_n > & (44)\\ &= \frac{1}{2\pi}\sum_{k=1}^{2N} d_{[\frac{n+1}{2}]} < (S_v S_E)^s e_n, e_n >, & (45)\end{aligned}$$

where $< \cdot, \cdot >$ is the vector scalar product. Define L_i as the space of amplitudes of incoming waves and L_o as the space of amplitudes of outgoing waves. Then

$$\left\{ \begin{array}{llll} S_E: & L_i & \to & L_o, \\ S_v: & L_o & \to & L_i, \end{array} \right. \tag{46}$$

and thus

$$S_v S_E: \quad L_i \quad \to \quad L_i. \tag{47}$$

The vector e_n has only one non-zero component at index n. Then the vector $S_E e_n$ has a non-zero component at index $n + (-1)^{n+1}$. The vector $S_V S_E e_n$ has non-zero components at the endpoints equivalent to $x_{n+(-1)^{n+1}}$, say at the points $x_{i_1}, x_{i_2}, ..., x_{i_v}$. Then the vector $S_E S_V S_E e_n$ has non-zero components at indexes $i_1 + (-1)^{i_1+1}, i_2 + (-1)^{i_2+1}, ..., i_v + (-1)^{i_v+1}$. We see that $< S^2 e_n, e_n >$ is different from zero only if there exist a closed path of discrete length 2 that starts at e_n and ends at e_n. Take all powers of S and we finally get:

$$\frac{1}{2\pi i}\mathrm{Tr}(S^s iD) = \sum_{s=1}^{\infty}\sum_{n=1}^{2N} d_{[\frac{n+1}{2}]} \sum_{p\in P_n^s}\left(\prod_{\sigma_{ij}^m\in T(p)} \sigma_{ij}^m\right) e^{ikl(p)}. \tag{48}$$

For a periodic orbit, p of degree g and with discrete length of the primitive orbit q then p will occur q times in the right sum. Once for each e_n that is a part of p and thus

$$\frac{1}{2\pi i}\mathrm{Tr}(S^s iD) = \sum_{p\in P} l(\mathrm{prim}(p)) \left(\prod_{\sigma_{ij}^m \in T(p)} \sigma_{ij}^m \right) e^{ikl(p)}. \tag{49}$$

- $k < 0$ For the negative powers, $S_V^n = S_V^{-n}$, since S_V is unitary according to Theorem (1) and $S_V = S_V^{-1}$. S_E^{-n} is almost equal S_E^n, with the difference that the exponents have opposite signs. So, the terms with negative k sums up to:

$$\sum_{p\in P} l(\mathrm{prim}(p)) \left(\prod_{\sigma_{ij}^m \in T(p)} \sigma_{ij}^m \right) e^{-ikl(p)}. \tag{50}$$

Proposition I: *(Theorem 1 from [11]) Let $H(\Gamma)$ be the Laplace operator on a finite connected metric graph Γ, then the following two trace formulae establish the relation between the spectrum $\{k_j^2\}$ of $H(\Gamma)$ and the set of periodic orbits P, the number of edges N, the number of vertices, M and the total length $\mathscr{L}$:*

$$u(k) \equiv 2\delta(k) + \sum_{n=1}^{\infty} (\delta(k-k_n) + \delta(k+k_n)) \tag{51}$$

$$= -(N-M)\delta(k) + \frac{\mathscr{L}}{\pi} + \frac{1}{2\pi}\sum_{p\in P}\left(A_p e^{ikl(p)} + A_p e^{-ikl(p)}\right), \tag{52}$$

and

$$\hat{u}(l) \equiv 2 + \sum_{n=1}^{\infty} \left(e^{-ik_n l} + e^{ik_n l}\right) \tag{53}$$

$$= -(N-M) + 2\mathscr{L}\delta(l) + \sum_{p\in P} (A_p\delta(l-l(p)) + A_p\delta(l+l(p))), \tag{54}$$

where A_p is independent of energy and given by (55).

$$A_p = l(\mathrm{prim}(p)) \left(\prod_{\sigma_{ij}^n \in T(p)} \sigma_{ij}^m \right) \tag{55}$$

3 Two non-isometric but isospectral graphs

An interesting question, not only from a mathematical point of view but also for say a musician, is whether one can decide the shape of a drum from the tones that it produces, or if there for the Laplace operator with Dirichlet b.c. exists a one to one correspondence between the set of all possible domains and the set of eigenvalues to the operator. Kac posed this question in 1966 [7] and it is now known that the answer to the question is in general 'no', but under certain regularity conditions on the domain, the inverse problem has essentially unique solutions. Here we are going to show that the answer is in general 'no', also for graph Laplacians.

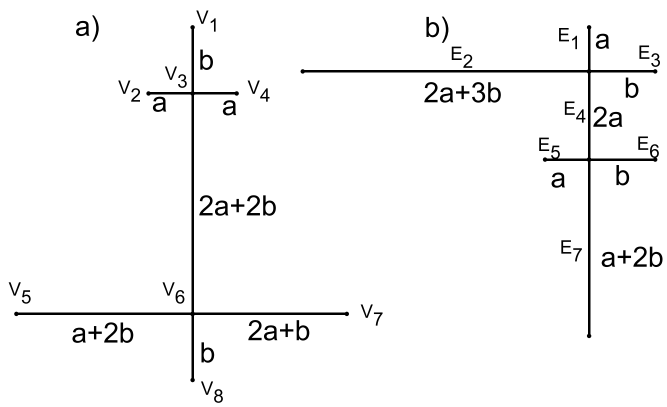

Figure 5: Two isospectral but non-isometric graphs, constructed with the lengths a and b. $V_1, ..., V_8$ are vertices and $E_1, ..., E_7$ are edges. Every edge, E_n, have an associated interval $[x_{2n-1}, x_{2n}] \in \mathbb{R}$. The graphs are trees with $\chi = 8 - 7 = 1$

In 1995 Chapman demonstrated how to produce isospectral domains for the Laplace operator [3]. Two graphs that are constructed with this method are illustrated in figure 5. These graphs were presented in [5], but the authors were not able to prove that the Laplace operators on the graphs are isospectral. This was later proved in [15] in the case of Dirichlet b.c. at the loose endpoints. Henceforth, we consider Laplacians with standard b.c. at all vertices.

