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The Laplacian on Isotropic Quantum Graphs: Solutions and Applications

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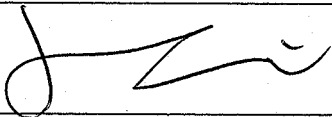
The Laplacian on Isotropic Quantum Graphs: Solutions and Applications

A thesis submitted in partial fulfillment of the requirement
for the degree of Bachelors of Science in Mathematics from
The College of William and Mary

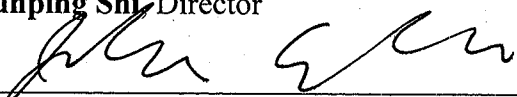
by

Patrick King

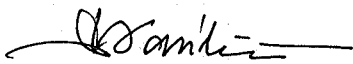
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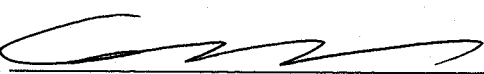
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April 23, 2012

The Laplacian on Isotropic Quantum Graphs:
Solutions and Applications

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April 23, 2012

Abstract

The quantum graph has been demonstrated to be widely applicable in the field of mathematical physics. The Laplacian in particular has use everywhere from quantum mechanics to wave phenomena. Restricting our study to several classes of isotropic quantum graphs, where every edge is the same length, we present complete solutions of several of these classes of graphs.

Contents

1	Introduction	1
1.1	Motivation	1
1.2	Preliminaries	3
1.2.1	Metric Graphs	3
1.2.2	Spectral Theory	6
1.2.3	Useful Properties	11
2	Analytical Results	21
2.1	Elementary Results	21
2.1.1	The One Dimensional Line	21
2.1.2	The Circle	24
2.2	The n -Star	27
2.3	The n -Path	29
2.4	The n -Petal	31
2.5	Complete Quantum Graphs	33
3	Numerical Simulation and Applications	41
3.1	Tools for Visualization	41
3.1.1	Specifying the Graph	42
3.1.2	Plotting Tools	43
3.1.3	Animation	44

3.2	Computer Algebra	44
4	Conclusion	47
4.1	Acknowledgements	49
A	General Solutions	51
A.1	n -Star	51
A.2	n -Path	54
A.3	n -Petal	56
B	Matlab Code	61
B.1	4-Complete Graph	61
B.2	6-Star Animation	63
C	Mathematica Code	67

List of Figures

1.1	A general graph and a directed graph.	3
1.2	Several differently shaped but still identical graphs.	4
1.3	Examples of multiple edges and self looping.	5
1.4	Exterior derivative directions. Arrows indicate the positive direction at the vertex for each edge.	8
1.5	Two identical graphs with exactly opposite direction conventions.	16
2.1	The 3-Line.	21
2.2	Line Solutions.	23
2.3	The 6-Ring.	25
2.4	Ring Solutions.	26
2.5	The 6-Star.	27
2.6	Solutions for the 6-Star.	29
2.7	The 4-Path.	29
2.8	Solutions to the 3-Path.	30
2.9	The 3-Petal.	31
2.10	Solutions to the 3-Petal.	32
2.11	The 5-Complete Graph.	33
2.12	The 5-Complete Graph, with Direction and Labeling Conventions.	34
2.13	Solutions to the 4-Complete graph.	37

Chapter 1

Introduction

1.1 Motivation

The quantum graph is a relative newcomer in the venerable field of partial differential equations, having been invented during the last century. Applications in mesoscale physics such as chemical bonding [7], photonic crystals, and quantum chaos [3] make the quantum graph an exciting idea, if still relatively obscured within the wide field of mathematical physics. Some more mundane applications can be found in the context of heat transport and wave phenomena as studied on thin wires. Such applications are naturally of interest to the applied mathematician or physicist.

The general mathematician, however, might be more motivated by the confluence of ideas from what are usually quite separate branches of mathematics - partial differential equations and graph theory. The quantum graph is, at its core, a problem in spectral theory: that is, eigenvalues and eigenfunctions of a generalized operator. Veterans of solving partial differential equations would certainly recognize these eigenvalue problems. Complete solution of almost any partial differential equation requires knowing its eigenvalues and corresponding eigenfunctions. [6]

The quantum graph is, essentially, a metric graph on whose edges an eigenvalue prob-

lem for an operator is solved. This is what makes this a “quantum” structure. This eigenvalue problem will, properly posed, yield a discrete set of eigenvalues, at “quantized” levels. This invites comparison to the discrete energies found in quantum theory, such as the spectrum of atomic hydrogen. Of course not all operators are useful or interesting to study, so we need to decide on an operator to use.

As far as operators are concerned, few enjoy as wide applicability as the Laplacian. Constituting the spatial part of the iconic wave and diffusion equations, the Laplacian is a relatively simple differential operator consisting of the second unmixed derivatives of a function. Befitting its lofty position within mathematics, its characteristics and properties are rather well known. In addition to its more classical applications, those who have studied quantum mechanics will readily recognize the Laplacian as part of the Hamiltonian operator of the Schrödinger equation. [2] More generally, the Laplacian is in a sense the simplest elliptic operator, and thus has many applications in general potential theory.

As with other classical problems in spectral theory, the domain is where the most interesting parts of the problem are found. The Laplacian, being a simple and useful operator, is a perfect choice for exploring the behavior of the quantum graph precisely because it leaves out complication. Using the Laplacian allows us to most clearly see how the structure of the graph affects the solutions while also allowing us to explore specific applications.

The central purpose of this paper is to obtain concrete results. Rather than establishing very general yet vague properties common to all operators, we restrict our study to specific cases. Wherever possible we state closed form solutions for all possible cases. By doing so we determine the concrete behavior of these quantum graphs, whose properties we study in great detail.

1.2 Preliminaries

The quantum graph is a structure which rests on very general notions in functional analysis. Unlike the more ordinary domains and applications of the Laplacian, where most of the finer points of spectral theory can be safely assumed to hold, quantum graphs extend the problem to a very different situation. We must examine every part of the problem.

1.2.1 Metric Graphs

What makes the quantum graph distinct is the graphical structure of the problem. Mathematically, graphs are simply a collection of vertices and edges. [9] An edge joins two vertices together, and can be thought of as a line between them. A vertex is simply a point, to which edges may or may not be connected. Graphs are usually described by their set of edges \mathcal{E} and their set of vertices \mathcal{V} . If we decide that the “orientation” of the edges matters - that is, we say an edge is directed from vertex A to vertex B , and not vertex B to vertex A - then we call the graph a directed graph.

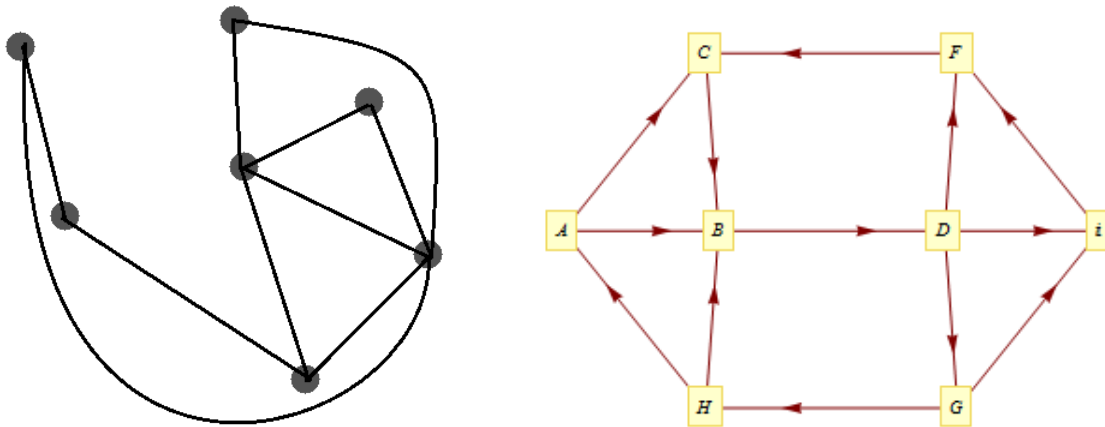


Figure 1.1: A general graph and a directed graph.

The definition of a graph does not specify many things, leaving much room for specialization and variety. If we are to solve problems on the graph, we should consider a more restrictive structure. We need a notion of distance on the edges - a general graph cannot tell you how “long” an edge is or how far apart two points are. A metric can tell us these things, and a graph equipped with such is called a metric graph. For our purposes, it is useful to stick to real number intervals. The following definition should suffice.

Definition 1.1. Let Γ be a graph, where $\mathcal{E} = \{e_i : 1 \leq i \leq n\}$ is the set of edges of Γ and $\mathcal{V} = \{v_j : 1 \leq j \leq m\}$ is the set of vertices of Γ . Γ is a metric graph if each edge $e_i \in \mathcal{E}$ is associated with an interval $[0, L_i]$ and the points 0 and L_i are associated with vertices. If an edge e_i is associated with a vertex v_j , then we say that $e_i \in v_j$. If x is a point on edge e_i , then we say that $x \in e_i$.

