Spectra of Quantum Graphs via a Scattering Matrix Approach

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Abstract

A common approach to study the structure of a graph or a network, $\mathcal{G}$, is through the analysis of the spectrum of linear operators on the vector space of functions on it. In this project, we are interested in quantum graphs, where vertices are connected by length-parametrized edges, together with the self-adjoint Neumann-Kirchhoff Laplacian. Following the ideas of Kottos and Smilansky, we explore the spectrum of this operator using a scattering matrix approach in some specific examples, particularly, the cycles, the line segments and the star graphs. We notice that in star graphs where edges are not rationally related, we have a truly infinite spectrum whereas when edges are rationally related, the spectrum has some sort of periodicity. We also propose the idea of Cayley metric graph in order to understand the infinite multiplicity in the case where the corresponding combinatorial graph of the quantum graph is Cayley.

1 Introduction

A widely used approach to explore the structure of a graph $\mathcal{G}$, is via the analysis of the spectrum, the set of all eigenvalues, of linear operators on the vector space of functions on G. For combinatorial graphs, one mostly consider the spectrum of the adjacency matrix, or the closely related combinatorial Laplacian. In this project, we are concerned with metric graphs, which are 1-dimensional structures where vertices, or nodes, are connected by length-parametrized edges. In this context, a natural self-adjoint operator arises, which is the Neumann-Kirchhoff Laplacian. A metric graph, together with the Laplacian, defines a quantum graph. Following the ideas of Kottos and Smilansky (1), we explore the spectrum of this operator using a scattering matrix approach.

The motivating example is as follows. Consider the simplest metric graph where there are only two vertices jointed by an single edge. Then the infinite spectrum of the Laplacian operator on the metric graph obtained by the scattering matrix approach will just be an infinite copy of the spectrum of the corresponding combinatorial graph related in a close way, though not exactly the same. In other words, each eigenvalue of the corresponding combinatorial graph, will have an infinite multiplicity in the infinite spectrum of the Laplacian operator on the metric graph. Following this observation, it is natural for one to ask if we can generalize this relationship and what properties lead to the infinite multiplicity. In order to answer these questions, we introduce the idea of Cayley metric graph at the end of this paper. This paper is organized as the following: Section 2 discusses some of the issues related to self-adjoint operators in infinite dimensional cases. Section 3 talks about the mathematical set up of this project. In particular, the idea of using quantum graphs and a scattering matrix approach to obtain the spectrum of the graph in Kottos and Smilansky. Section 4 are specific examples of quantum graphs of our interests. Namely, the cycles, the line segments, and the star graphs. Section 5 provides the statistical description of some star graphs, which are widely studied in quantum graph literature. Section 6 discusses further directions of this project. In particular, we propose the idea of a Cayley metric graph by combining the ideas of different kinds of graphs together.

2 Self-Adjoint Operators

2.1 Problems for Self-adjoint Operators in Infinite Dimension

This section will discuss some of the problems of self-adjoint operators that arise in the infinite dimensional cases, following the ideas in (2). Recall the standard spetral theory in linear algebra that if A is a self-adjoint $n \times n$ matrix,then there exists an orthonormal basis $\{v_j\}_{j=1}^n$ for $\mathbb{C}^n$ and real numbers $\lambda_1, ..., \lambda_n$ such that $Av_j = \lambda_j v_j$. We may state the result equivalently in basis-independent language as follows. Suppose $\mathbf{H}$ is a finite-dimensional Hilbert space and A is a self-adjoint linear operator on $\mathbf{H}$, meaning that $\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle$ for all $\phi, \psi \in \mathbf{H}$. Then there exists an orthonormal basis of $\mathbf{H}$ consisting of eigenvectors for A with real eigenvalues.

Since there is a standard notion of orthonormal bases for general Hilbert spaces, one might hope that a similar result would hold for self-adjoint operators on infinite-dimensional Hilbert spaces. However, there are simple examples showing that a self-adjoint operator may not have any eigenvectors. Consider the following example. Let $\mathbf{H} = L^2([0, 1])$ and an operator A on $\mathbf{H}$ defined by

$$(A\psi)(x) = x\psi(x).$$

Then A is a self-adjoint operator on H, but A has no eigenvectors. This is

because if $x\psi(x) = \lambda\psi(x)$, then ψ would have to be supported on the set where $x = \lambda$, which is a measure zero set. Therefore, only the zero element of $L^2([0,1])$ satisfies $A\psi = \lambda\psi$.

At the same time, there is another serious problem with self-adjoint operators in the infinite-dimensional case. In quantum mechanics, most of the self-adjoint operators A are unbounded operators, which means that there is no constant C such that $\|A\psi\| \leq C\|\psi\|$ for all ψ. For example, let X be the position operator on $L^2(\mathbb{R})$ such that $(X\psi)(x) = x\psi(x)$. Let 1_E denote the indicator function of set E. then we have:

$$\|X1_{[n,n+1]}\| \geq \|1_{[n,n+1]}\|$$

for all $n \in \mathbb{N}$. Hence X cannot be bounded. However, it can be shown that if a self-adjoint operator A is defined on all of $\mathbf{H}$, then A must be bounded. Therefore, if A is self-adjoint and unbounded, it cannot be defined on all of $\mathbf{H}$. As a result, we define an "unbounded operator on $\mathbf{H}$" to be a linear operator from a dense subspace of H, known as the domain of A, to $\mathbf{H}$. However, the notion of self-adjointness for such an operator is more complicated than in the bounded case. That is to say, the obvious requirement, $\langle\phi, A\psi\rangle = \langle A\phi, \psi\rangle$ for all ϕ, ψ in the domain of A, is not the "correct" condition. In particular, it is not sufficient to guarantee the spectral theorem for A. Instead, we will define the adjoint A^* of any unbounded operator A, to be an unbounded operator with its own domain. Then an unbounded operator is called self-adjoint, if the domains of A and A^* are the same and A and A^* agree on their common domain. In other word, being self-adjoint not only means that A and A^* agree whenever they are both defined, but also that the domains of A and A^* agree.

2.2 Unbounded Self-Adjoint Operators

In quantum mechanics, most of the operators, including those describing position, momentum, and energy, are not defined on the whole corresponding Hilbert space, but only on a dense subspace of it. In the case of the position operator as mentioned above, given $\psi \in L^2(\mathbb{R})$, the function $X\psi(x) = x\psi(x)$ could easily go wrong and fail to be in $L^2(\mathbb{R})$. Nonetheless, the space of functions ψ's in $L^2(\mathbb{R})$ for which $x\psi(x)$ is again in $L^2(\mathbb{R})$ is a dense subspace in $L^2(\mathbb{R})$. A common property of these operators is that they are not bounded, meaning that there is not constant C such that

$$\|A\psi\| \leq C\|\psi\|$$

for all ψ for which the operators A are defined. Because of the operators are not bounded, we cannot use the bounded linear transformation theorem to extend them to the whole Hilbert space. In this section, we will discuss the "appropriate" notion of self-adjointness for unbounded operators, as discussed above, for which the spectral theorem will hold. As we have already mentioned, the natural candidate for a definition of being self-adjoint, $\langle\phi, A\psi\rangle = \langle A\phi, \psi\rangle$ for all

ϕ, ψ in the domain of A, is not the right one. For any unbounded operator A, we have to define another unbounded operator A^*, called the adjoint of A on its own naturally defined domain. Then A is defined to be self-adjoint if A and A^* are the same operators with the same domain.

Let us give the precise definition of an unbounded self-adjoint operator, together with conditions for self-adjointness. An unbounded operator A on $\mathbf{H}$ is a linear map of some dense subspace, or namely, the domain of A, $\mathrm{Dom}(A) \subseteq \mathbf{H}$ into $\mathbf{H}$. In fact, as "unbounded" implies "not necessarily bounded," we permit the case in which $\mathrm{Dom}(A) = \mathbf{H}$ and thus A is bounded.Consider the following two cases:

1. If A is bounded, for any ϕ,the linear functional $\langle \phi, A\cdot \rangle$ is also bounded. Then by Riesz Theorem, there is a unique χ such that

$$\langle \phi, A\cdot \rangle = \langle \chi, \cdot \rangle$$

Define the adjoint A^* of A by setting $A^*\phi = \chi$.