Theorem II: *The length spectra, i.e. the set of all possible lengths of the periodic orbits are equal for the graphs in figure 5 and given by*

$$2an + 2bk, \quad n, k \in \mathcal{N} \tag{56}$$

Proof: Start from the vertex V_3. An arbitrary number of orbits of length $2a$ and $2b$ can be added from there, and thus, periodic orbits of length $2an + 2bk$ can be constructed on either graph, where n and k are natural numbers. These are all possible periodic orbits since, every periodic orbit on either graph have to contain an even number of a's and b's. $\square$

According to the trace formula, (54), the sums

$$\sum_{p\in P} A_p e^{ikl(p)} \tag{57}$$

have to be equal for both graphs, in order to be isospectral. Thus, Theorem 2 can not guarantee that the Laplacians to the graphs in figure 5a and b are isospectral.

To fully describe the spectrum of the two Laplace operators on the graphs, we have to consider the differential equation $-\varphi'' = \lambda\varphi$ on all edges along with the standard boundary conditions (8). For the graphs in figure 5 this can be formulated as:

$$\left\{\begin{array}{c} -\varphi_n'' = \lambda\varphi_n, \quad n = 1, ..., 7, \\ \varphi_1(x_2) = \varphi_2(x_4) = \varphi_3(x_5) = \varphi_4(x_7), \\ \partial\left(\varphi_1(x_2) + \varphi_2(x_4) + \varphi_3(x_5) + \varphi_4(x_7)\right) = 0, \\ \varphi_4(x_8) = \varphi_5(x_{10}) = \varphi_6(x_{11}) = \varphi_7(x_{13}), \\ \partial\left(\varphi_4(x_8) + \varphi_5(x_{10}) + \varphi_6(x_{11}) + \varphi_7(x_{13})\right) = 0, \\ \partial\varphi_1(x_1) = \partial\varphi_2(x_3) = \partial\varphi_3(x_6) = \partial\varphi_5(x_9) = \partial\varphi_6(x_{12}) = \partial\varphi_7(x_{14}) = 0. \end{array}\right. \tag{58}$$

The differential expression on the edges have solutions of the form $\varphi_n = A\cos(k(x - x_{2n-1})) + B\sin(k(x - x_{2n-1}))$. Together with the conditions in the last line of (58) we have

$$\begin{array}{rcl} \varphi_1 &=& A_1\cos\left(k(x-x_1)\right), \\ \varphi_2 &=& A_2\cos\left(k(x-x_3)\right), \\ \varphi_3 &=& A_3\cos\left(k(x-x_5)\right), \\ \varphi_4 &=& A_4\cos\left(k(x-x_7)\right) + A_4'\sin\left(k(x-x_7)\right). \end{array} \qquad \begin{array}{rcl} \varphi_5 &=& A_5\cos\left(k(x-x_9)\right), \\ \varphi_6 &=& A_6\cos\left(k(x-x_{11})\right), \\ \varphi_7 &=& A_7\cos\left(k(x-x_{13})\right), \end{array} \tag{59}$$

These functions together with the boundary conditions give, for graph 5 a):

$$\left\{\begin{array}{c} \varphi_1(b) = \varphi_2(a) = \varphi_3(a) = \varphi_4(0), \\ \frac{d}{dx}\varphi_1(b) + \frac{d}{dx}\varphi_2(a) + \frac{d}{dx}\varphi_3(a) - \frac{d}{dx}\varphi_4(0) = 0, \\ \varphi_4(2a+2b) = \varphi_5(a+2b) = \varphi_6(2a+b) = \varphi_7(b) = 0, \\ \frac{d}{dx}\varphi_4(2a+2b) + \frac{d}{dx}\varphi_5(a+2b) + \frac{d}{dx}\varphi_6(2a+b) + \frac{d}{dx}\varphi_7(b) = 0. \end{array}\right. \tag{60}$$

Let $\cos(kx)$ be abbreviated by $c(x)$ and $\sin(kx)$ by $s(x)$. Then the function φ is an eigenfunction to the Laplacian with the standard boundary conditions, on graph 5 a) iff:

$$\begin{pmatrix} c(b) & -c(a) & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & c(a) & -c(a) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & c(a) & -1 & 0 & 0 & 0 & 0 \\ s(b) & s(a) & s(a) & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & c(2a+2b) & s(2a+2b) & -c(a+2b) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & c(a+2b) & -c(2a+b) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & c(2a+b) & -c(b) \\ 0 & 0 & 0 & s(2a+2b) & -c(2a+2b) & s(a+2b) & s(2a+b) & s(b) \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \\ A_4' \\ A_5 \\ A_6 \\ A_7 \end{pmatrix} = 0. \tag{61}$$

The corresponding condition for the Laplacian with standard boundary conditions on graph 5 b) is

$$\begin{pmatrix} c(a) & -c(2a+3b) & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & c(2a+3b) & -c(b) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & c(b) & -1 & 0 & 0 & 0 & 0 \\ s(a) & s(2a+3b) & s(b) & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & c(2a) & s(2a) & -c(a) & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & c(a) & -c(b) & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & c(b) & -c(a+2b) \\ 0 & 0 & 0 & s(2a) & -c(2a) & s(a) & s(b) & s(a+2b) \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \\ A'_4 \\ A_5 \\ A_6 \\ A_7 \end{pmatrix} = 0. \tag{62}$$

We are now ready to prove the main result:

Theorem III: *The Laplace operators to the graphs shown in Figure 5 are isospectral in the case when standard boundary conditions are imposed at all vertices (including loose endpoints).*
Proof: The determinants to the matrices in (61) and (62) are:

$$\begin{aligned} \det(S) \;=\; & \cos(ka)\Big(\\ & -\tfrac{1}{8}\left[\sin(6ka+3kb)+\sin(4ka+3kb)+\sin(4ka+kb)-\sin(2ka+kb)\right] \\ & -\tfrac{1}{4}\left[-\sin(4ka+5kb)+\sin(2ka+5kb)+\sin(kb)\right] \\ & -\tfrac{1}{2}\left[\sin(6ka+7kb)+\sin(6ka+5kb)\right]\Big) \end{aligned} \tag{63}$$

The result is obtained by an expansion of the terms in the determinants with trigonometric identities, for example $\sin(a+b)=\sin(a)\cos(b)+\cos(a)\sin(b)$, as far as possible and then by sorting the terms and combining them again. The equality of the determinants verifies that the spectrum is equal for the two operators when $\lambda \neq 0$. In the case when $\lambda = 0$, the spectral multiplicity is 1 for both graphs according to [10], Theorem 1. $\square$

The same result has been proved in the case of Dirichlet boundary conditions at the loose endpoints and standard boundary conditions at the inner vertices. In that case:

$$\begin{aligned} \det(S) \;=\; & \sin(ka)\Big(\\ & -\tfrac{1}{8}\left[\cos(6ka+3kb)-\cos(4ka+3kb)+\cos(4ka+kb)+\cos(2ka+kb)\right] \\ & -\tfrac{1}{4}\left[-\cos(4ka+5kb)-\cos(2ka+5kb)+\cos(kb)\right] \\ & -\tfrac{1}{2}\left[\cos(6ka+7kb)-\cos(6ka+5kb)\right]\Big), \end{aligned} \tag{64}$$

and thus, the spectrum of the Laplace operators on the graphs are equal when $\lambda \neq 0$. For any tree with Dirichlet boundary conditions and standard boundary conditions at the inner vertices, the only function corresponding to the eigenvalue $\lambda = 0$ is the function $\varphi = 0$. This result can be obtained by slightly modifying the proof of Theorem 1 in [10]. This fact was not discussed, neither in [15] or [5] but it is essential for a rigorous proof.

The eigenfunctions to the Laplace operator with standard boundary conditions at all vertices can be divided into two classes, according to whether they vanish at the inner vertices or not. We call eigenfunctions, φ, *localised* if they are supported by a certain non-intersecting path, i.e. if they are supported on no more than two edges that are connected to the same vertex. Each path that supports a localised eigenfunction has to start and end at a loose end point or the boundary conditions can not be met. There are in total $\begin{pmatrix} 6 \\ 2 \end{pmatrix} = 15$ paths that can support localised eigenfunctions, see table (1). All eigenfunctions that are zero at the inner vertices can be expressed by linear combinations of the localised eigenfunctions. The approach with localised eigenfunctions is very useful if only a subset of the spectrum to the Laplace operator is needed. We have found six different types of localized eigenfunctions on the graphs. They are:

		Graph a		Graph b	
#	Path	lengths	type	lengths	type
1	$V_1 - V_3 - V_2$	b,a	i	a,(2a+3b)	ii
2	$V_1 - V_3 - V_4$	b,a	i	a,b	i
3	$V_1 - V_3 - V_6 - V_5$	a,2a+2b,a+2b	iii	a,2a, a	vi
4	$V_1 - V_3 - V_6 - V_7$	b,2a+2b,2a+b	iv	a,2a,b	i
5	$V_1 - V_3 - V_6 - V_8$	b,2a+2b,b	iv	a,2a,a+2b	iii
6	$V_2 - V_3 - V_4$	a,a	vi	2a+3b,b	iv
7	$V_2 - V_3 - V_6 - V_5$	a,2a+2b,a+2b	iii	2a+3b,2a,a	ii
8	$V_2 - V_3 - V_6 - V_7$	a,2a+2b,2a+b	i	2a+3b,2a,b	iv
9	$V_2 - V_3 - V_6 - V_8$	a,2a+2b,b	i	2a+3b,2a,a+2b	i
10	$V_4 - V_3 - V_6 - V_5$	a,2a+2b,a+2b	iii	b,2a,a	i
11	$V_4 - V_3 - V_6 - V_7$	a,2a+2b,2a+b	i	b,2a,b	iv
12	$V_4 - V_3 - V_6 - V_8$	a,2a+2b,b	i	b,2a,a+2b	i
13	$V_5 - V_6 - V_7$	a+2b,2a+b	v	a,b	i
14	$V_5 - V_6 - V_8$	a+2b,b	i	a,a+2b	iii
15	$V_7 - V_6 - V_8$	2a+b,b	iv	b,a+2b	i

Table 1: Intervals in the graphs in figure 5, that can support localised eigenfunctions, together with a type parameter (i-vii) and the lengths of the edges of the paths.

Type i: Take for example the path $V_1 - V_3 - V_2$ on graph a. The boundary conditions yield that $\cos(ka) = 0$ and $\cos(kb) = 0$ and hence, for $\lambda = k^2$ to be an eigenvalue to the Laplace operator on the graph, k must satisfy:

$$\left\{ \begin{array}{l} k = \frac{\pi}{a}\left(\frac{1}{2} + n_1\right), \\ k = \frac{\pi}{b}\left(\frac{1}{2} + n_2\right). \end{array} \right. \tag{65}$$

Type ii: The conditions on k are:

$$\left\{ \begin{array}{l} k = \frac{\pi}{a}\left(\frac{1}{2} + n_1\right), \\ k = \frac{\pi}{3b}\left(\frac{1}{2} + n_2\right). \end{array} \right. \tag{66}$$