In a sense, metric graphs associate each edge with a one dimensional interval. (More on this interval later.) If we know how to measure distances on these intervals then we know how to measure distance between any points on the entire graph. This provides us with an important analytic foundation from which we can build the machinery of differential equations.

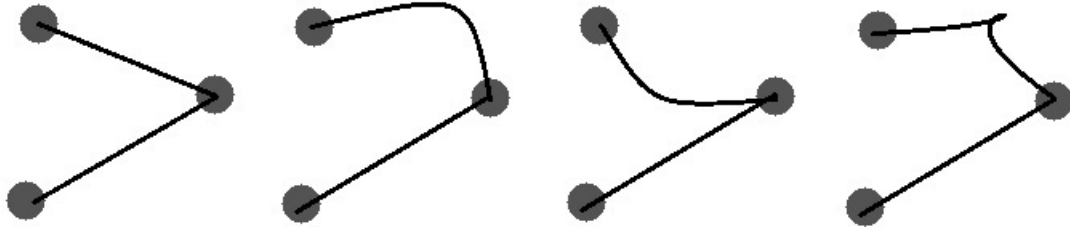


Figure 1.2: Several differently shaped but still identical graphs.

Even with this notion of distance the metric graph still does not place much restriction on the shape of the edge itself. While vertices are simply points, the edges are simply

associated with one dimensional intervals and so can be as strangely shaped as one desires. Since there is only a single dimension associated with each edge, the shape does not actually matter. In Figure 1.2, even though the graphs look very different, the solutions on each will take the same values as long as they have the same length edges.

As we are looking for concrete results, we should concern ourselves with the types of graphs we consider. In the literature, it is common to exclude both self-loops (edges whose endpoints are the same vertex; alternatively, vertices connected to themselves) and multiple edges connecting two vertices. However, since they can be used to construct simple classes of graphs and their behavior is interesting, we decided to include these and not forbid them. We will certainly be treated to some interesting behavior. Some examples are given in Figure 1.3.

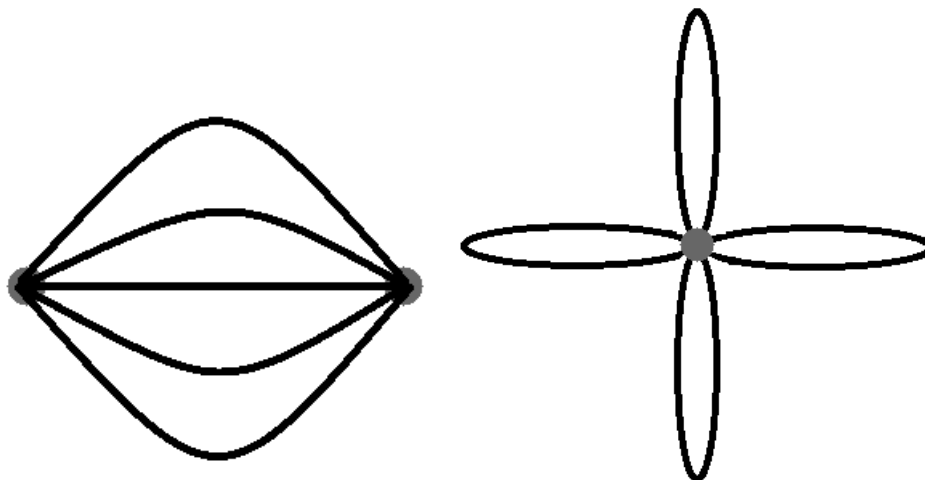


Figure 1.3: Examples of multiple edges and self looping.

As hinted at before, in principle every edge can have a different length. This is wonderfully general but woefully difficult to deal with when one is actually finding the solutions to these quantum graphs. In the most general form the edges can even have infinite length. [5] We will restrict our study to quantum graphs whose edges are all the same length.

Definition 1.2. Let Γ be a metric graph. Γ is *isotropic* if every edge has the same length, denoted L .

Another equivalent term for this behavior is *equilateral*, but we feel that the term *isotropic* makes more sense from the diffusive or physical perspective. By making every edge the same length, we have an additional symmetry to the problem which we can exploit. It also makes characterizing the problem much simpler, as will become clear shortly. In accord with our goal of finding concrete results, this symmetry allows us to find closed form expressions for both eigenvalues and eigenfunctions of entire classes of quantum graphs.

Another possibility the astute reader might notice is that these definitions do not in principle prohibit graphs with an infinite number of edges or vertices. While such cases might be interesting in some cases, we will in general assume that the graphs we study are *finite*, meaning that the graph has only a finite number of vertices and edges. In fact, implicit in our assumption, we only consider *compact* graphs, which are finite graphs with finite edge lengths. [9] Additionally, we only consider graphs which are *connected*, meaning that every pair of vertices on the graph has a path between them. Disconnected parts of graphs do not affect the spectrum, and are thus irrelevant. Some cases in which edges are allowed to be of infinite length are considered in Kuchment. [4]

1.2.2 Spectral Theory

As we stated before, we will choose the Laplacian as the operator of choice on our graph. In rectangular coordinates, the Laplacian is

$$\Delta = \sum_i \frac{\partial^2}{\partial x_i^2}. \tag{1.1}$$

Obviously for a one dimensional space this reduces to $\Delta = \frac{\partial^2}{\partial x^2}$. Actually, many prefer to define the negative Laplacian as the operator of choice, since this gives a more natural

definition of the eigenvalue problem. (This will become clear later. The idea is that, since the eigenvalues of the positive Laplacian are all strictly nonpositive, then we either define the eigenvalues as negative or we define the Laplacian as negative to make the eigenvalues strictly increasing. This fact will be demonstrated later.)

With these considerations, we can define the (one dimensional) eigenvalue problem as

$$u''(x) = -\lambda u(x). \tag{1.2}$$

where λ is a constant and $u(x)$ is a function satisfying this relation. Any λ which can satisfy this equation for some $u(x)$ is called an eigenvalue and the corresponding $u(x)$ is called an eigenfunction. Normally $u(x)$ is not permitted to be equal to zero; one can see that this would trivially satisfy this problem for any constant λ . We call the set of all permissible λ the *spectrum*. The one dimensional Laplacian eigenvalue problem is quite well understood in terms of Sturm-Liouville theory. [6]

Even though the edges of graphs seem decidedly one dimensional, there is actually nothing in practice which would prevent us from using a higher dimensional Laplacian. In fact, some applications involve solving two linked eigenvalue problems at once on a single vertex. In Bolte and Kerner, the authors study two particle quantum graphs, where each “dimension” roughly corresponds to the position of one particle. This then leads to a two-dimensional Laplacian as part of their two-particle Schrödinger operator. [1] This example shows that, in practice, we are not limited to one dimension. However, as will become abundantly clear, it is sufficient for our purposes to simply study quantum graphs with one dimension on each edge.

When we are talking about continuity and derivatives on metric, we must be very careful about what we mean. Graph structure forces us to evaluate what we mean by continuity and differentiation. Continuity will manifest itself as boundary conditions on vertices, which will become clear shortly. Differentiation should be considered directional in nature, as illustrated by Figure 1.4. Inside the edge differentiation can be taken to be

natural; that is, the usual form of differentiation that we are used to. The ends of the edges are more interesting. For any arbitrary edge, the vertices are located at the points 0 and L_e , where L_e is the length of the edge. We define the outward normal derivatives to be

$$\begin{aligned}\frac{\partial u_i(0)}{\partial n} &= -\frac{du_i(0)}{dx}, \\ \frac{\partial u_i(L_e)}{\partial n} &= \frac{du_i(L_e)}{dx}.\end{aligned}\tag{1.3}$$

As a convenient shorthand, we will absorb both of these definitions into the notation $\partial_n(x)$, which denotes the outward normal derivative of the function $u(x)$.

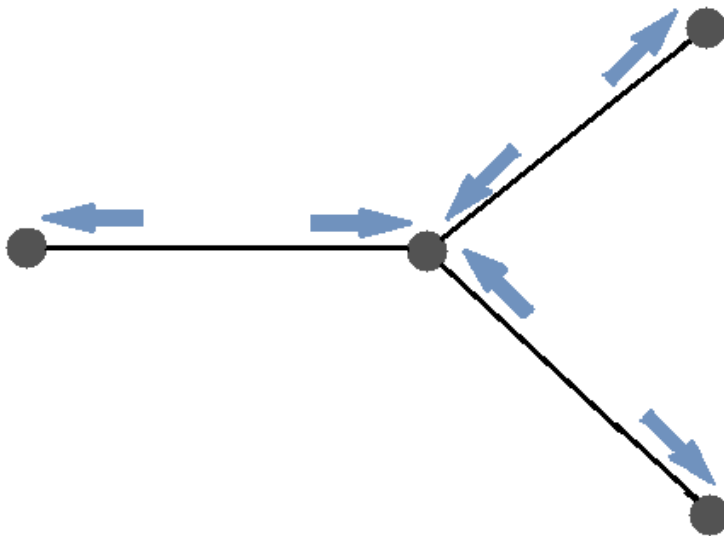


Figure 1.4: Exterior derivative directions. Arrows indicate the positive direction at the vertex for each edge.