2. If A is unbounded instead, $\langle \phi, A\cdot \rangle$ is not necessarily bounded, but might still be bounded for some vectors ϕ. If $\langle \phi, A\cdot \rangle$ happens to be bounded for some $\phi \in \mathbf{H}$, then the bounded linear transformation theorem guarantees that this linear functional has a unique bounded extension from $\mathrm{Dom}(A)$ to all of $\mathbf{H}$. Then again, the Riesz theorem implies that there is a unique χ such that this linear functional is a "inner product with χ." This reasoning leads to the following definition:

Definition 2.1. *Let A be an operator defined on a dense subspace $Dom(A) \subseteq \boldsymbol{H}$. Let $Dom(A^*)$ be the space of all $\phi \in \boldsymbol{H}$ for which the linear functional*

$$\psi \mapsto \langle \phi, A\psi \rangle, \psi \in Dom(A)$$

is bounded. Then for $\phi \in Dom(A^*)$, define $A^*\phi$ to be the unique vector such that $\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle$ for all $\psi \in Dom(A)$.

Note that $\langle \phi, A\cdot \rangle$ is bounded means that there exists a constant C such that $|\langle \phi, A\psi \rangle| \leq \|\psi\|$ for all $\psi \in \mathrm{Dom}(A)$. The operator A^* is linear in its domain, and we call it the **adjoint** of A.

There is another way to think about the definition of A^*. Let ϕ be a vector, if there exists another vector χ such that $\langle \phi, A\psi \rangle = \langle \chi, \psi \rangle$ for all $\psi \in \mathrm{Dom}(A)$, then we say $\phi \in \mathrm{Dom}(A^*)$ and $A^*\phi = \chi$. Once again, by Riesz theorem, such a χ exists if and only if $\langle \phi, A\cdot \rangle$ is bounded, meaning that the two ways of thinking about the adjoint A^* are equivalent.

It is worth mentioning that given an operator A defined on a dense subspace, its adjoint A^* does not necessarily have to be densely defined. However, this situation is not a usual problem for operators of interests in practice.

Definition 2.2. *An unbounded operator A on $\boldsymbol{H}$ is **symmetric** if*

$$\langle \phi, A\psi \rangle = \langle A\phi, \psi \rangle$$

for all $\phi, \psi \in Dom(A)$.

If A is symmetric, then A^* is seen as an extension of A in the following sense:

Definition 2.3. *An unbounded operator A is called an **extension** of an unbounded operator B if*

$$1. Dom(B) \subseteq Dom(A)$$

$$2. A = B \text{ on } Dom(B)$$

Proposition 2.1. *An unbounded operator A is symmetric if and only if A^* is an extension of A.*

Proof. Given A is symmetric, for all $\phi \in \mathrm{Dom}(A)$, we get that

$$|\langle \phi, A\psi \rangle| \leq \|A\phi\| \|\psi\|$$

by Cauchy-Schwarz inequality, meaning that $\phi \in \mathrm{Dom}(A^*)$. In this case, the unique vector $A^*\phi$ for which $\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle$ is just $A\phi$. Hence A and A^* agrees on $\mathrm{Dom}(A)$.

In terms of the backward direction, given A^* is an extension of A, for all $\phi \in \mathrm{Dom}(A)$, we have:

$$\langle \phi, A\psi \rangle = \langle A^*\phi, \psi \rangle = \langle A\phi, \psi \rangle$$

for all $\psi \in \mathrm{Dom}(A)$, which means that A is symmetric. □

Definition 2.4. *An unbounded operator A on $\boldsymbol{H}$ is **self-adjoint** if*

$$1. Dom(A) = Dom(A^*)$$

$$2. A^*\phi = A\phi \text{ for all } \phi \in Dom(A)$$

Equivalently,we can say that an operator A is self-adjoint if A^* equals A, given that the equality of unbounded operators has to include the equality of domains. As Proposition 2.1 suggests, every self-adjoint operator is symmetric, but the opposite direction is not true. There are many symmetric operators that are not self-adjoint, as a symmetric operator is self-adjoint if and only if Dom (A) = Dom(A^*). In practice, it is sometimes difficult to show that D(A^*) is not larger than D(A).

3 Quantum Graphs and Scattering Approach

This section will introduce some background mathematics which motivate this project, following the ideas in (3). The first part introduces the set up of examples in the beginning section. Namely, the metric graph, the Neumann-Kirchhoff Laplacian, and the use of scattering matrix approach to calculate the spectrum of the graph. The second part introduces the two kinds of graphs of general interests, Cayley graph and homogeneous graph.

3.1 Metric graph, Neumann-Kirchhoff Laplacian and scattering matrix approach

3.1.1 Metric graph and Neumann-Kirchhoff Laplacian

In this section, we introduce the main players of the quantum graph theory: metric graphs and differential operators on them. A graph consists of a set of points called vertices and a set of segments connecting some of the vertices, which are called edges. In combinatorial graphs, vertices are the main players and the edges merely indicate some relations between them. In contrast, in metric graphs, we focus our attention on the edges. They act no longer just as abstract relations between vertices, but rather as physical "wires" connecting them. Quantum graphs are essentially metric graphs equipped with differential operators. The main operator under consideration acts as the second derivative along the edges with certain conditions at vertices. In fact, these conditions generalize the boundary conditions for ODEs, hence we will discuss what are the "appropriate" conditions.

Moreover, one should be aware that the points of a metric graph $\mathcal{G}$ are not only its vertices, but also all intermediate points x on the edges as well. Hence when we consider functions on it, we consider them as defined along the edges, rather than just at the vertices, as in the combinatorial cases. In particular, one can talk about continuous functions and define the standard space of continuous functions on the metric graph. The presence of the cooridnate x along the edges makes it possible for one to define the Lebesgue measure dx on the graph in a natural way. Having this measure, one can then define some other standard function spaces on the graph. Let $H^k(e)$ denote the standard Sobolev space of functions on the edge e that have all their distributional derivatives up to the order k in $L^2(e)$.

Definition 3.1. *The **Sobolev space** $H^1(\mathcal{G})$ consists of all continuous functions on G that belong to $H^1(e)$ for each edge e such that*

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

The continuity condition imposed on functions in the Solobev space $H^1(\mathcal{G})$ means that any function f from this space has the same value at a vertex v on all edges adjacent to v, and therefore, its value $f(v)$ at v is well-defined. In fact, this is a natural condition for one-dimensional H^1-functions, which are continuous in the standard one-dimensional setting.

However, on the other hand, there seems to be no natural definition of higher-order Solobev spaces $H^k(\mathcal{G})$, where k is greater than 1. The reason is that, unlike in the one-dimensional case, there are no natural conditions that functions should satisfy at vertices. In fact, such vertex conditions will depend on a particular Hamiltonian studied. Hence one will often start with spaces

where smoothness is enforced only along edges, without any junction conditions at vertices at all.

Let's formally define a metric graph: a **metric graph** $\mathcal{G}$ includes a set of vertices $V \subseteq \mathcal{G}$, where $\mathcal{G}\backslash V$ is a union of finitely many open intervals. Let $\mathcal{E}$ be a set of oriented edges. For every $e \in \mathcal{E}$, denote L(e) as the length of the edge. Specifically, We will call a metric graph infinite if it has infinitely many vertices, or equivalently, infinitely many edges. Otherwise, the graph is called finite, and a finite graph whose edges all have finite lengths is called compact. For the sake of our purpose, we mainly consider the case of compact graphs, which are also compact as topological space. We define two smooth functions:

$$e\colon [0, L(e)] \to \mathcal{G}$$

$$\bar{e}\colon [0, L(e)] \to \mathcal{G}$$

namely, the same edge as e, but parametrized in the opposite direction by

$$\bar{e}(t) = e(L(e) - t)$$

We assume that $\mathcal{E}$ is symmetric, which means that $\bar{e} \in \mathcal{E}$ whenever $e \in \mathcal{E}$. We also assume that there is no multiple edges with the same end points. Then for every $v_1, v_2 \in V, e, e^{'} \in \mathcal{E}$, define the adjacency matrices of the vertices and edges respectively as

$$c(v_1, v_2) = c(v_2, v_1) = \begin{cases} 1 & \exists e \in \mathcal{E}\colon e(0) = v_1, \bar{e}(0) = v_2 \\ 0 & \text{otherwise} \end{cases}$$

$$c(e, e') = c(e', e) = \begin{cases} 1 & e(0) = e'(0) \\ 0 & otherwise \end{cases}$$

Once we have a metric graph $\mathcal{G}$, it becomes a quantum one after being equipped with an additional structure: assignment of a differential , or sometimes more general, operator on $\mathcal{G}$. This operator is often called the Hamiltonian in physics. In most cases, though not always, the Hamiltonian is required to be self-adjoint. When studying quantum graphs, the most commonly used operator is the negative second derivative acting on each edge:

$$f(x) \mapsto -\left(\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right)$$

where x is the coordinate x along an edge.