Type iii: Consider path number 3 on the graph in figure 5 a): $V_1 - V_3 - V_6 - V_5$. On $V_1 - V_3$ it is required that $\cos(ka) = 0$ on $V_6 - V_5$ it is further required that

$\sin(2kb) = 0$. These restrictions are sufficient for the boundary conditions to be fulfilled on $V_3 - V_6$ as well. Thus, k is the solution to:

$$\begin{cases} k = \frac{\pi}{a}\left(\frac{1}{2} + n_1\right), \\ k = \frac{n_2\pi}{2b}. \end{cases} \tag{67}$$

Type iv: Analogous to type iii above but a and b are interchanged.

$$\begin{cases} k = \frac{\pi}{b}\left(\frac{1}{2} + n_1\right), \\ k = \frac{n_2\pi}{2a}. \end{cases} \tag{68}$$

Type v: The conditions on k are:

$$\begin{cases} k = \frac{\pi}{a+2b}\left(\frac{1}{2} + n_1\right), \\ k = \frac{\pi}{2a+b}\left(\frac{1}{2} + n_2\right) \end{cases} \tag{69}$$

Type vi: k is the solutions to $\cos(ka) = 0$ and thus

$$k = \frac{\pi}{a}\left(\frac{1}{2} + n_1\right). \tag{70}$$

The direct problem for the localised eigenfunctions is reduced to the problem of finding eigenvalues for the one-dimensional Laplace operator on compact intervals with Dirichlet boundary conditions at certain points.

Lemma I: *Localised functions of the types (i)-(v) exist iff $\frac{a}{b}$ is a rational number.*
Proof: For type (i), the two conditions on k in (65) yields:

$$\frac{\pi}{a}\left(\frac{1}{2} + n_1\right) = \frac{\pi}{b}\left(\frac{1}{2} + n_2\right), \tag{71}$$

and we get

$$\frac{a}{b} = \frac{1 + 2n_1}{1 + 2n_2}. \tag{72}$$

The right hand side of (72) is rational and we conclude that (65) have solutions iff $\frac{a}{b}$ is rational. This result is obtained for type (ii)-(v) in the same way. □

We can show the result in another way as well. Let l be the total length of all edges in a path. The eigenfunction to the Laplace operator with Dirichlet b.c. on the interval $[0, l] \in \mathbb{R}$ is $\varphi = \cos(kx)$, $k = 0, 1, 2....$ This function do never vanish at points that divide the interval into irrational parts and hence, the extra conditions from the types mentioned can never be met if a/b is irrational.

For example, let $a = \sqrt{2}$ and $b = 1$; then, the path $V_1 - V_3 - V_2$ have $l = a + b$, and thus $\cos(\frac{n\pi}{l})$ can never be zero at $x = \sqrt{2}$ since $\frac{l}{a} = \frac{a+b}{a} = 1 + \frac{b}{a} = 1 + \frac{1}{\sqrt{2}}$ is irrational.

We have thus given an example of two isospectral but non-isometric graphs. They were proven isometric by solving the direct problem, which we saw had the same solutions. This demonstrates that the inverse problem does not have a unique solution. For the graphs considered, we could also conclude that the spectrum corresponding to localised eigenfunctions is limited to $k = \frac{\pi}{a}\left(\frac{1}{2} + n\right)$ when a/b is an irrational number. Type vi is special and this can be seen in (63) which can be factorized by $\sin(ka)$.

4 Four graphs with different Euler characteristics

This section will discuss questions regarding the Euler Characteristic, χ that we earlier defined as $\chi = M - N$, where M is the number of vertices and N is the number of edges in a graph.

Consider for a moment the graph that consists of only one edge and thus two vertices. The Euler characteristic for this graph is 1. All connected graphs can be constructed from this graph by three operations:

1. Decorating the graph i.e. adding a vertex on an existing edge. This will leave χ unchanged since the decorated edge will be split in two.

2. Addition of an edge between two nodes. This will decrease χ by one.

3. Addition of an edge with a loose endpoint. This leaves χ unchanged.

So, for a connected graph:

$$-N \leq \chi \leq 1. \tag{73}$$

The trace formula (1) reveals that χ can be determined from the spectrum and the following theorem gives an explicit formula:

Proposition II: *(Theorem 4 from [9]) Let Γ be a finite compact metric graph and $L(\Gamma)$-the corresponding Laplace operator (with standard boundary conditions). Let $q \in L_\infty(\Gamma)$ be a real valued potential and $S = L(\Gamma) + Q$-the corresponding Schrödinger operator, where Q is the operator of multiplication by q. Then the Euler characteristic $\chi(\Gamma)$ of the graph Γ is uniquely determined by the spectrum $\lambda_n(S)$ of the operator S and can be calculated using the limit*

$$\chi(\Gamma) = 2 \lim_{t\to\infty} \sum_{n=0}^{\infty} cos\sqrt{\lambda_n(S)}/t \left(\frac{sin\sqrt{\lambda_n(S)}/2t}{\sqrt{\lambda_n(S)}/2t} \right)^2, \tag{74}$$

where the following convention is used:

$$\lambda_m = 0 \Rightarrow \frac{sin\sqrt{\lambda_n(S)}/2t}{\sqrt{\lambda_n(S)}/2t} = 1. \tag{75}$$

In what follows we are going to determine χ to the graphs shown in Figure 6 using the following properties instead:

Proposition III: *(Theorem 1 from [10]) Let Γ be a compact metric graph with Euler characteristic χ, and let $L(\Gamma)$ be the corresponding Laplace operator. Then $\lambda = 0$ is an eigenvalue with spectral multiplicity $m_s(0) = 1$ and algebraic multiplicity $m_a(0) = 2 - \chi$.*

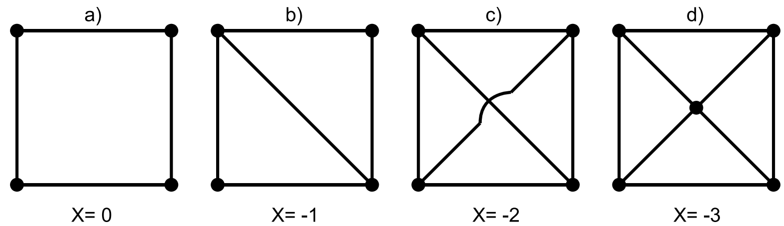

Figure 6: Four graphs with different Euler characteristics. For simplicity, all edges have the length 1.