In the context of the Laplacian eigenvalue problem, we should take our domain to be, on each edge, some subset of the Hilbert space $L^2(0, L_e)$, where L_e is again the length of the edge in question. The inner product on this space is

$$\langle f, g \rangle = \int_0^{L_e} f(x)g(x)dx \quad (1.4)$$

We need our functions to be \mathcal{C}^2 in the interior of the edge so that we admit continuous first and second derivatives; the boundary conditions require only \mathcal{C}^1 continuity on the boundary. Distance in this space is understood in the same sense as in Euclidean space, and inherits a useful inner product structure by virtue of being a subset of a Hilbert space. Then these individual subspaces are combined according to the structure of the graph. Graph structure naturally prohibits a simple sum of these spaces - this combination can only be understood as a combination consistent with the structure of the graph edges. We denote the subspace on a particular edge as

$$\mathbb{E}_e = \mathcal{C}^2(0, L_e) \cap \mathcal{C}^1[0, L_e], \quad e \in \mathcal{E}, \quad (1.5)$$

where L_e is the length of the edge. This is what we are really thinking of when we mentioned the “interval” earlier. On each edge, there is a generally different eigenfunction, and we denote this solution $u_i(x)$ on edge e_i and $x \in \mathbb{E}_{e_i}$. The complete space of the graph is obviously not constructed by simple addition but in the manner dictated by the combinatorial properties of the graph; that is, an orthogonal direct sum. [5]

$$\mathbb{E}(\Gamma) = \bigoplus_{e_i \in \mathcal{E}} \mathbb{E}_{e_i} \quad (1.6)$$

Armed with our new functional space, we almost have enough to define the quantum graph. There is one remaining piece. We need to make our operator, the Laplacian, have a property known as self-adjointness on our graph. There are several reasons for this - self-adjoint operators have a discrete spectrum and have several quite useful properties. This is determined by the choice of boundary conditions, and is considered part of the definition of the operator. Any choice of boundary conditions which makes the operator self adjoint is sufficient for a quantum graph.

Definition 1.3. Let Γ be a metric graph whose edges are associated with the edge space $\mathbb{E}(\Gamma)$. The graph Γ and a self-adjoint Laplacian Δ comprise a quantum graph.

Of course we now have to determine what boundary conditions to impose to make our Laplacian self-adjoint. Naturally on each edge the interior $(0, L_e)$ should not have any boundary conditions. The vertices represent special points where the structure of the graph changes and so we should impose conditions on them. We call vertices with degree 1 (vertices with only one edge connected to them, excluding self-loops) endpoints. Vertices with more edges connected to them (2 or more) are called joints. (Actually, the case where the degree of the vertex is 2 is a special case, which will be described shortly.)

Joints require careful treatment, and we need to develop some sense of continuity. Since we define our solutions on all the edges, including the ones meeting at a joint, then continuous solutions should have the same value at the vertex, which can be called the *continuity* conditions. At a given vertex v , then for all edges e_i, e_j connected to vertex v_k ,

$$u_i(x) = u_j(x) : x \in v_k. \quad (1.7)$$

We also should determine conditions for the first derivatives of the functions at this boundary. We can impose what are called *Kirchoff* conditions on the derivatives. (These conditions are also called “natural”, “free”, or even “Neumann”, depending on who you ask.) This condition (derived in Ruedenberg and Scherr [7]) is the most natural condition which we have to extend our notion of continuity. The derivation can be likened to continuity of fluid flow in tubes as the limit of the radius of the tube approaches zero. For edges e_i associated with a joint v ,

$$\sum_{e_i \in v} \partial_n u_i(x) = 0 : x \in v_k. \quad (1.8)$$

In other words, the sum of the outward normal derivatives at a joint is equal to zero.

Returning to our endpoints, it seems natural to impose Neumann boundary conditions, which are in essence a realization of Kirchoff boundary conditions for one edge. For the

part of the solution defined on the edge associated with endpoint v ,

$$\partial_n u_i(x) = 0 \quad : \quad x \in v_k. \quad (1.9)$$

It can be shown that if we take these boundary conditions on our quantum graphs for joints and endpoints then our Laplacian is self-adjoint. (We can also choose Dirichlet boundary conditions on the endpoints, where the value of the function at the endpoint is fixed at zero; these conditions also yield a self-adjoint Laplacian. However, Neumann conditions are more natural considering our joint conditions.)

Finally, for notation purposes, it will be useful to partition the set of vertices into two sets: one of endpoints and one of joints. If \mathcal{V} is the set of vertices, then $\mathcal{V} = \mathcal{F} \cup \mathcal{J}$, where \mathcal{F} is the set of endpoints and \mathcal{J} is the set of joints. The notation $v \in \mathcal{F}$ indicates that v is an endpoint, and similarly $v \in \mathcal{J}$ indicates that v is a joint. This notation allows us to easily distinguish between joints and endpoints when describing the problem. We can now state the general quantum graph problem. For $u = (u_1, u_2, \dots, u_n) \in \mathbb{E}(\Gamma)$,

$$\left\{ \begin{array}{lll} u_i''(x) = -\lambda u_i(x), & x \in e_i, \quad u_i \in \mathbb{E}_{e_i}, & \forall e_i \in \mathcal{E}, \\ u_i(x) = u_j(x), & x \in v_k, & \forall v_k \in \mathcal{V}, \quad e_i, e_j \in v_k \\ \sum_i \partial_n u_i(x) = 0, & x \in v_k, & \forall v_k \in \mathcal{J}, \\ \partial_n u_i(x) = 0, & x \in v_k, & \forall v_k \in \mathcal{F}. \end{array} \right. \quad (1.10)$$

1.2.3 Useful Properties

While the preceding sections are useful in the sense that the reader is on the right theoretical ground, this section is actually the most useful in practice as it illuminates several specific properties which are of great use in problem solving. A priori, the eigenvalue λ has no conditions on it. However, given the specification of the eigenvalue problem and our specified boundary conditions, we can learn more about it. Given an eigenvalue and

eigenfunction pair, we can deduce several properties. (In fact, these properties hold for graphs with any length edges, not just isotropic ones.)

Theorem 1.4. *Any eigenvalue λ of a quantum graph is a real number. Furthermore, $\lambda \geq 0$.*

Proof. Take any eigenvalue λ and associated eigenfunction $u(x) = (u_i(x))$ solution. Then

$$u_i''(x) = -\lambda u_i(x).$$

Take also the complex conjugate of the eigenfunctions, $\bar{u}_i(x)$. Multiplying this on the right, we obtain for every edge e_i

$$u_i''(x)\bar{u}_i(x) + \lambda u_i(x)\bar{u}_i(x) = 0.$$

We can then integrate over our entire graph, utilizing the inner product of the Hilbert space. We can sum over all the integrals on every edge to obtain

$$\sum_{i=1}^n \int_0^L u_i''(x)\bar{u}_i(x)dx + \lambda \sum_{i=1}^n \int_0^L u_i(x)\bar{u}_i(x)dx = 0.$$

We can then integrate the first term by parts over each edge to obtain

$$\sum_{i=1}^n u_i'(x)\bar{u}_i(x) \Big|_0^L - \sum_{i=1}^n \int_0^L u_i'(x)\bar{u}_i'(x)dx + \lambda \sum_{i=1}^n \int_0^L u_i(x)\bar{u}_i(x)dx = 0.$$

We now need to consider the boundary term. Notice that a given L or 0 corresponds to a given vertex. The value at the vertex is fixed by continuity conditions, and so we sum the derivatives at this fixed vertex. Denoting the position of the vertex as $x = v_j$ for a particular vertex, and i indexing over all edges associated with this vertex, we can thus regroup this sum as a double sum:

$$\sum_{i=1}^n u_i'(x)\bar{u}_i(x) \Big|_0^L = \sum_{v_j \in \mathcal{V}} \bar{u}_i(v_j) \sum_{e_i \in v_j} u_i'(v_j).$$

The second term is zero for both joints (with Kirchoff conditions) and endpoints (with Neumann conditions). (Notice also that this is true for Dirichlet conditions, using the

first sum.) This is then zero, and the boundary term vanishes. Rearranging the negative term, we now have

$$\lambda \sum_{i=1}^n \int_0^L u_i(x) \overline{u_i}(x) dx = \sum_{i=1}^n \int_0^L u_i'(x) \overline{u_i'}(x) dx.$$

By assumption $u_i(x)$ are not zero, so $\sum_{i=1}^n \int_0^L u_i(x) \overline{u_i}(x) dx \neq 0$. We can then divide this to characterize λ .

$$\lambda = \frac{\sum_{i=1}^n \int_0^L u_i'(x) \overline{u_i'}(x) dx}{\sum_{i=1}^n \int_0^L u_i(x) \overline{u_i}(x) dx}. \quad (1.11)$$

Both the top and bottom integrals are all nonnegative real numbers for every edge; particularly they are zero only if $u_i'(x) = 0$. Hence, $\lambda \geq 0$.