Another very commonly used operator is a general Schrödinger operator:

$$f(x) \mapsto -\left(\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right) + V(x)f(x)$$

where $V(x)$ is an electric potential.

For both of the two above operators, the direction of the edge is irrelevant. This will not be the case if one wants to include first order derivative terms, for example, like magnetic potentials, or to consider first order operators like $\frac{\mathrm{d}f}{\mathrm{d}x}$. In such cases, one need to assume the graph to be directed and consider directed edges b and coordinates x_b in the correponding direction. For instance, the magnetic Schrödinger operator can be defined as:

$$f(x_b) \mapsto (\frac{1}{i}\frac{\mathrm{d}}{\mathrm{d}x_b} - A_b(x_b))^2 f(x_b) + V(x_b)f(x_b)$$

where V is the electric potential and A is the magnetic potential. Note that A is an one-dimensional vector field, which is to say that it changes sign when the direction of the oriented edge is reversed: $A_b(x_b) = -A_{\hat{b}}(x_{\hat{b}})$, where $\hat{b}$ denotes the edge coordinate parametrized in the opposite direction, i.e. $x_{\hat{b}} = L_b - x_b$.

The discussion about the domains of self-adjoint operators makes it clear that the definition of the quantum graph Hamiltonian is not complete until the domain is specified. The classical case of differential operators on a graph with only one edge suggests that the domain description should involve smoothness conditions along the edge and some boundary conditions at the vertices, analogous to the boundary conditions for a single interval. Moreover, the requirement of being self-adjoint will impose additional restrictions on the vertex conditions.

Definition 3.2. ***Quantum graph*** *is a metric graph equipped with a Hamiltonian $\mathcal{H}$ with "appropriate" vertex conditions. In other words, a quantum graph Γ is a triple: (metric graph $\mathcal{G}$, Hamiltonian $\mathcal{H}$, vertex conditions).*

In order to make the definition of the Hamiltonian operator complete, we need to describe its domain. Assuming that $\mathcal{H}$ acts as the negative second order derivative operator, it is natural to require a function f belongs to the Sobolev space $H^2(e)$ on each edge e. Consider the second derivative operator defined on the direct sum $\oplus_{e\in\mathcal{E}} C_0^\infty(e)$ of the spaces of smooth functions on edges vanishing with all their derivatives at the vertices. By squeezing the functions to a shorter segment than e and then modify them to make them infinitely differentiable, we get that the closure of the operator in $L^2(\Gamma)$ has the domain $\oplus_{e\in\mathcal{E}} H_0^2(e)$, where $H_0^2(e)$ is the order 2 Sobolev space on the edge e of functions vanishing with their first derivatives at the ends of the edges. Defined in this way, the operator is symmetric. Now the remaining task is to find boundary conditions at the vertices that would produce self-adjoint extensions of this operator.

We employ the most commonly used conditions, which are called **Neumann-Kirchhoff**. Let $\Psi : \mathcal{G} \to \mathbb{C}$ and $e \in \mathcal{E}$. Define $\Psi_e : [0, L(e)] \to \mathbb{C}, \Psi_e(t) = \Psi(e(t))$. Also define $\Psi''(e(t)) = \Psi''(\bar{e}(L(e)-t)) = \left(\frac{\mathrm{d}^2\Psi_e(t)}{\mathrm{d}t^2}\right)_{t=t_0} = \left(\frac{\mathrm{d}^2\Psi_{\bar{e}}(t)}{\mathrm{d}t^2}\right)_{t=L(e)-t_0}$.

Then let us define the Neumann-Kirchhoff Laplacian, denoted By Δ. Consider $\mathcal{D}$ = The space of twice differentiable functions on $\mathcal{G}\backslash V$ such that all the functions satisfy the following two boundary conditions:

(1. continuity)

$$\lim_{t\to 0} \Psi_e(s) = \Psi(v), \forall v \in V, \forall e \in \mathcal{E} \text{ such that } e(0) = v$$

(2. current conservation)

$$\sum_{e\in\mathcal{E}:e(0)=v} \Psi_e'(0) = 0, \forall v \in V$$

A operator $\Delta : \Psi \in D \to \Psi''$ is the Neumann-Kirchhoff Laplacian. Here, in the second condition, the sum is taken over the set of all edges e connected to the vertex v and the derivatives are assumed to be taken in the directions away from the vertex, which we shall call the outgoing edges.

One important property of the Neumann-Kirchhoff Laplacian is that it is self-adjoint.

Theorem 3.1. *The Neumann-Kirchhoff Laplacian is self-adjoint.*

We wish to explore the spectrum of the Laplacian. It consists of eigenvalues of the operator. An eigenvalue λ of the operator is a real number such that

$$-\Psi'' = \lambda\Psi$$

It turns out that $\lambda \geq 0$, so let $k^2 = \lambda$.

Proposition 3.1. *$\Psi \in D$ such that $-\Psi'' = \lambda\Psi$ is determined by its values on the vertices.*

Proof. Suppose $\Psi : \mathcal{G} \to \mathbb{C}$ satisfies $-\Psi'' = \lambda\Psi$ and the two boundary conditions. Then $\forall e \in E, \Psi_e(t) = a(e)e^{-ikt} + b(e)e^{ikt}$.

Boundary condition 1 implies that $\begin{cases} \Psi_e(0) = \Psi(e(0)) \\ \Psi_e(L(e)) = \Psi(\bar{e}(0)) \end{cases}$

$$\Rightarrow \begin{cases} a + b = \Psi(e(0)) \\ ae^{-ikL(e)+} + be^{ikL(e)} = \Psi(\bar{e}(0)) \end{cases}$$

It follows that:

$$\begin{cases} a = \frac{1}{2i\sin(kL(e))}(\Psi(e(0))e^{ikL(e)} - \Psi(\bar{e}(0))) \\ b = -a + \Psi(e(0)) \end{cases}$$

Substitute a, b back into the general solution to the differential equation and simplify:

$$\Psi_e(t) = \frac{\Psi(e(0))\sin(kL(e) - t) + \Psi(\bar{e}(0))\sin(kt)}{\sin(kL(e))}.$$

This means that $\Psi_e(t)$ is determined by the values of Ψ at the endpoints of e, e(0) and $\bar{e}(0)$. □

But how to determine the eigenvalues k^2? Let us use the second boundary condition. Using the above expression of $\Psi_e(t)$, we get that

$$\Psi'_e(0) = \frac{1}{\sin(kL(e))}[-k\Psi(e(0))\cos(kL(e)) + k\Psi(\bar{e}(0))].$$

Since

$$\sum_{e\in\mathcal{E}:e(0)=v} \Psi'_e(0) = 0, \forall v \in V,$$

plug in the expression for $\Psi'_e(0)$:

$$\sum_{e\in\mathcal{E}:e(0)=v} \frac{-\Psi(v)\cos(kL(e)) + \Psi(\bar{e}(0))}{\sin(kL(e))} = 0, \forall v \in V$$

or

$$\sum_{e\in\mathcal{E}:e(0)=v} \frac{\Psi(\bar{e}(0))}{\sin(kL(e))} = \Psi(v) \sum_{e\in\mathcal{E}:e(0)=v} \cot(kL(e)), \forall v \in V$$