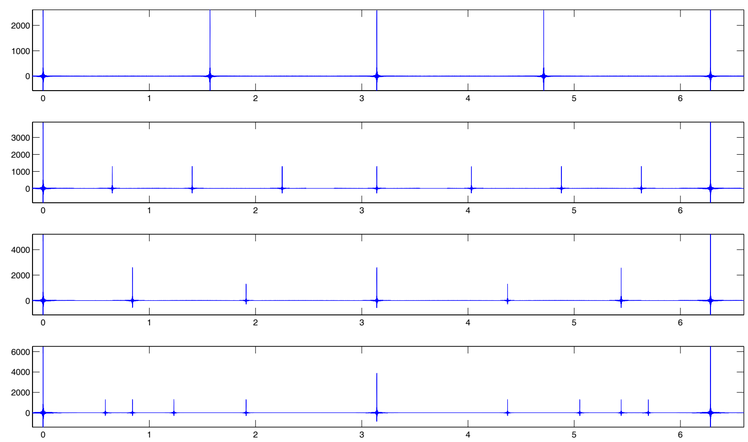

Figure 7: Estimation of the trace formula for the four graphs in figure 6. From top to bottom, a), b), c) and d). The 9193 first terms from (79) are used. Maple and Matlab were used in order to calculate the scattering matrices and produce the graphics.

Let u be the distribution that contains the spectrum to the Laplace operator on the graphs shown in figure 6. There is a suitable expression for u in equation (41):

$$u = \frac{1}{2\pi} Tr[(\sum_{k=-\infty}^{\infty} S^k)D]. \tag{76}$$

The expression does have a more simple form when $l_1 = l_2 = ... \equiv 1$ since then:

$$S_e = \underbrace{\begin{pmatrix} 0 & 1 & & & \\ 1 & 0 & & & \\ & & 0 & 1 & \\ & & 1 & 0 & \\ & & & & \dots \end{pmatrix}}_{\tilde{S}_e} e^{ik}, \tag{77}$$

and

$$u = \frac{1}{2\pi} Tr[(\sum_{k=-\infty}^{\infty} (S_v \tilde{S}_e)^k) e^{ik}] \quad (78)$$

$$= \frac{1}{\pi} Tr[(\sum_{k=0}^{\infty} (S_v \tilde{S}_e)^k) cos(k)]. \quad (79)$$

For $l_j = 1$, the spectrum is 2π-periodic on the k-axis i.e. if $(k_j)^2$ is an eigenvalue then $(k_j + 2\pi n)^2$ is also an eigenvalue. In addition, if $k_j + 2\pi n \neq 0$ for any n, then the multiplicities of $k_j + 2\pi n$ coincide (Theorem 2, [9]).

We introduce two approximations in order to carry out the calculations. Let u_t be a truncation of (79) so that:

$$u_t = \frac{1}{\pi} Tr[(\sum_{k=0}^{2048} (S_v \tilde{S}_e)^k) cos(k)]. \quad (80)$$

If φ is a function with support in $k = 0$ but not in any other k_n which is a zero to $det(S - I) = 0$, then $m_a(0)$ can be calculated from:

$$u[\varphi] = \int_{-\infty}^{\infty} u(k)\varphi(k)dk = \varphi(0)m_a(0). \quad (81)$$

A function φ for which the condition on the support holds in this case is $\varphi = \theta(k + 0.02) - \theta(k - 0.02)$. We arrive at

$$u[\varphi] = \int_{-0.02}^{0.02} u(k)\varphi(k)dk \approx \sum_{n=-120}^{120} u_t(n\Delta)\Delta \equiv \tilde{m}_a(0). \quad (82)$$

Where $\Delta = \frac{0.04}{242}$.

Carrying out these calculations for the graphs shown in Figure 6 yields:

Graph in Figure 6	a)	b)	c)	d)
$\tilde{m}_a(0)$	2.02	3.02	4.03	5.03

We see that the Euler characteristics for the graphs can be calculated accurately by $\chi = 2 - \tilde{m}_a(0)$.

5 Edges of length zero

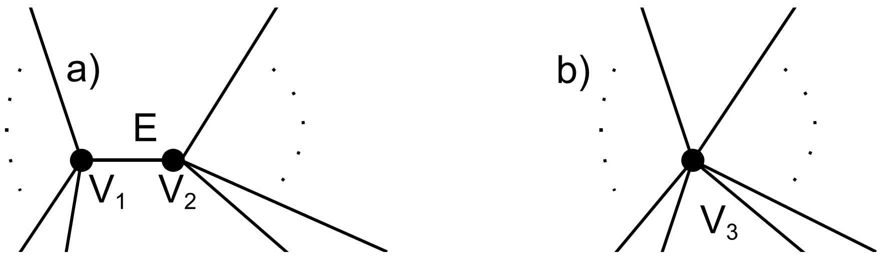

Figure 8: We prove that the two graphs have the same scattering properties in the limit when the length of E tends to zero and the valencies fulfil $v_1 + v_2 = v_3 + 2$.

In this section we are going to discuss what happens to the spectrum of a graph Laplacian in the limit when the length of an edge (or several) say E tends to zero. It is natural to consider the *reduced graph*, Γ_R which can be obtained from Γ by removing the edge $E = [x_1, x_2]$ and substituting the vertices connected to E say V_1 and V_2 by a new vertex $V_3 = V_1 \cup V_2 \setminus \{x_1, x_2\}$ with valency $v_3 = v_1 + v_2 - 2$. This procedure is illustrated in Figure 8.