□

Equation 1.10 has a quite suggestive form. It is, in some sense a Rayleigh quotient since each of these integrals is the inner product on each edge space. The additive nature of the integral suggests that we can think of this sum of integrals over the edges as in fact an integral over the entire domain - exactly the form of the Rayleigh quotient in classical eigenvalue problems. This makes intuitive sense, since traditional integrals are additive. We can also demonstrate that zero is always an eigenvalue of any quantum graph - a trivial solution obtained regardless of the intrinsic structure of the graph.

Theorem 1.5. *Zero is always an eigenvalue of any quantum graph. Furthermore, the only eigenfunction solution corresponding to a zero eigenvalue is $u_i(x) = C$ for every edge on the quantum graph.*

Proof. Suppose that zero is an eigenvalue. Then the eigenvalue equation becomes

$$u_i''(x) = 0.$$

Per standard treatment of differential equations we can integrate this to obtain, for some integration constant B ,

$$u'_i(x) = B_i.$$

In general, using the result from Theorem 1.4, zero is an eigenvalue only if $u'_i(x) = 0$. So, since $u'_i(x) = 0$, we can integrate again to obtain, for another integration constant C_i ,

$$u_i(x) = C_i.$$

Thus zero is an eigenvalue and is associated with a constant eigenfunction. Continuity conditions in conjunction with the connectedness of our graphs demand that this constant be the same on every edge of any graph, so for $\lambda = 0$, $u_i(x) = C$ for all edges $e_i \in \mathcal{E}$.

□

This result has important implications for problem solving. Each of the subproblems that are solved on each edge are a Sturm-Liouville problem. Since we know the solution for $\lambda = 0$, and since λ is not less than zero, then we know that all the nontrivial eigenvalues are greater than zero, and so we know the form of solution we should look for when we solve problems. [6] This form, or “ansatz” as it is called in differential equations, is

$$u_i(x) = C_{1,i} \cos(kx) + C_{2,i} \sin(kx). \tag{1.12}$$

Here k is the square root of λ , and $C_{1,i}, C_{2,i}$ will be determined by the collective boundary conditions of the graph. This gives us the starting point from which we can determine the algebraic system of equations that determines the solutions of the problem. In general, it is also important to remember another useful property of eigenfunctions: for any two given eigenfunctions $u_1(x)$ and $u_2(x)$ with common eigenvalue λ , then any linear combination of the two is also an eigenfunction of λ . This follows directly from the linearity of derivatives; it is a simple exercise to verify.

Another useful property we can prove is that the spectrum of the Laplacian quantum graph is discrete. This is another property which the quantum graph shares with its more

classical brethren.

Theorem 1.6. *The spectrum of the quantum graph satisfies $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_m \leq \lambda_{m+1} \leq \dots$. Additionally, $\lim_{m \rightarrow \infty} \lambda_m = \infty$.*

We offer this result without proof as it is a trivial result, provided one knows that these facts are true for the one-dimensional Laplacian eigenvalue problem. [8] Since each edge is essentially an individual Laplacian eigenvalue problem with non-homogeneous Neumann (or Dirichlet) boundary conditions, and since these properties hold for such problems, then it follows that these properties generalize to the whole graph. Applying algebraic conditions, such as forcing the eigenvalues to be the same on all edges and coupling the vertex conditions together do not change the conditions under which these facts are true.

Up until this point we have simply stated that the edges of the graph have a defined point labeled 0 and L . This can be thought of as a “direction” of the edge. The astute reader will note that, in general, this choice might not be arbitrary. It could be the case that direction matters. This is not a trivial problem - we would be in some trouble if the solutions of the graph depended on this direction choice, since then we would, in principle, have to solve the problem with every possible direction convention to obtain every solution. This is, to say the least, a much more complex problem.

Fortunately we can prove that the choice is arbitrary. Indeed, this is quite useful - one might imagine that solving the problem with one convention is quite difficult but with another it is easy. This is of great value when solving problems.

Theorem 1.7. *Let Γ be a Laplacian quantum graph. The eigenvalues and eigenfunctions of Γ are identically determined by any direction convention applied to Γ .*

Proof. Let Γ be a Laplacian quantum graph. Suppose we were to find eigenfunction solutions and eigenvalues using a given direction convention. Take any such eigenvalue - eigenfunction pair. The eigenfunction can either be constant or a linear combination of sines and cosines.

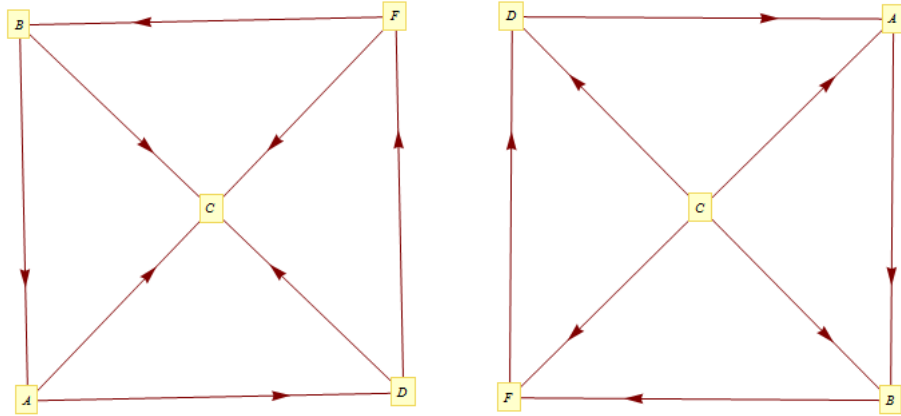


Figure 1.5: Two identical graphs with exactly opposite direction conventions.

Case 1. $\lambda \neq 0$.

Then

$$u_i(x) = a_i \cos(kx) + b_i \sin(kx).$$

These constants a_i and b_i are uniquely determined for this i th edge and satisfy all the boundary conditions. Suppose we were to reverse the direction convention. This would be equivalent to the transformation

$$x \rightarrow L - x.$$

This transformation does two things. First it switches the location of the vertices associated with this edge. If v_1 was at position $x = 0$ and v_2 was at $x = L$, in the new variable v_1 is at $x = L$ and v_2 is at $x = 0$. This also effectively reverses the edge. Now suppose we express our old solution in terms of this new variable. Then

$$U_i(L - x) = a_i \cos(kL - kx) + b_i \sin(kL - kx).$$

First we should check that it satisfies the eigenvalue problem. Calculating the first and second derivatives, we have

$$U'_i(L - x) = a_i k \sin(kL - kx) - b_i k \cos(kL - kx),$$

$$U_i''(L-x) = -a_i k^2 \cos(kL-kx) - b_i k^2 \sin(kL-kx).$$

By inspection, we can conclude that

$$U_i''(L-x) = -k^2 U_i(L-x).$$

We can see that, since $k^2 = \lambda$, then this equation satisfies the eigenvalue problem in this new variable with the same eigenvalue λ . Next we check the boundary conditions. Continuity is the easiest, so we should start with that. We should find that $u_i(0) = U_i(L)$ and $u_i(L) = U_i(0)$.

$$u_i(0) = a_i,$$

$$U_i(L) = a_i \cos(kL - kL) + b_i \sin(kL - kL) = a_i,$$

$$u_i(L) = U_i(L),$$

$$u_i(L) = a_i \cos(kL) + b_i \sin(kL),$$

$$U_i(0) = a_i \cos(kL - 0) + b_i \sin(kL - 0) = a_i \cos(kL) + b_i \sin(kL),$$

$$u_i(L) = U_i(0).$$

So we know that the new equation satisfies the continuity at the boundaries. Now we check the derivative boundary conditions. They will be satisfied if $u_i'(0) = -U_i'(L)$ and $u_i'(L) = -U_i'(0)$. The negative sign can be explained by the chain rule, but alternatively in terms of the outward derivative. Remember that the sign of the derivative depended on whether the derivative was at 0 or L . Switching them will invert the sign to keep our direction convention. So,

$$u_i'(0) = b_i k,$$

$$U_i(L) = a_i k \sin(kL - kL) - b_i k \cos(kL - kL) = -b_i k,$$

$$u_i'(0) = -U_i'(L),$$

$$u_i'(L) = -a_i k \sin(kL) + b_i k \cos(kL),$$

$$U_i'(0) = a_i k \sin(kL - 0) - b_i k \cos(kL - 0) = a_i k \sin(kL) - b_i k \cos(kL),$$

$$u'_i(L) = -U'_i(0).$$

So we have verified that the new equation satisfies all the boundary conditions, and is thus a solution to the quantum graph with the new direction convention. Now we check that every solution to the new graph is constructed in this way from the old graph. Suppose there is a solution to the new graph which cannot be expressed this way. Then, for some

$$U_i(L - x) = A_i \cos(kL - kx) + B_i \sin(kL - kx),$$

we know that this cannot be constructed from a solution on the original graph. However, it is quite easy to show that $A_i \cos(kx) + B_i \sin(kx)$ is indeed a solution of the original graph, making it part of the solution set; however this means that $U_i(L - x)$ can be constructed from that solution and this is a contradiction. Thus every solution of the new graph can be constructed from the solutions of the old one. Thus this given solution is determined identically by either direction convention. Since this was done for arbitrary solution u_i , then this applies to every solution.