Using the definition of the adjacency matrix for vertices, c(v,v'), we can rewrite the above equation as:

$$\sum_{v'} \frac{c(v,v')}{\sin(kL(v,v'))}\Psi(v') - [\sum_{v'} c(v,v')\cot(kL(v,v'))]\Psi(v) = 0, \forall v \in V,$$

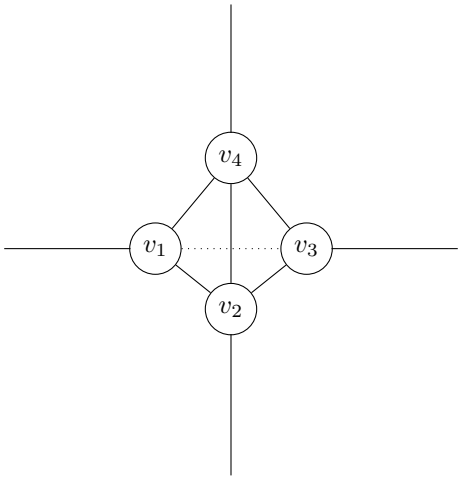
Then define:

$$F(v) = \textstyle\sum_{e\in\mathcal{E}:e(0)=v} \cot(kL(e))$$
$$G(v,v') = \frac{c(v,v')}{\sin(kL(v,v'))}$$
$$\delta(v,v') = \begin{cases} 1 & v' = v \\ 0 & v' \neq v \end{cases}$$
$$H(k)_{v,v'} = G(v,v') - \delta(v,v')F(v)$$

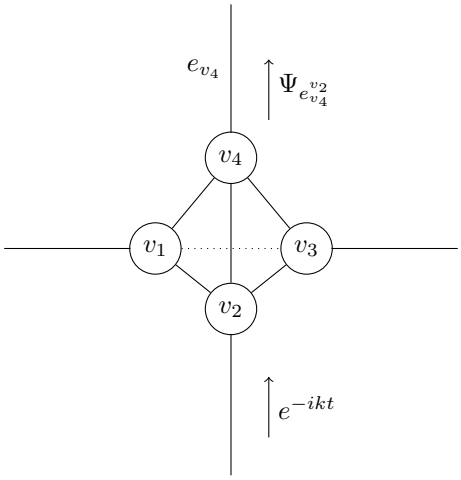
Thus a solution $\Psi \neq 0$ of $-\Psi'' = k^2\Psi$ with the Neumann-Kirchhoff boundary conditions exists $\Leftrightarrow \exists \Psi_v = \begin{bmatrix} \Psi(v_1) \\ \cdots \\ \Psi(v_N) \end{bmatrix} = \Psi|_v \neq 0$ such that $H(k)\Psi_v = 0$ (matrix equation.)

3.1.2 Scattering approach

In this section, we will introduce a matrix S related to the vertices with respect to the scattering process. This matrix is the key to calculate the spectrum of the graph. Given a graph $\mathcal{G}$, attach one lead/edge to each vertex and denote the edge attached to $v \in V$ by $e_v : [0, \infty) \to \bar{\mathcal{G}} = \mathcal{G} \cup \{leads\}$. The figure below is an illustration of the idea.



Let $\mathcal{E}_{int} = \mathcal{E}$ denote the original interior edge of $\mathcal{G}$ and let $\mathcal{E}_{ext}$ denote the external edges (leads).
Define $\Psi^v_{e'}(t) = \delta(v, v')e^{-ikt} + S(v, v')e^{ikt}$, where $e, e' \in \mathcal{E}_{ext}, e'(0) = v'$. This is the solution of $-\Psi'' = k^2\Psi$ restricted to $e' = e_{v'}$ for the incoming wave along e_v with the wave number k. Schematically:



Proposition 3.2. $S = [iI - H(k)][iI + H(k)]^{-1}$
In particular, as H(k) is Hermitian and symmetric, S is unitary and symmetric.

Proof. Apply the two boundary conditions, namely, continuity and current conservation, we get that

$$\begin{cases} 1.\Psi^v(v') = \delta(v,v') + S(v,v') & \forall v, v' \in V \\ 2.\sum_{e' \in \mathcal{E}: e'(0)=v} \Psi^v_{e_{v'}}(0) = \sum_{e' \in \mathcal{E}_{int}, e'(0)=v'} (\Psi^v_{e'})'(0) + (\Psi^v_{e_{v'}})'(0) = 0 \end{cases}$$

$$\forall e' \in \mathcal{E}_{int}, e'(0) = v' \Rightarrow \begin{cases} (\Psi^v_{e'})'(0) = \frac{k}{\sin(kL(e'))}[-\Psi^v(v')\cos(kL(e')) + \Psi^v(\bar{e'}(0))] \\ (\Psi^v_{e_{v'}})'(0) = -ik\delta(v,v') + ikS(v,v') \end{cases}$$

Since $\sum_{e' \in \mathcal{E}_{int}, e'(0)=v'} (\Psi^v_{e'})'(0) + (\Psi^v_{e_{v'}})'(0) = 0$,
we get:

$$\sum_{e' \in \mathcal{E}_{int}, e'(0)=v'} \frac{-\Psi^v(v')\cos(kL(e')) + \Psi^v(\bar{e'}(0))}{\sin(kL(e'))} - i\delta(v,v') + iS(v,v') = 0$$

$$\Rightarrow \sum_{v'' \in V} c(v',v'') \frac{-\Psi^v(v')\cos(kL(v',v'')) + \Psi^v(v'')}{\sin(kL(v',v''))} - i\delta(v,v') + iS(v,v') = 0$$

$$\Rightarrow -F(v')\Psi^v(v') + \sum_{v'' \in V} G(v',v'')\Psi^v(v'') - i\delta(v,v') + iS(v,v') = 0$$

$$\Rightarrow [\sum_{v''} H(k)_{v',v''}\Psi^v(v'')] - i\delta(v,v') + iS(v,v') = 0$$

$$\Rightarrow [\sum_{v''} H(k)_{v',v''}(\delta(v,v'') + S(v,v''))] - i\delta(v,v') + iS(v,v') = 0$$

So:

$$\sum_{v'' \in V} H(k)_{v',v''}\delta(v,v'') + \sum_{v'' \in V} H(k)_{v',v''}S(v,v'') - i\delta(v,v') + iS(v,v') = 0$$

Notice that:

$\sum_{v'' \in V} H(k)_{v',v''}\delta(v,v'') = H(k)_{v,v'}, \sum_{v'' \in V} H(k)_{v',v''}S(v,v'') = (SH(k))_{v,v'}$

Therefore, H(k) + SH(k) - iI + iS = 0

$\Rightarrow S(H(k) + iI) = iI - H(k)$

We conclude that $S = [iI - H(k)][iI + H(k)]^{-1}$. $\square$

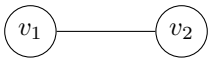
Define $\zeta(k) = det[I - S(k)]$. In kottos and Smilansky, they argue that the graph eigenvalues are the numbers k^2 where k are the roots of the function $\zeta(k) = 0$.

4 Examples

4.1 The Cycles

Following the idea above, we will calculate the eigenvalues of the basic examples, the cycles of n vertices.

Consider the most basic example, where there is only two vertices v_1 and v_2 connected by one edge whose length is L.