We know about scattering in a single vertex from the proof of the trace formula. An incoming wave results in a reflected wave and transmitted waves that can be described through the vertex scattering matrix. In the same way, we can have a scattering matrix for a compact graph with with infinite edges attached.

Theorem IV: *The scattering matrix for the double star graph shown in Figure 8 a) tends to the scattering matrix for the reduced (star) graph shown in figure 8 b) when the length of E tends to zero.*

Proof: We denote the reflection and transmission coefficients for vertex V_m by r_m and t_m respectively. The standard boundary conditions (8) give

$$r_m = \frac{2 - v_m}{v_m}, \quad t_m = \frac{2}{v_m}, \tag{83}$$

where v_m is the valency of V_m. Transmission and reflection in the graph shown in figure 8 b) is described by r_3 and t_3 while there are more possibilities for the graph shown in 8 a). We define the amplitude of an transmitted wave that enter the structure from an infinite edge attached to V_1 and leave the structure on an infinite edge attached to V_2 as t_{12}. We define t_{21}, t_{11} and t_{22} analogously. The reflection coefficients for the structure will be denoted by r_{11} and r_{22}. We have to verify that

$$t = t_{11} = t_{12} = t_{21} = t_{22}, \tag{84}$$

and

$$r = r_{11} = r_{22}, \tag{85}$$

when the length of E, d tends to zero. We start with an expansion of the coefficient t_{12}.

$$t_{12} \quad = \quad t_1 e^{ikd} t_2 + t_1 e^{ikd} r_2 e^{ikd} r_1 e^{ikd} t_2 + \ldots \tag{86}$$

$$= \quad \frac{t_1 t_2 e^{ikd}}{1 - r_1 r_2 e^{2ikd}}, \tag{87}$$

for which it holds that

$$\lim_{d\to 0} \frac{t_1 t_2 e^{ikd}}{1 - r_1 r_2 e^{2ikd}} = \frac{t_1 t_2}{1 - r_1 r_2}. \tag{88}$$

The expression is symmetric in the sense that t_1 and t_2 can be interchanged and thus $t_{12} = t_{21}$. In the same way we find that

$$t_{11} = t_1 + \frac{r_2 t_1 e^{2ikd}}{1 - r_1 r_2 e^{2ikd}}, \tag{89}$$

so

$$\begin{aligned}
\lim\nolimits_{d\to 0} \quad & t_1 + \frac{r_2 t_1 e^{2ikd}}{1 - r_1 r_2 e^{2ikd}} & (90)\\
= \quad & t_1 + \frac{r_2 t_1}{1 - r_1 r_2} & (91)\\
= \quad & \frac{t_1(1 + r_2(t_1 - r_1))}{1 - r_1 r_2} & (92)\\
= \quad & \frac{t_1 t_2}{1 - r_1 r_2}. & (93)
\end{aligned}$$

The expression is symmetric and equal to (88) and thus it holds that $t_{11} = t_{12} = t_{21} = t_{22}$. If we use (83) we find that

$$\frac{t_1 t_2}{1 - r_1 r_2} = \frac{2}{v_3}, \tag{94}$$

and we see that (84) is true. In the case of reflection

$$\begin{aligned}
r_{11} \quad &= \quad r_1 + t_1 e^{ikd} r_2 e^{ikd} t_1 + t_1 e^{ikd} r_2 e^{ikd} r_1 e^{ikd} r_2 e^{ikd} t_1 + ... & (95)\\
&= \quad r_1 + \frac{t_1^2 r_2 e^{2ikd}}{1 - r_1 r_2 e^{2ikd}}, & (96)
\end{aligned}$$

so

$$\begin{aligned}
\lim_{d\to 0} r_1 + \frac{t_1^2 r_2 e^{2ikd}}{1 - r_1 r_2 e^{2ikd}} \quad &= \quad r_1 + \frac{t_1^2 r_2}{1 - r_1 r_2} & (97)\\
&= \quad \frac{r_1 + r_2 + 2 r_1 r_2}{1 - r_1 r_2}. & (98)
\end{aligned}$$

Since the last expression is symmetric, we see that $r_{11} = r_{22}$. If we use (83) we finaly get

$$\frac{r_1 + r_2 + 2 r_1 r_2}{1 - r_1 r_2} = \frac{2 - v_3}{v_3}. \tag{99}$$

This conclues that (85) is fulfilled and that all possibilities are considered. □
We turn our considerations to the spectral problem for the Laplacian on the graph in figure 9 a). It has six edges and six vertices, three of valency 3 and three of valency 1. The volume of the graph is always 3 but the shape is altered by the parameter a that determine the length of central edges and also change

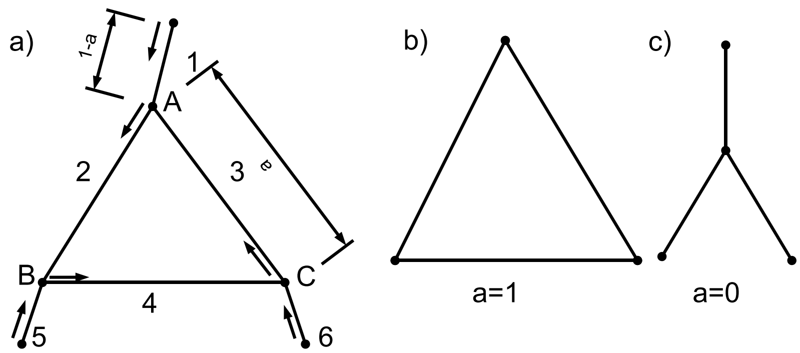

Figure 9: A one-parameter graph. The letters denote vertices; the numbers edges and the arrows indicate positive direction in local coordinate systems on the edges. Note that the graphs are presented with different scales and that the total length always is 3.