Case 2. $\lambda = 0$.

Clearly the solution determined with the new direction convention will be the same constant, satisfying all the boundary conditions. Thus every constant solution is determined identically for either direction convention.

Having proved this for an inversion of any edge direction convention on any characterization of the quantum graph, then inductively this argument can be applied repeatedly to obtain that all direction conventions on a given quantum graph determine all of the solutions identically.

□

Having proved this useful result, then we may now choose a direction on the quantum graph arbitrarily, and take the convention which makes solving the graph easiest.

Earlier we mentioned that vertices of quantum graphs with degree 2 are “special cases.” In fact, the presence of these “interior” vertices do not change the solution at all.

To understand why, we should examine these vertices more closely. Each of these vertices has two edges connected to it. If we label one solution $f_i(x)$ and $f_j(x)$, and we let x_v be the location of the vertex, then our boundary conditions demand that

$$f_i(x_v) = f_j(x_v), \quad \frac{\partial f_i}{\partial x}(x_v) = \frac{\partial f_j}{\partial x}(x_v). \quad (1.13)$$

The second condition follows from the summation of the outward normal derivatives: no matter what direction convention we choose, one direction will oppose the other. Since we only have two terms, and their sum must be zero, then it follows that this must be true. However, these conditions simply enforce continuity - in fact, every point on any edge satisfies the same conditions. In other words, any continuous function with a continuous first derivative which satisfies the endpoint boundary conditions satisfies the boundary conditions on this vertex. We can state this more formally in a theorem.

Theorem 1.8. *Let v_1 be a vertex in quantum graph Γ with degree 2, having edges e_1 and e_2 , each terminating at vertices v_2 and v_3 respectively. The subgraph consisting of $\{v_1, v_2, v_3\}$ and $\{e_1, e_2\}$ is equivalent to a single edge e between vertices v_2 and v_3 , whose length is the sum of the lengths of e_1 and e_2 .*

Proof. Define a direction convention where on edge 1, L_1 corresponds to the location of v_1 , and on edge 2, 0 corresponds to the location of v_1 .

Suppose $u_1(x)$ and $u_2(x)$ are any two eigenfunctions on edge 1 and edge 2 respectively associated with any eigenvalue λ . By virtue of being a solution, $u_1(x)$ satisfies boundary conditions at v_1 and v_2 , and $u_2(x)$ satisfies boundary conditions at v_2 and v_3 . Consider the central vertex v_2 . By our direction conventions, we have that

$$u_1(L_1) = u_2(0),$$

$$\frac{du_1(L_1)}{dx} = \frac{u_2(0)}{dx}.$$

In addition, by the definition of the eigenvalue problem, $u_i''(x) = -\lambda u_i(x)$; since this is true, then we can also conclude that

$$u_1''(L_1) = u_2''(0).$$

These three equations taken together constitute the conditions for \mathcal{C}^2 continuity. We can then construct a new edge, of length $L_1 + L_2$, and with vertices v_2 and v_3 . If we construct the function

$$u(x) = \begin{cases} u_1(x), & x \in [0, L_1], \\ u_2(x - L_1), & x \in [L_1, L_1 + L_2]. \end{cases}$$

We know that this is a \mathcal{C}^2 function, and that this also satisfies the eigenvalue equation for λ and satisfies boundary conditions at v_2 and v_3 . Thus $u(x)$ is a solution of the new edge e and so every solution constructed from these two edges is a solution of the new edge.

We next show that we can construct a solution from one edge for these two edges. Take edge e of length $L_1 + L_2$ for arbitrary L_1 and L_2 . For some eigenvalue λ , we have some eigenfunction $u(x)$. This eigenfunction necessarily satisfies the boundary conditions at the vertices of e , which we shall call v_2 and v_3 .

Suppose we partition our solution into two parts: one interval $[0, L_1]$, and the other $[0, L_2]$.

Define $u_1(x)$ and $u_2(x)$ as

$$\begin{aligned} u_1(x) &= u(x), \quad x \in [0, L_1], \\ u_2(x) &= u(x + L_1), \quad x \in [0, L_2]. \end{aligned}$$

Since $u(x)$ is a \mathcal{C}^2 function, then it follows that $u_1(L_1) = u_2(0)$ and $u_1'(L_1) = u_2'(0)$. These are exactly the boundary conditions on two edges connected by a vertex. Thus every solution on the single edge is a solution on the two edges.

As the solution sets are identical, then it is clear then that the two subgraphs are equivalent.

□

Since these two situations are equivalent, then often it is more useful to “contract” the two edges into a single edge.

Chapter 2

Analytical Results

2.1 Elementary Results

Some of the simplest quantum graphs can be considered to be almost trivial. These graphs correspond to structures encountered in the classical theory of the Laplacian - the straight line or the circle. They are worth mentioning, however, since they illustrate some important properties for general graphs.

2.1.1 The One Dimensional Line

The simple one dimensional line - or, as some prefer, the one dimensional box - is the simplest possible quantum graph. Obviously, when viewed from the perspective of partial differential equations, this corresponds to a single interval in \mathbb{R} . On the other hand, we can also think of it as a single edge with two vertices. Such a structure is naturally quite well known and its solution is easy, for both Dirichlet and Neumann boundary conditions.



Figure 2.1: The 3-Line.

Choosing Neumann conditions, then on a domain of length L , the problem is stated thus:

$$\begin{cases} u''(x) = -\lambda u(x) & x \in (0, L), \\ u'(0) = u'(L) = 0. \end{cases} \quad (2.1)$$

The eigenvalues are of the form

$$\lambda_m = \frac{m^2\pi^2}{L^2}, \quad m = 0, 1, 2, \dots \quad (2.2)$$

The eigenfunctions are

$$u(x) = \cos\left(\frac{m\pi x}{L}\right). \quad (2.3)$$

If we were to choose Dirichlet conditions then the solutions are very similar: the eigenvalues are identical but the eigenfunctions are instead sine functions instead of cosines.

These solutions do not require the formalism of quantum graphs to find. Why mention them? The answer lies in considering a natural extension of the line: suppose we were to link several of these edges together in a chain. Now, in order to solve the problem, we need to specify vertex conditions, which we will do according to our conventions above. Then we state the problem as:

$$\begin{cases} u_i''(x) = -\lambda u_i(x), \\ u_i(x_j) = u_k(x_j), & x_j \in \mathcal{V}, \\ \sum_i \partial_n u_i(x_j) = 0, & x_j \in \mathcal{J}, \\ u_i'(x_j) = 0, & x_j \in \mathcal{F}. \end{cases} \quad (2.4)$$

Interestingly enough, we find that the solution of this problem is the same as the solution for the simple line above. This follows from Theorem 1.8. Simply stated, this means that any quantum graph formed by connecting edges together in a line is equivalent to a single line with the same endpoint conditions.

Definition 2.1. Let Γ be a quantum graph. If Γ contains n edges, then Γ is called an n -line if Γ contains 2 endpoint vertices and every non-endpoint vertex is connected to exactly 2 edges.

Corollary 2.2. Let Γ be a quantum graph. If Γ is an n -line, then Γ is equivalent to Γ' , where Γ' is a 1-line whose length is the sum of the lengths of the edges of Γ .

This has interesting implications. First, we have found, albeit trivially, all the solutions for a class of quantum graphs. (Incidentally, this does not depend on isotropy, so each edge can have arbitrary length. All that matters is the sum of the lengths.) Additionally, this indicates that the shape of this line - that is, the “angles” between adjacent edges at an interior vertex - does not change the solution. The solution to a straight line is the same as a convoluted one, provided that they are the same length.

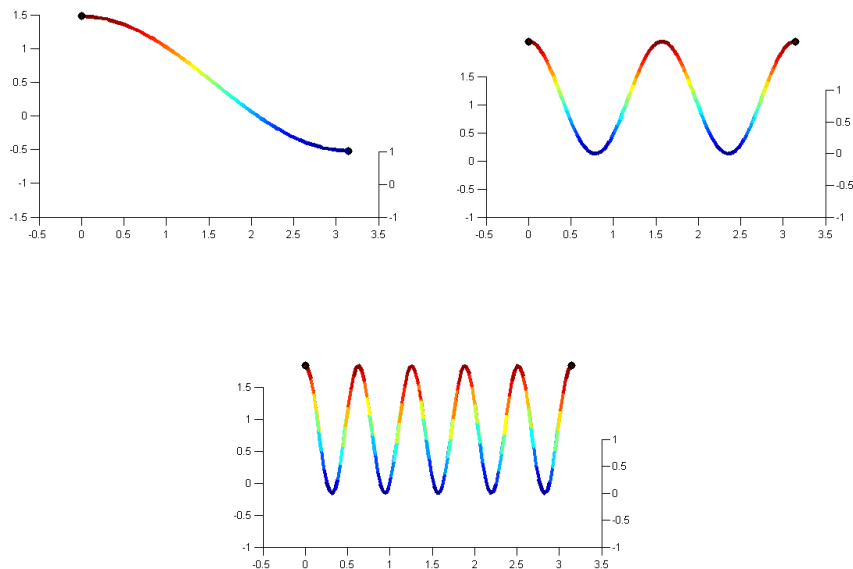


Figure 2.2: Line Solutions.