Then by definition, we have the following:

$$G = G(v_1, v_2) = \frac{1}{\sin(kL)}$$

$$G(v_i, v_i) = 0 \text{ for i = 1, 2}$$

$$F = F(v_1) = F(v_2) = \cot(kL)$$

$$H(k)_{v_i,v_i} = -F \text{ for i = 1, 2}$$

$$H(k)_{v_1,v_2} = H(k)_{v_2,v_1} = G$$

So:

$$H(k) = \begin{pmatrix} -\cot(kL) & \frac{1}{\sin(kL)} \\ \frac{1}{\sin(kL)} & -\cot(kL) \end{pmatrix}$$

Given:

$$S(k) = [iI - H(k)][iI + H(k)]^{-1}$$

plug in everything, we get that:

$$S(k) = e^{-ikL} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which is symmetric and unitary.
Then

$$\zeta(k) = det[I - S(k)] = 0 = det(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}) - \begin{pmatrix} 0 & e^{-ikL} \\ e^{-ikL} & 0 \end{pmatrix}) = 1 - e^{-i2kL}$$

We get that

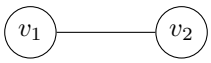
$$e^{-i2kL} = 1$$
$$k = \frac{\pi}{L}m, m \in \mathbb{Z}$$

Hence the eigenvalues of the graph where two vertices are connected by an interval of length L are

$$k^2 = \frac{\pi^2}{L^2}m^2, m \in \mathbb{N}$$

Similarly, we can solve for the spectrum of the following cycles, each edge with the same length L:

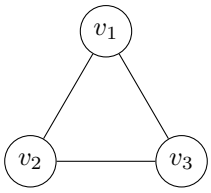
(n = 2)



$$k = \frac{2m}{2L}\pi, m \in \mathbb{N}$$

$$k^2 = \frac{(2m)^2}{(2L)^2}\pi^2, m \in \mathbb{N}$$

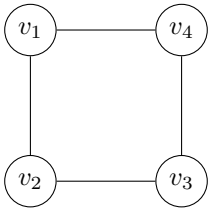
(n = 3)



$$k = \frac{2m}{3L}\pi, m \in \mathbb{N}$$

$$k^2 = \frac{(2m)^2}{(3L)^2}\pi^2, m \in \mathbb{N}$$

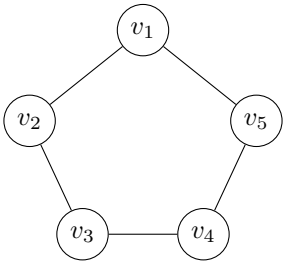
(n = 4)



$$k = \frac{2m}{4L}\pi, m \in \mathbb{N}$$

$$k^2 = \frac{(2m)^2}{(4L)^2}\pi^2, m \in \mathbb{N}$$

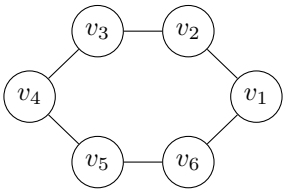
(n = 5)



$$k = \frac{2m}{5L}\pi, m \in \mathbb{N}$$

$$k^2 = \frac{(2m)^2}{(5L)^2}\pi^2, m \in \mathbb{N}$$

(n = 6)



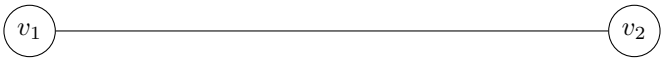
$$k = \frac{2m}{6L}\pi, m \in \mathbb{N}$$

$$k^2 = \frac{(2m)^2}{(6L)^2}\pi^2, m \in \mathbb{N}$$

One quickly notice that if the total lengths of the cycles are the same, namely, if the total lengths of the cycles are all L, which means each segment is L/n, then k and k^2 will be the same for all the cycles, and they are exactly the ones for the cycle with only one vertex. This is precisely due to the Neumann-Kirchhoff boundary conditions. When the boundary conditions hold at a vertex of degree 2, in this cases, at all the vertices, the vertex actually can be eliminated, hence combining two adjacent edges into one smooth edge. The boundary conditions exactly guarantee that the adjacent H^2 pieces of the function match into a single H^2 function on the resulting longer edge: the continuity condition ensures the natural continuity and the current conservation condition ensures the continuity of the first derivative.

4.2 Line Segments with Different Numbers of Nodes

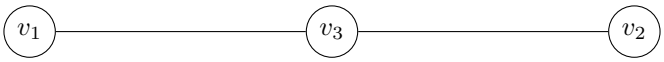
Given the observation above, we should also consider the example where we start with a single line segment with two vertices at the ends, and keep adding new nodes in the middle. Consider the case when each time, we add a new node, but each segment has the length L. Then we have:
(n = 2)



$$k = \frac{2m}{2L}\pi, m \in \mathbb{N}$$

$$k^2 = \frac{(2m)^2}{(2L)^2}\pi^2, m \in \mathbb{N}$$

(n = 3)



$$k = \frac{2m}{4L}\pi, m \in \mathbb{N}$$

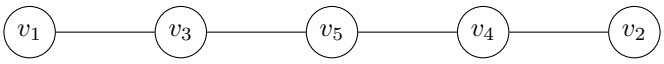
$$k^2 = \frac{(2m)^2}{(4L)^2}\pi^2, m \in \mathbb{N}$$

(n = 4)

$$k = \frac{2m}{6L}\pi, m \in \mathbb{N}$$

$$k^2 = \frac{(2m)^2}{(6L)^2}\pi^2, m \in \mathbb{N}$$

(n = 5)



$$k = \frac{2m}{8L}\pi, m \in \mathbb{N}$$

$$k^2 = \frac{(2m)^2}{(8L)^2}\pi^2, m \in \mathbb{N}$$

(n = 6)

$$k = \frac{2m}{10L}\pi, m \in \mathbb{N}$$

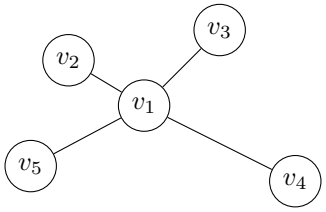
$$k^2 = \frac{(2m)^2}{(10L)^2}\pi^2, m \in \mathbb{N}$$

Observe that just like the cycle graphs, if the total lengths of the segments are the same, namely, if the lengths of the total segments are all L, which means each segment is $L/(n-1)$, then k and k^2 will be the same for all the cases, and they are exactly the ones for the single segment with two vertices at the ends, or namely ,the 2-cycle. Again, this is precisely due to the Neumann-Kirchhoff boundary conditions. When the boundary conditions hold at a vertex of degree 2, in this cases, at all the vertices, the vertex actually can be eliminated, hence combining two adjacent edges into one smooth edge. The boundary conditions exactly guarantee that the adjacent H^2 pieces of the function match into a single H^2 function on the resulting longer edge: the continuity condition ensures the natural continuity and the current conservation condition ensures the continuity of the first derivative.

Moreover, we also notice that the line graphs and the cycle graphs are different, as they have different eigenvalues. This is because the boundary conditions on the line do not allow the ends to be identified to form a cycle, unless we impose additional conditions on the endpoint vertices.

4.3 The Star Graphs

Since any arbitrary graph locally, i.e. near a vertex, looks like a star graph, quantum star graphs are often studied in the literature. Consider a star graph as below. We impose Neumann-Kirchhoff conditions at all vertices of the graph.



Taking the boundary conditions as given, we can rewrite the eigenvalue function as:

$$\left(\frac{\mathrm{d}^2\Psi_e}{\mathrm{d}t^2}\right) = k^2\Psi_e(t), k \in \mathbb{R}$$

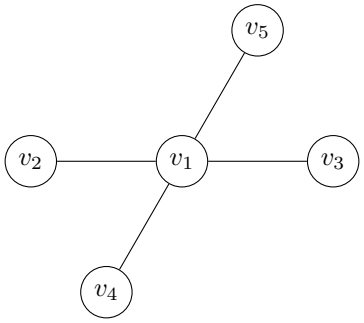
Consider the function Ψ_e on the edge e going from a peripheral to the central vertex. At the peripheral vertex, we have the Neumann-Kirchhoff condition $\Psi_e'(0) = 0$. Together with the above equation, it implies that on the edge e the eigenfunction Ψ_e must have the form $\Psi_e(t) = A_e \cos(kt)$. The outgoing derivative of $\Psi_e(t)$ at the central vertex $t = L(e)$ is equal to $A_e \sin(kL(e))$. This means that the two boundary conditions at the central vertex become:

$$\begin{cases} A_1 \cos(kL_1) = A_2 \cos(kL_2) = ... = C \\ \sum_{b=1}^{\mathcal{E}} A_b k \sin(kL_b) = 0 \end{cases}$$

If we divide the second equation by C, we get that k^2 is an eigenvalue if

$$F(k) = \sum_{b=1}^{\mathcal{E}} \tan(kL_b) = 0$$

Notice that the case $C = 0$ requires a separate consideration which let us conclude that if a value of k is a pole for n out of $\mathcal{E}$ summands in $F(k)$, then k^2 is an eigenvalue of multiplicity n-1. Particularly, if L_b's are not rationally related, then all eigenvalues of the star graph are simple and k^2 is an eivenvalue if and only if $F(k) = 0$.