the length of the outer edges so that the total length $\mathscr{L} = 3$. Figure 9 b) and c) shows two extreme cases when the parameter $a = 1$ and $a = 0$ respectively. In the first case, the loose edged disappear and in the second one the graph reduces to a tree i.e. the cycle disappears. Our aim is to understand how the spectrum of the graph b) and c) can be obtained as a limit of the spectrum in a). We apply the direct method that was used in Section 3 to find the spectrum. The functions on the edges are

$$\begin{array}{rclrcl} \varphi_1 &=& A_1\cos(kx), & \varphi_2 &=& A_2\cos(kx) + A_2'\sin(kx), \\ \varphi_5 &=& A_5\cos(kx), & \varphi_3 &=& A_3\cos(kx) + A_3'\sin(kx), \\ \varphi_6 &=& A_6\cos(kx), & \varphi_4 &=& A_4\cos(kx) + A_4'\sin(kx). \end{array} \tag{100}$$

With the abbreviations $c(x) \equiv \cos(kx)$, $s(x) \equiv \sin(kx)$ and $b \equiv (1-a)$ the conditions on the coefficients are

$$\begin{pmatrix} c(b) & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c(b) & 0 & 0 & -c(a) & -s(a) & 0 & 0 & 0 & 0 \\ -s(b) & 0 & -1 & -s(a) & c(a) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & c(b) & 0 \\ 0 & -c(a) & -s(a) & 0 & 0 & 0 & 0 & c(b) & 0 \\ 0 & -s(a) & c(a) & 0 & 0 & 0 & -1 & -s(b) & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & c(b) \\ 0 & 0 & 0 & 0 & 0 & -c(a) & -s(a) & 0 & c(b) \\ 0 & 0 & 0 & 0 & -1 & -s(a) & c(a) & 0 & -s(b) \end{pmatrix} \begin{pmatrix} A_1 \\ A_2 \\ A_2' \\ A_3 \\ A_3' \\ A_4 \\ A_4' \\ A_5 \\ A_6 \end{pmatrix} = \mathbf{0} \tag{101}$$

When $a = 1$, the determinant of the matrix in the equation system (101) is

$$2(\cos(3k) - 1) \tag{102}$$

and the solution to this equation give the same k as the decorated circle of length 3, i.e.

$$k = \frac{2n\pi}{3}, \quad n \in \mathscr{Z}, \tag{103}$$

and the spectrum to graph b) is thus equal to the spectrum of the reduced graph.

Eigenvalues to the Laplacian on the reduction of graph c) can be determined from the equation

$$\cos^2(kx)\sin(kx) = 0, \tag{104}$$

and thus, the eigenvalues are

$$\lambda = \frac{n^2\pi^2}{4}. \tag{105}$$

Let $a = 0$, then the determinant of the matrix in (101) is zero. This means that there is at least one non-zero vector in the nullspace to the matrix for every k. The vector is the one that corresponds to $A_2' = A_3' = A_4'$. The corresponding function has the properties that it has no value anywhere, but a derivative in the three vertices that was brought together. Is this an eigenfunction to the graph Laplacian? It is not mathematically meaningful since φ has no support and hence $||\varphi|| = 0$. The difference between the algebraic and spectral multiplicities is related to the Euler characteristic. It is clear that the Euler characteristics for graphs shown in figure 9 a) and c) are different.

Lemma II: *Let Γ_1 be a compact graph with scattering matrix $S^{(1)}$ and an edge E of length d. If Γ_2 is the reduced graph to Γ_1 with respect to E then*

$$\lim_{d\to 0} det(S^{(1)}) = -det(S^{(2)}) \tag{106}$$

Proof: $S_V^{(1)}$ and $S_V^{(2)}$ are unitary by Theorem 1 and furthermore real and symmetric so their determinants are therefore equal to one. As $d \to 0$, the block that corresponds to E in $S_E^{(1)}$ tends to $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ and thus

$$\lim_{d\to 0} S_E^{(1)} = \begin{pmatrix} 0 & 1 & \\ 1 & 0 & \\ & & S_E^{(2)} \end{pmatrix} \tag{107}$$

so

$$\lim_{d\to 0} det\, S_E^{(1)} = det \begin{pmatrix} 0 & 1 & \\ 1 & 0 & \\ & & S_E^{(2)} \end{pmatrix} = -det\, S_E^{(2)} \tag{108}$$

□

It does not hold that $det(A) = det(B)$ implies $det(A-I) = det(B-I)$. Take for example $A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ and $B = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & 2 \end{pmatrix}$. Hence, Lemma 2 will not reveal how the trace formula handles edges of length zero.

5.1 Connecting symmetric graphs

We let three symmetric graphs with known scattering properties be connected to each other as in Figure 10. At this point, we require that each of them have three infinite edges, or *connectors*. We say that graphs are symmetric iff their scattering matrices have the form:

$$S = \begin{pmatrix} r & t & t \\ t & r & t \\ t & t & r \end{pmatrix}. \tag{109}$$

The scattering matrix was introduced for a single vertex when the trace formula

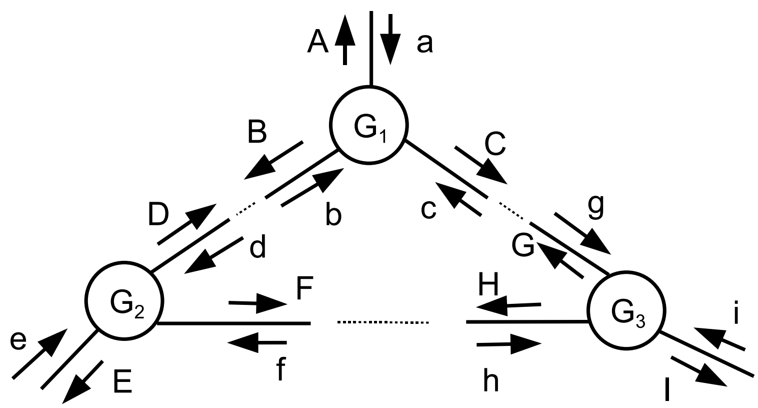

Figure 10: Three symmetric graphs $G_1 = G_2 = G_3$ are connected to a new graph. It is possible to determine the scattering properties of this combination. The letters denote amplitude coefficients to incoming and outgoing waves.