As can be seen in Figure 2.2, the solutions to the line look like freely vibrating strings; this is why Neumann conditions are sometimes called “free” conditions. On these plots,

the horizontal axis corresponds to the spatial extent of the domain: $0 < x < L$. In these plots, for convenience, we choose length $L = \pi$. (Note: in this plot, and in all subsequent plots, the solutions are represented by both height and color. This is for clarity. The color is simply a scale relative to the infimum and supremum points of the solution. This is explained further in the next chapter.)

2.1.2 The Circle

The circle is a similar problem to the one dimensional line: it can be solved without using the methods of quantum graphs. One can choose any point on the circle and choose it to be the origin; in terms of quantum graphs, this will be our vertex. The circle then is a type of self-loop, which actually introduces some interesting behavior on quantum graphs. We can more rigorously define the circle as an n -cycle, which consists of several vertices connected in a cycle. Formally we define the n -cycle thus:

Definition 2.3. Let Γ be a quantum graph. If Γ contains n vertices and every vertex is connected to exactly two edges and has no self-loops, then Γ is an n -cycle.

This figure illustrates the example of the 6-cycle, along with a direction convention. Incidentally, similar to the n -line, we can use the result of Theorem 1.8 to characterize all of the solutions of the n -cycle.

Corollary 2.4. *Let Γ be a quantum graph. If Γ is an n -cycle, then Γ is equivalent to Γ' , where Γ' is a 1-cycle whose length is the sum of the lengths of the edges of Γ .*

Thus to characterize all of the solutions of the n -cycle, one needs only to specify the length of the cycle and the solutions of the 1-cycle. The 1-cycle has a standard type of boundary conditions, called periodic boundary conditions. We can cite the solutions. The problem is stated as

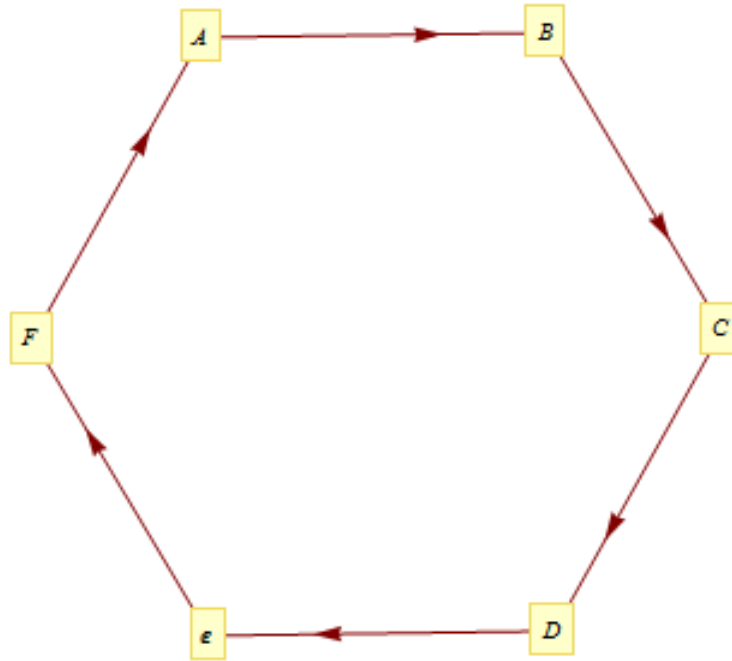


Figure 2.3: The 6-Ring.

$$\begin{cases} u''(x) = -\lambda u(x) & x \in (0, L), \\ u(0) = u(L), \\ u'(0) = u'(L). \end{cases} \quad (2.5)$$

The eigenvalues have the form

$$\lambda_m = \frac{(2m)^2 \pi^2}{L^2} : m = 0, 1, 2, \dots \quad (2.6)$$

Eigenfunction solutions can be determined by linear combinations of these two basis eigenfunctions. (The eigenspace is thus two-dimensional for each eigenvalue $\lambda_m > 0$.)

$$u(x) = \cos\left(\frac{2m\pi x}{L}\right),$$

$$u(x) = \sin\left(\frac{2m\pi x}{L}\right). \quad (2.7)$$

So again we have characterized the solutions for an entire class of quantum graphs. It should be emphasized that these solutions for both the n -line and n -cycle are true for arbitrary graphs of this form, isotropic or not. It is an interesting fact that a combinatorially nontrivial graph - let's say, a 100-cycle - has solutions completely determined from a quite simple analytic problem.

Here are some solutions plotted on the cycle. In fact, we do not even have to specify where the vertex is; the choice is arbitrary. One can impose further conditions that the solution take a certain value at the vertex, but this is not a general condition. Since the vertex condition is in essence a statement of continuity, then the circle problem can be interpreted as finding the solutions to the Laplacian that “fit” on the circle.

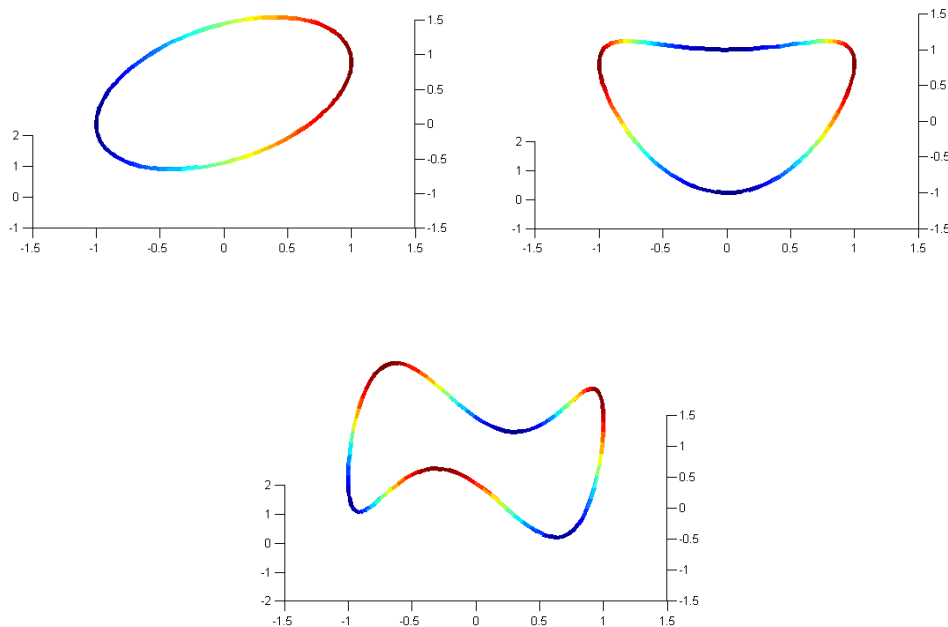


Figure 2.4: Ring Solutions.

2.2 The n -Star

Having looked at these trivial cases, we should now look at some more interesting graphs. In graph theory the idea of a star graph is one of the simpler structures. Such a graph consists of many edges only connected together at a central vertex. Of course, a picture communicates the idea much more effectively. If we have six edges, then the graph would look like

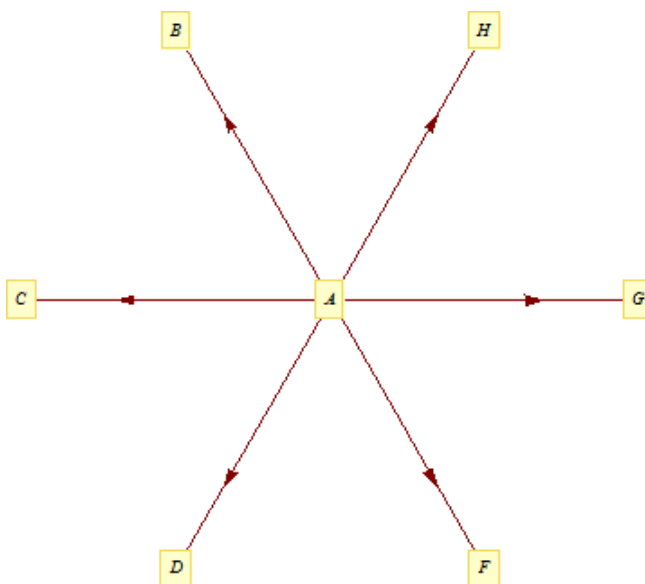


Figure 2.5: The 6-Star.