If we consider the case where all the edges have the same length L, we get that either $\tan(kL) = 0$ or $\cos(KL) = 0$. So:

$$k = \frac{2m}{4L}\pi, m \in \mathbb{N}$$

$$k^2 = \frac{(2m)^2}{(4L)^2}\pi^2, m \in \mathbb{N}$$

which is the same as the spectrum of the 4-cycle, by coincidence.

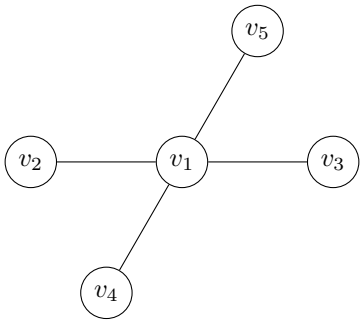
5 Statistical Description of Spectra of Star Graphs

This section will elaborate on the theoretical result of the spectra of star graphs in the previous section. Recall that k^2 is an eivenvalue if and only if

$$F(k) = \sum_{b=1}^{\mathcal{E}} \tan(kL_b) = 0$$

.
We consider the following different cases of the edge lengths for star graphs, and obtain the spectra numerically in R by taking a look of the roots of F.

5.1 Star graphs with equal length edges



As we have seen in the previous section, if we consider the case where all the edges have the same length L, we get that either $\tan(kL) = 0$ or $\cos(kL) = 0$. So:

$$k = \frac{2m}{4L}\pi, m \in \mathbb{N}$$

$$k^2 = \frac{(2m)^2}{(4L)^2}\pi^2, m \in \mathbb{N}$$

.

In R, numerically, we get that for a four-edge star graph whose four edges all have the same length $L = 1$, the graph of the function $F(k)$ with respect to k is

as follows, which clearly has a periodicity that we have seen in the theoretical solution.

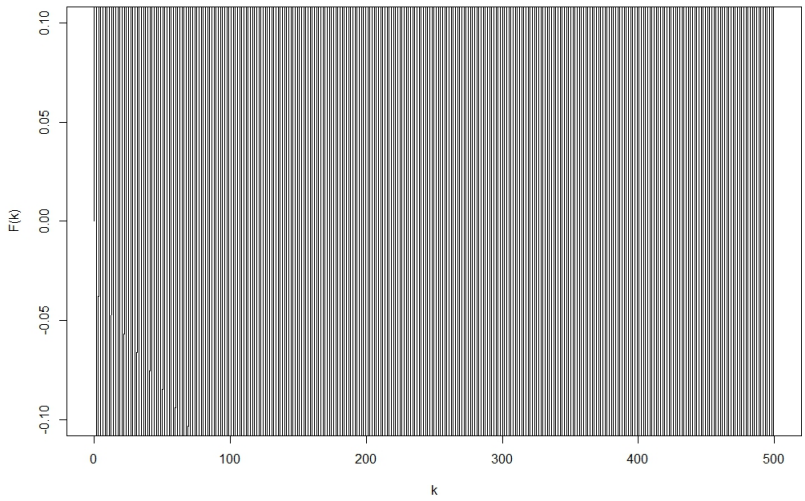


Figure 1: F(k) of a four-edge star graph with equal-length edges

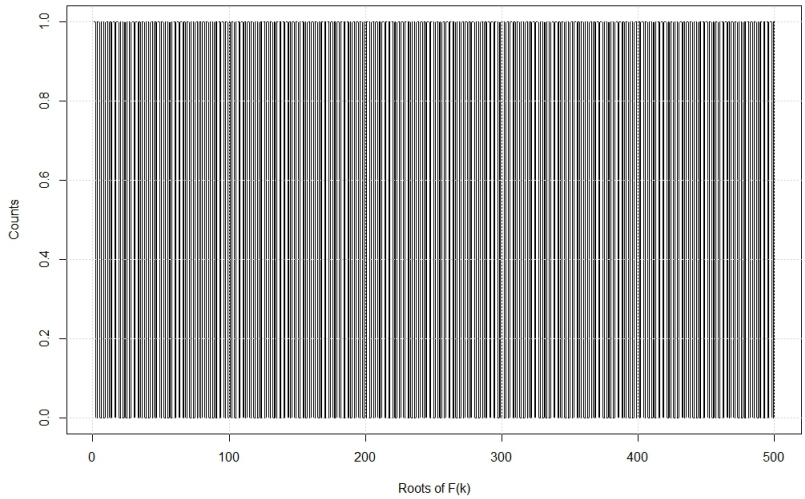


Figure 2: Spectrum statistics of a four-edge star graph with equal-length edges

5.2 Star graphs whose edge lengths are rationally related

It is natural to ask what will happen if the edge lengths are rationally related. That is to say, what will happen if the edge lengths are rationally related? Will the spectrum of a star graph show some kinds of periodicity? Let us first consider the four-edge star graph where $L_{e_1} = L_{e_2} = L_{e_4} = 1$ and $L_{e_4} = 2$. Then we get the spectrum as follows:

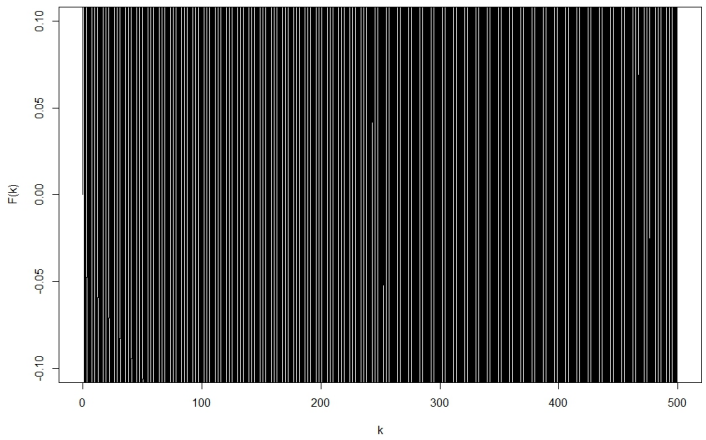


Figure 3: F(k) of a four-edge star graph with edge lengths $\{1, 1, 1, 2\}$

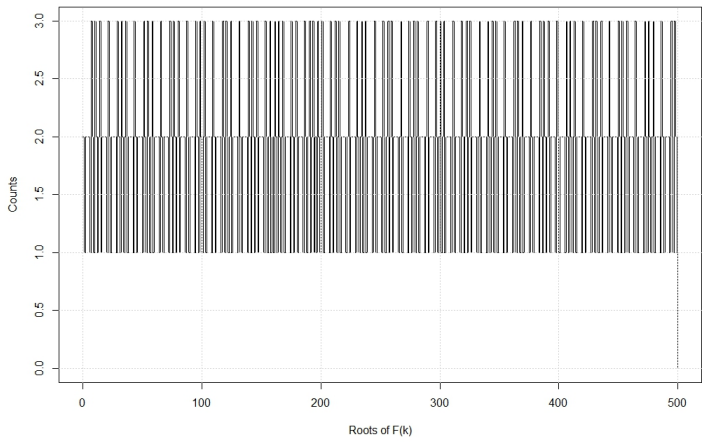


Figure 4: Spectrum statistics of a four-edge star graph with edge lengths $\{1, 1, 1, 2\}$

Then let us consider the case where $L_{e_1} = L_{e_2} = 1$, $L_{e_3} = L_{e_4} = 2$. The

spectrum is the following:

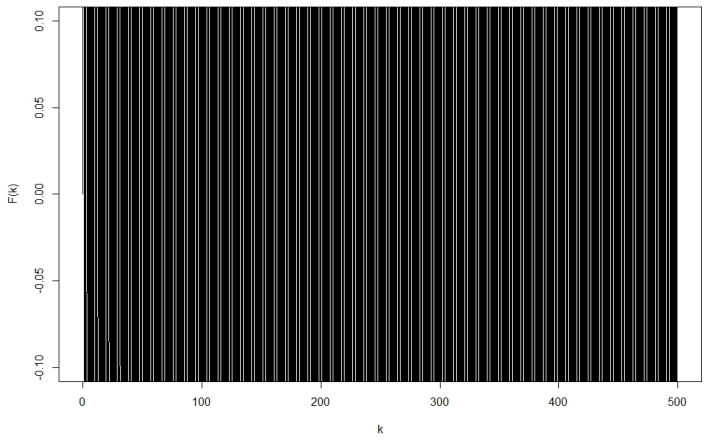


Figure 5: F(k) of a four-edge star graph with edge lengths $\{1, 1, 2, 2\}$

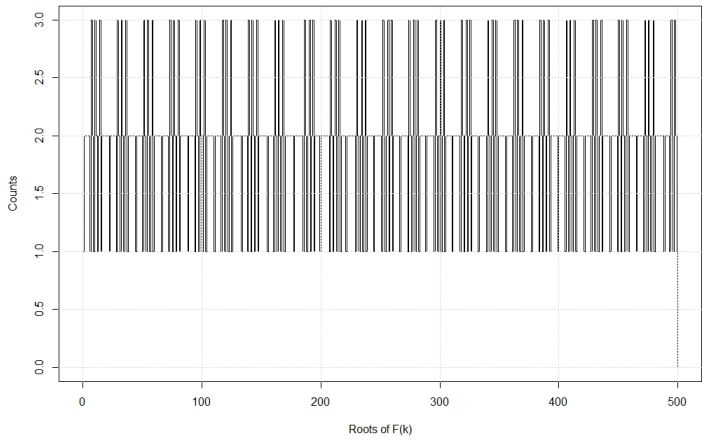


Figure 6: Spectrum statistics of a four-edge star graph with edge lengths $\{1, 1, 2, 2\}$

Finally, consider the case where $L_{e_1} = 1$, $L_{e_2} = L_{e_3} = L_{e_4} = 2$

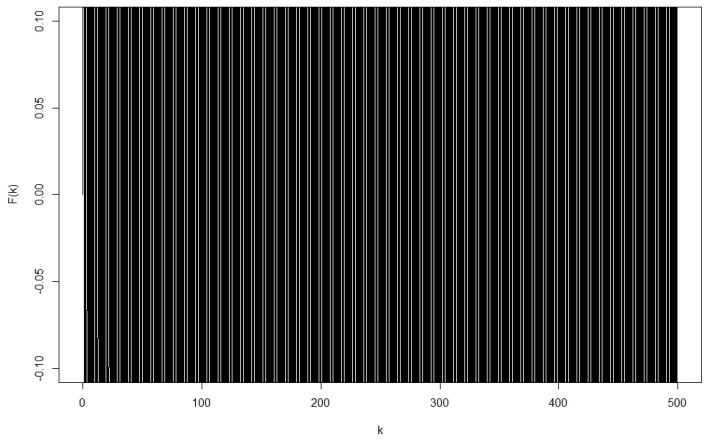


Figure 7: F(k) of a four-edge star graph with edge lengths $\{1, 1, 2, 2\}$

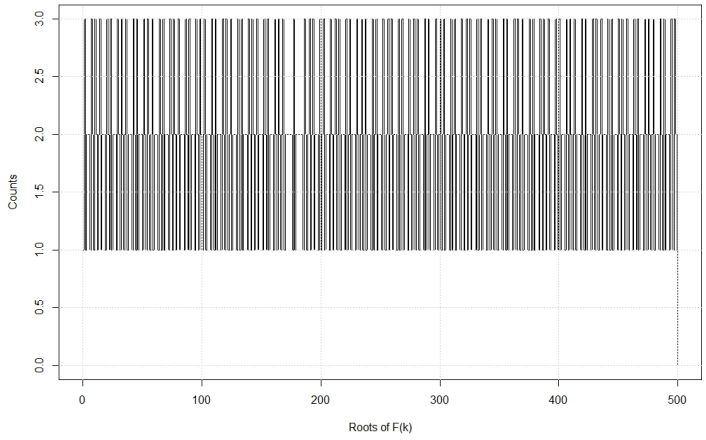


Figure 8: Spectrum statistics of a four-edge star graph with edge lengths $\{1, 1, 2, 2\}$

Note that in all cases, there is some kind of pattern, or periodicity in the spectrum, though not quite as simple as in the case of graphs with all equal-length edges.

5.3 Star graphs whose edge lengths are not rationally related

After considering the cases where the edge lengths are rationally related, then it is natural to ask what will happen if the edge lengths are not rationally related. That is to say, what will happen if the edge lengths are irrationally related? In section 4.3, we have shown that if the edges are not rationally related, then all eigenvalues of the star graph are simple. But what about the periodicity of the spectrum of a star graph?

Let us first consider the four-edge star graph where $L_{e_1} = L_{e_2} = L_{e_4} = 1$ and $L_{e_4} = \sqrt{2}$. Then we get the spectrum as follows:

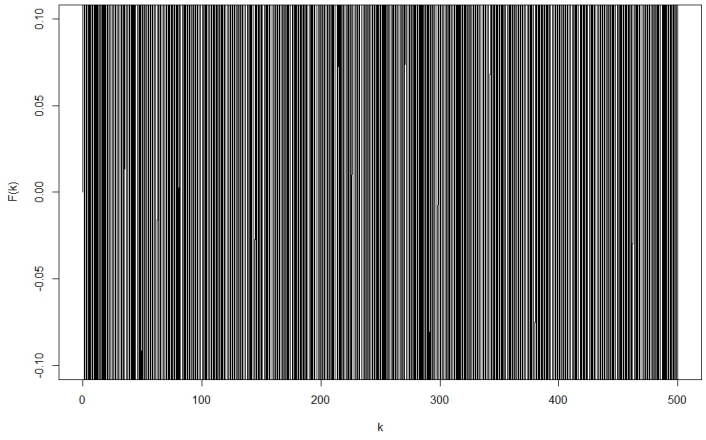


Figure 9: F(k) of a four-edge star graph with edge lengths $\{1, 1, 1, \sqrt{2}\}$

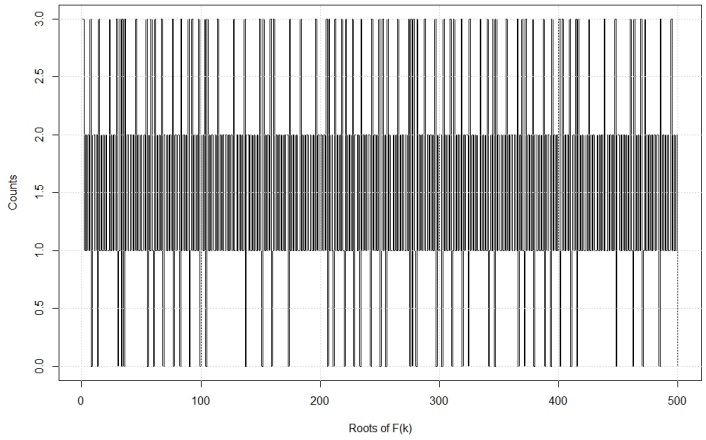


Figure 10: Spectrum statistics of a four-edge star graph with edge lengths $\{1, 1, 1, \sqrt{2}\}$

Then let us consider the case where $L_{e_1} = L_{e_2} = 1$, $L_{e_3} = \sqrt{2}$, $L_{e_4} = \sqrt{3}$. The spectrum is the following:

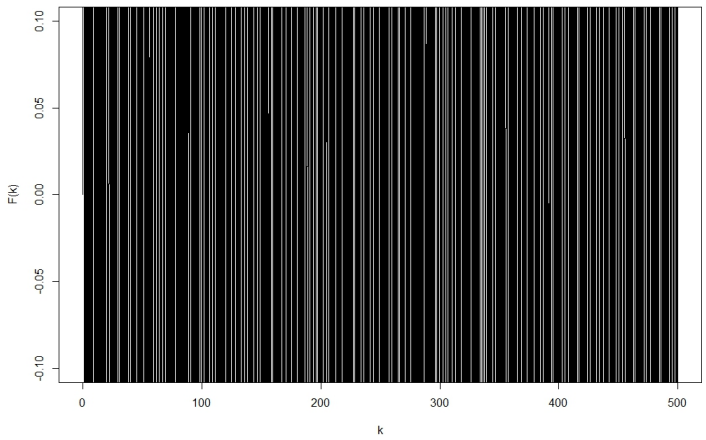


Figure 11: F(k) of a four-edge star graph with edge lengths $\{1, 1, \sqrt{2}, \sqrt{3}\}$