was derived. This definition can be extended to the case of compact graphs with several infinite edges attached. Here we do so, and let the scattering matrices describe the relationship between the coefficients of incoming and outgoing waves to graphs. We stress that the graphs can have any finite number of edges and vertices as long as they are symmetric. For example, three triangular graphs like the one in figure 11 a) can be joined together and form b). If we then let the lengths of the connecting edges shrink to zero, the resulting graph is c). Consider figure 10 again. If we as a first step not consider interaction between the graphs, it holds that:

$$\begin{pmatrix} A \\ B \\ \vdots \\ I \end{pmatrix} = \begin{pmatrix} S & & \\ & S & \\ & & S \end{pmatrix} \begin{pmatrix} a \\ b \\ \vdots \\ i \end{pmatrix}. \tag{110}$$

Now we continue and let the graphs be connected. We let one wave enter the structure from above, i.e. $a = 1$, $e = 0$ and $i = 0$. We see that the reflection coefficient to the structure, $\hat{r}$ will be equal to A and that the transmission coefficient $\hat{t}$ will be equal to E or I. The way we connect the three graphs and the symmetries in the problem gives another 14 equations:

from symmetry:	from connectivity:
B=C, b=c	b=D, B=d,
D=G, d=g	c=G, C=g,
F=H, f=h	f=H, F=h,
E=I, e=i.	

And we finaly get

$$\hat{r} = \frac{tr^3 - r^2 - 3\,t^2r^2 - r^3 + 2\,t^2r + r^4 - t^3r + r + 2\,t^4 - tr^2}{-t^3 - t^2r + tr^2 - r + r^3 - tr + 1 - r^2}, \tag{111}$$

and

$$\hat{t} = -\frac{t^2\,(-1 - t + r)}{-t^3 - t^2r + tr^2 - r + r^3 - tr + 1 - r^2}. \tag{112}$$

Finaly, we give an example. Put together three star graphs with valency 3. A star graph is a graph that consists of one vertex only, with attached infinite edges. The star graph with valency three has $r = -1/3$ and $t = 2/3$. Formula (111) and (112) yield $\hat{r} = -1/3$ and $\hat{t} = 2/3$. This is in perfect order with Theorem 4.

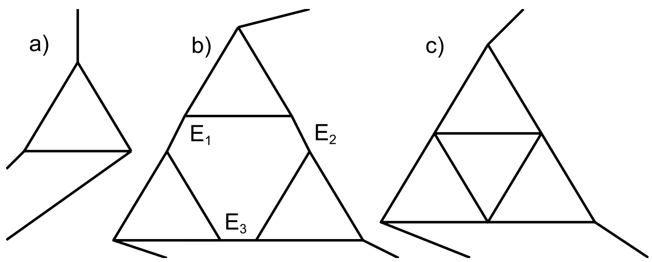

Figure 11: a) An example of a symmetric graph. b) Three such graphs are joined together. The length of the edges goes to zero, and the result is c).

6 Discussion, Applications and Conclusions

In Section 3 we proved that two graphs can be isospectral even if they are not isometric. It is an interesting question to find out other equivalence classes of isospectral graphs as well as conditions that guarantee that two isospectral graphs are isometric. One of the first steps in this direction is the proof that the Euler characteristic is determined by the spectrum. This is illustrated in Section 4 where several explicit calculations have been carried out. The recursive formula for the scattering parameters that was found in 5 can be applied to the scattering problem on Sierpinski triangles and it should be possible to generalize the result for other kind of symmetric graphs as well.

It is beyond the scope of this paper to discuss the accuracy of the model and also application but many references can be found in [16, 8].

Graph Laplacians promise to be very useful. They have the same eigenvalues as discrete approximations:

Proposition IV: *(Theorem 2 from [13]) For a finite compact quantum graph Γ_c with a discrete model Γ_h it holds that*

$$\lambda_i^h \to \lambda_i^c \quad as \quad h \to 0 \tag{113}$$

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

And the discrete approximations can approximate Laplacians of higher order i.e. not only one-dimensional Laplacians:

Proposition V: *(Theorem from [4]) Let M be a closed Riemannian manifold of dimension d. Take a sequence of $1/n$-nets in M, $(\Gamma_n, l_n), 1 \leq n \leq \infty$, with length functions $l_n \equiv 1/n$. There exist a constant $C(d)$ depending only on the dimension d, such that:*

$$\frac{1}{C} \limsup_{n\to\infty} \lambda_k(\Gamma_n, l_n) \leq \lambda_k(M) \ \leq C \liminf_{n\to\infty} \lambda_k(\Gamma_n, l_n), \tag{114}$$

for any $k \geq 0$. The constants $C(d)$ satisfy $C(d) \leq 2 \cdot 50^d$ for any $d \geq 1$.

The parameter estimation might suggest that this is a very rought estimation, but Fujiwara suspects that there exist nets in M such that $C = 1$ in the Theorem.

Symbols

Γ	Graph
v	Vertex
e	Edge
$\mathscr{Z}$	the set of integers, ..., $-2, -1, 0, 1, 2, ...$
$\mathscr{N}$	the set of natural numbers, $0, 1, 2, ...$
$\mathscr{L}$	the total length of a metric graph
χ	the Euler characteristic of a graph, $\chi = M - N$
$\mathscr{H}$	Hilbert space
$\oplus$	Orthogonal sum symbol
$\mathbb{C}$	The complex numbers
$\mathbb{R}$	The real numbers

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