From the perspective of the quantum graph, the star provides possibly the simplest case which exhibits quantum graph behavior which is not seen elsewhere, like in the line or circle. There is only one joint vertex, and the rest of the vertices are simple endpoints with ordinary Neumann boundary conditions. When we solve an n -star, then we will only have to incorporate one vertex with the new boundary conditions. For definiteness, we should adopt a more formal definition for this type of graph.

Definition 2.5. Let Γ be a quantum graph. If Γ has n edges, then Γ is called an n -star if

each edge is connected to the same common vertex and terminates at a unique endpoint vertex, with no edge being a self loop.

As the definition suggests, the n -star represents a class of graphs; that is, there are infinitely many distinct isotropic star graphs, all of which have common structure. In fact the common characteristics between n -stars allows us to characterize the solutions for any n in a fairly compact, closed form definition.

Theorem 2.6. *Let Γ be an isotropic n -star. Then Γ has two types of eigenvalues and eigenfunctions specified by, for $m = 1, 2, 3, \dots$,*

$$\lambda = \frac{m^2\pi^2}{L^2}, \quad u_i(x) = A \cos\left(\frac{m\pi x}{L}\right);$$

$$\lambda = \frac{(m - \frac{1}{2})^2\pi^2}{L^2}, \quad u_i(x) = B_i \sin\left(\frac{(m - \frac{1}{2})\pi x}{L}\right) : \sum_{i=1}^n B_i = 0 .$$

The proof of this theorem is in Appendix A.1. Figure 2.6 shows several plotted solutions of the 6-star for comparison. In order, they correspond to eigenvalues $\lambda = \frac{\pi^2}{L^2}$, $\lambda = \frac{\pi^2}{4L^2}$, and $\lambda = \frac{16\pi^2}{L^2}$.

As stated in the theorem, the n -star has two types of eigenvalues. Their form is suggestive: the first kind, which we call *integer* eigenvalues, correspond to the fundamental cosine solutions which directly satisfy Neumann conditions in a “natural” manner. The second kind, *half-integer* eigenvalues, represent a sine solution, whose form is not the same on each edge. Indeed, there is an external condition on the coefficients: their sum must be zero. Naturally this leads to an infinitude of possible eigenfunctions for a given half-integer eigenvalue, but since we know that any linear combination of eigenfunctions is also an eigenfunction, then we can obtain a basis for the eigenfunction “space.” The size of this space depends on how many edges there are; as it turns out, for n edges, then $(n - 1)$ linearly independent basis eigenfunctions are needed to span the complete space. With this in mind, we say that the half-integer eigenvalues are $(n - 1)$ dimensional.

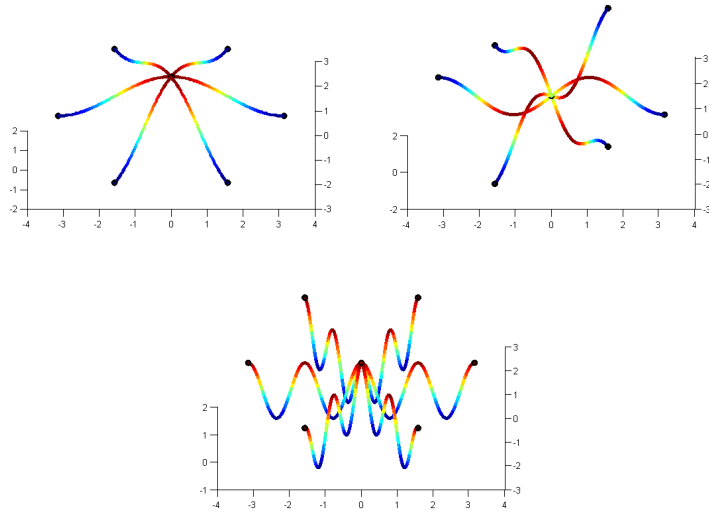


Figure 2.6: Solutions for the 6-Star.

2.3 The n -Path

Having looked at the n -star, we should search for other simple graphs. Suppose we take an n -star, and then connect every endpoint together, so that there is only two vertices in the graph. This looks like two points with n different paths between them.

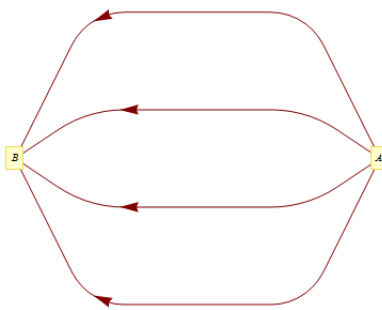


Figure 2.7: The 4-Path.

Following as before with a more formal definition, we precisely define the n -path as:

Definition 2.7. Let Γ be a quantum graph. If Γ has n edges, then Γ is called an n -path if Γ has exactly two vertices, where every edge is between those two vertices.

Unlike the star, the n -path does not have any endpoints at all. The proof of the solutions is given in Appendix A.2; as before we will cite the solutions in a theorem.

Theorem 2.8. Let Γ be an isotropic n -path. Then Γ has eigenvalues of the form $\lambda_m = \frac{m^2\pi^2}{L^2} : m = 1, 2, 3, \dots$, with eigenfunctions

$$u_i(x) = A \cos\left(\frac{m\pi x}{L}\right) + B_i \sin\left(\frac{m\pi x}{L}\right) : \sum_{i=1}^n B_i = 0.$$

Figure 2.8 shows some solutions. Now there is only one type of eigenvalue; but, we still retain a similar eigenfunction form: a one dimensional cosine solution, and an $(n - 1)$ dimensional sine solution. The eigenspace is n dimensional.

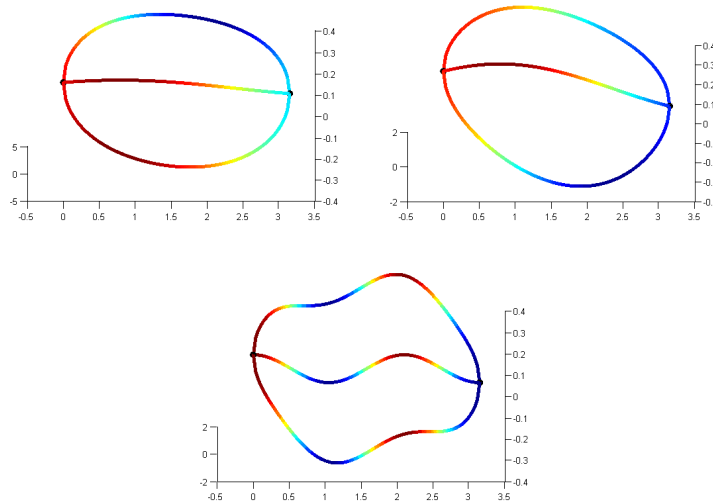


Figure 2.8: Solutions to the 3-Path.

2.4 The n -Petal

The n -petal is a departure from the previous two cases; it is the result self looping a single vertex several times. Figure 2.9 captures the idea.

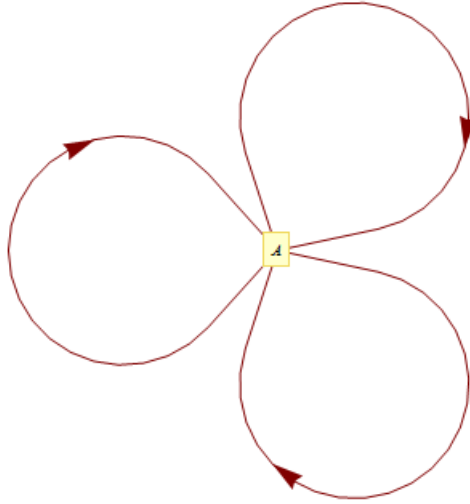


Figure 2.9: The 3-Petal.

As usual, a more precise definition is in order:

Definition 2.9. Let Γ be a quantum graph. If Γ has n edges, then Γ is called an n -petal if Γ has exactly one vertex, and every edge is a self-loop.

The self-looping complicates the problem: there is only one Kirchoff condition, but each edge contributes two terms to the sum of derivatives. We can state the solutions, derived in Appendix A.3:

Theorem 2.10. *Let Γ be an isotropic n -petal. Then for $m = 0, 1, 2, \dots$, the eigenvalues and eigenfunctions are given by*

$$\lambda = \frac{(2m)^2\pi^2}{L^2}, \quad u_i(x) = A \cos\left(\frac{2m\pi x}{L}\right); \quad (2.8)$$

$$\lambda = \frac{(2m)^2\pi^2}{L^2}, \quad u_i(x) = B_i \sin\left(\frac{2m\pi x}{L}\right) : B_i \text{ free}; \quad (2.9)$$

$$\lambda = \frac{(2m-1)^2\pi^2}{L^2}, \quad u_i(x) = B_i \sin\left(\frac{(2m-1)\pi x}{L}\right) : \sum_i B_i = 0. \quad (2.10)$$

This behavior is somewhat unusual - the unconstrained even sine solutions cancel each other out at the central vertex, leaving totally uncoupled eigenfunctions. The odd eigenvalues are $(n - 1)$ dimensional, while the even eigenvalues are $(n + 1)$ dimensional. Some solutions are given below in Figure 2.10.