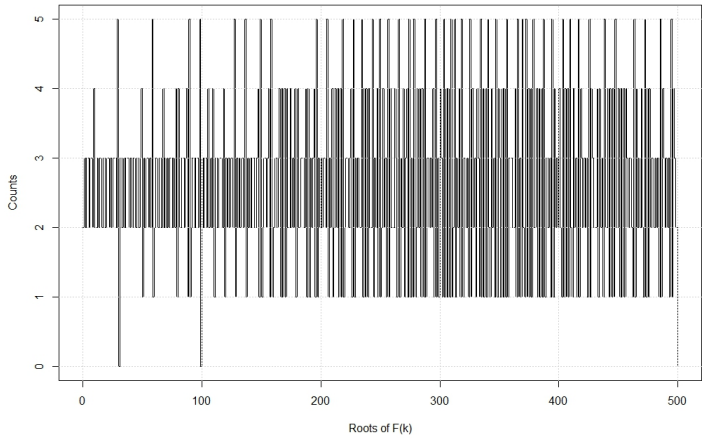


Figure 12: Spectrum statistics of a four-edge star graph with edge lengths $\{1, 1, \sqrt{2}, \sqrt{3}\}$

Finally, consider the case where $L_{e_1} = 1$, $L_{e_2} = \sqrt{2}$, $L_{e_3} = \sqrt{3}$, $L_{e_4} = \sqrt{5}$

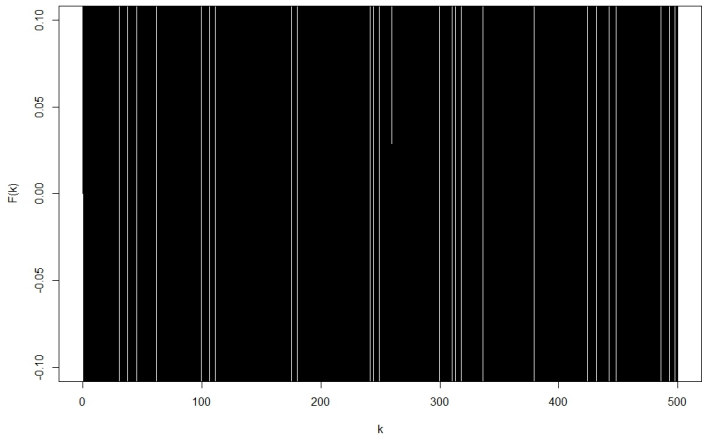


Figure 13: F(k) of a four-edge star graph with edge lengths $\{1, \sqrt{2}, \sqrt{3}, \sqrt{5}\}$

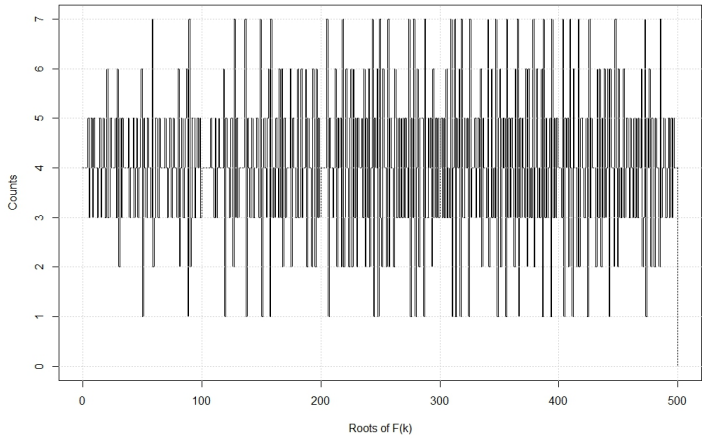


Figure 14: Spectrum statistics of a four-edge star graph with edge lengths $\{1, \sqrt{2}, \sqrt{3}, \sqrt{5}\}$

Notice that as the edges become less and less rationally related, the frequency of eigenvalues increase and they are more and more aperiodic. It shows that when the edges are not rationally related, we have a truly infinite spectrum for a star graph.

6 Further Directions

This section will first discuss further directions of this project. Remember that in the introduction, this project was motivated by the fact that in the examples of the cycles, the infinite spectrum of the Laplacian operator on the metric graph obtained by the scattering matrix approach will just be an infinite copy of the spectrum of the corresponding combinatorial graph related in some way, though not exactly the same. One special property about the cycle is that its corresponding combinatorial graph could be seen as a Cayley graph with an underlying group. Hence to understand this infinite multiplicity, We would like to use ideas from representation theory and propose the idea of Cayley metric graph, which combines the ideas of a Cayley graph and a metric graph. We conjecture some properties of Cayley metric graphs as well.

6.1 Cayley Metric Graphs

Let $\mathcal{G} = (V, \mathcal{E})$ be a metric graph, and let G be its symmetric group.

Definition 6.1. *A symmetry f of G is a homomorphism of $|\mathcal{G}| = \cup_{e\in\mathcal{E}}|e|$, the underlying metric space such that:*
1. f maps vertices to vertices: $f|_V : V \to V$ is a permutation of vertices.

2. f maps edges to edges: $f|_{e_i} : e_i \to e_j$, is smooth and perserve the Lebesgue measure m on the intervals.

In other word, f is a graph isometry of the metric graph.

We would like to conjecture the following:

Proposition 6.1. *G acts on the Hilbert space by an unitary representation that commutes with the Laplacian.*

Combining the notion of metric graph and Cayley graph, we introduce the notion of Cayle metric graph. Namely, we embed the combinatorial graph into the metric graph, where in this case, all the egdes have the same length L.

Let $\mathcal{G}_0$ be a Cayley graph, $\mathcal{G}$ be a metric graph such that $\mathcal{G}_0 \hookrightarrow \mathcal{G}$. Let $L^2(\mathcal{G})$ be the L^2 space on $\mathcal{G}$, and $L^2(\mathcal{G}_0)$ be the L^2 space on $\mathcal{G}_0$. Then we define the two inner products respectively by:

$$\langle f, g\rangle = \sum_{e\in\mathcal{E}} \int_0^L \bar{f} g dm$$

,

$$\langle f(v), g(v)\rangle = \sum_{v\in V} \bar{f(v)} g(v) = \langle f, g\rangle_0$$

.

Define a restriction map

$$R : L^2(\mathcal{G}) \to L^2(\mathcal{G}_0)$$
$$f \mapsto f|_v$$

and the canonical extension (or inclusion, which is not unique)

$$E_k : L^2(\mathcal{G}_0) \hookrightarrow L^2(\mathcal{G})$$

Let Δ denote the subspace of the Laplacian. Δ_0 denote the correponding subspace in $L^2(\mathcal{G}_0)$.

We would also like to conjecture the following two propositions:

Proposition 6.2. $\Delta_0 \circ R = R \circ \Delta$

Proposition 6.3. $\Delta \circ E_k = E_k \circ \Delta_0$

We are hoping to break up the unitary representation on the entire Hilbert space to the unitary representation on the eigenspace of Δ, which are standard for studying graph spectra.

6.2 Some Research Questions

Here, I list some research questions related to this project that would be interesting to continue studying.

1. How edge lengths affect the spectrum of a quantum graph? As we have seen in the examples of star graphs whose edges are rationally related, where there is some kind of periodicity. Does this periodicity has to do with the fact that we can subdivide each edge into equal segments without changing the topology?

2. What will happen if the graph is a homogeneous graph?

3. What will happen if the graph is a Cayley metric graph?

4. Under what conditions Can we obtain the spectrum of a metric graph from its corresponding combinatorial graph? Remember in the case where the edges are not rationally related, we have shown that all the eigenvalues are simple. In that case, we have a truly infinite spectrum, not an infinite copy of the spectrum of the correponding combinatorial graph.

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