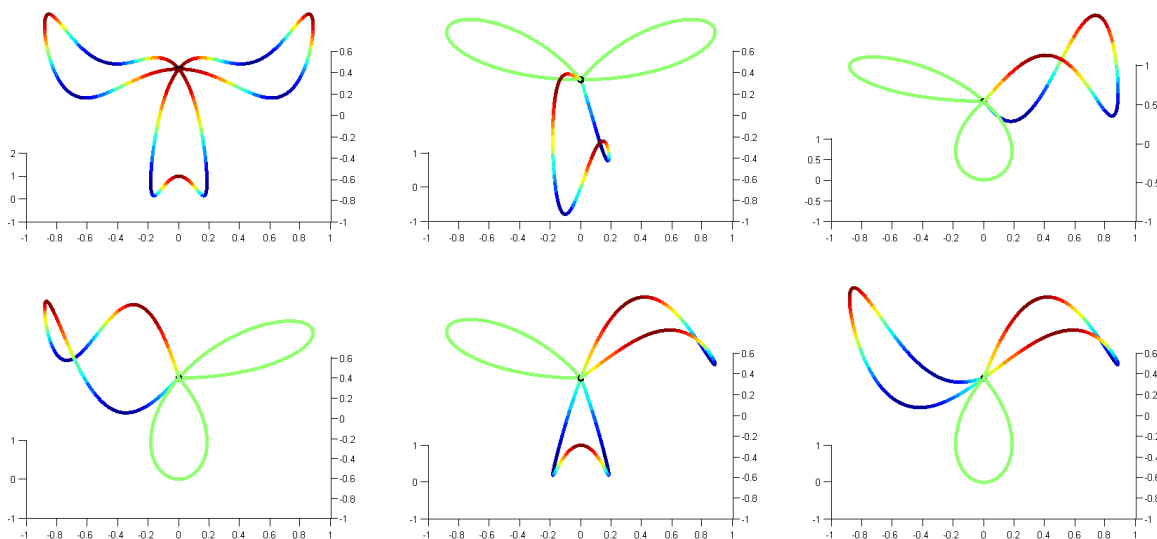


Figure 2.10: Solutions to the 3-Petal.

The six figures in Figure 2.10 are actually the simplest basis eigenfunctions for the eigenspace of the eigenvalues corresponding to $m = 2$. The strange behavior of the free sine solutions can be thought of as a “decoupling” behavior: the other edges are not affected by the solutions on a given edge, since their value vanishes at the vertex and their derivative contributions cancel each other out. Indeed, any of the sine solutions we have seen before can display decoupling behavior: an edge can be “decoupled” by

choosing zero as the coefficient on that edge and then choosing appropriate coefficients on the other edges.

2.5 Complete Quantum Graphs

Unlike the previous classes of graphs, complete quantum graphs present much more of a challenge. Part of this is due to the simplest complete quantum graphs are actually cases of other classes of quantum graphs; the first nontrivial (that is, different) complete quantum graph occurs at $n = 4$. (If $n = 1$, then the graph is a single point, and thus not interesting. For $n = 2$, the graph is the 1-line. $n = 3$ corresponds to a 3-cycle.) A more formal definition is given below.

Definition 2.11. Let Γ be a quantum graph. If Γ has n vertices, then Γ is an n -complete quantum graph if every vertex is connected to every other vertex by exactly one edge.

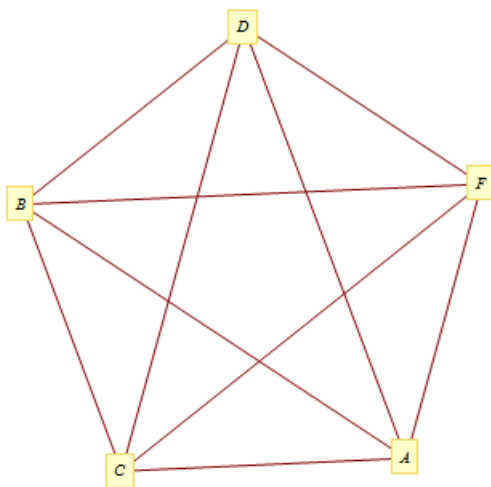


Figure 2.11: The 5-Complete Graph.

As always it is better to see an example of the graph visually. For the case $n = 5$, Figure 2.11 shows what the complete graph looks like.

In principle, finding the eigenvalues of the complete graph uses the same process as the other quantum graphs that we have looked at before. At each vertex we apply the joint and continuity boundary conditions which gives us a system of equations. However, the complete graph contains far more equations than the previous cases. Rather than solving it by hand it is useful to use a computer algebra system such as **Mathematica** to assist our computation of the results.

To find the spectrum of the complete graph, we should label each vertex and then determine the equations that follow from the boundary conditions. As with all of our quantum graphs, we look for solutions of the form $a_i \cos(kx) + b_i \sin(kx)$, which gives two constants for each edge. Since the degree of each vertex of a complete graph is the same and there is identical structure everywhere, there is not a natural labeling or direction convention which makes computation easier.

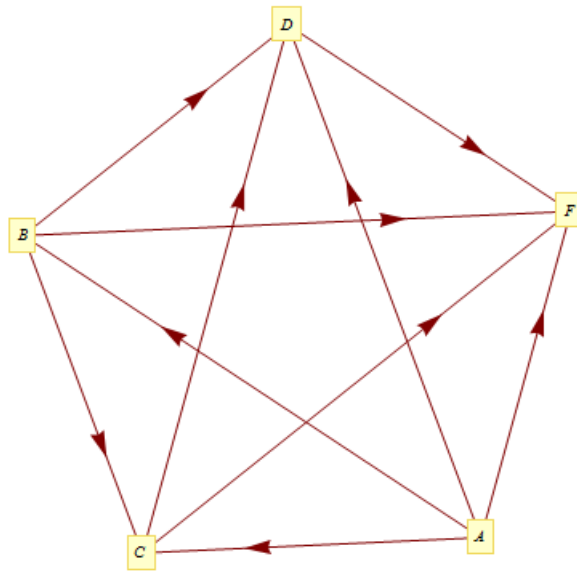


Figure 2.12: The 5-Complete Graph, with Direction and Labeling Conventions.

We introduce a type of ordering on our vertex labeling through alphabetical order.

That is, vertex A is “greater” than vertex B or C , and in that sense the edge connecting them has the direction such that 0 is located at vertex A and L is located at vertex B or C . Similarly, we number the edges starting from A to B , then A to C , and so on until all other vertices have been connected to A ; then the numbering continues from B to C , B to D , and so on. If we use the directed graph as the ordering, then the Figure 2.12 describes this convention for $n = 5$.

With a well-defined convention it is easier to program our equations into **Mathematica** consistently. As a system of equations determined by boundary conditions, the natural method of solution is to put the coefficients into a matrix form. A simple result from graph theory states that the number of edges in a graph with n vertices is given by $\frac{n(n-1)}{2}$. Conveniently, since there are two distinct coefficients per edge, then the number of distinct coefficients is $n(n-1)$. We should now examine the number of equations that the boundary conditions give us for each edge.

There are $(n-1)$ edges connected to each vertex. For continuity, we get equality between any two of the edges at the vertex. But one of these equalities is superfluous since equality is transitive. So, continuity contributes $n(n-2)$ equations to the system. On the other hand the Kirchoff boundary conditions at each vertex contributes exactly one equation, so Kirchoff conditions contributes n equations. In the complete graph there are no endpoints, so the total number of equations is exactly $n(n-1)$. This is precisely the number of coefficients. Thus the matrix of the system is square for any n -complete graph $((n^2 - n) \times (n^2 - n))$.

When determining the equations, we choose them such that they equal zero. Putting the equations into matrix form, then our system is now of the form

$$\mathbf{Ax} = 0, \tag{2.11}$$

where \mathbf{A} is the matrix of the system and \mathbf{x} is the vector of coefficients. An example matrix is given in Appendix C. To avoid the trivial solution where every coefficient is

zero, then the matrix \mathbf{A} must be singular, and thus its determinant should be zero. Since our equations will have terms involving $\cos(kL)$ and $\sin(kL)$, so requiring $\det \mathbf{A}$ to vanish will restrict the values of k and determine the eigenvalues of the graph. This makes this equation the characteristic equation of the complete quantum graph.

As an example, we can use the $n = 5$ complete quantum graph. When we compute the determinant of the matrix in **Mathematica**, we obtain a characteristic equation for $n = 5$, given by

$$256k^5 \cos^5\left(\frac{kL}{2}\right) (1 + 4 \cos(kL))^4 \sin^7\left(\frac{kL}{2}\right) = 0. \quad (2.12)$$

This equation gives us the quantization conditions for the eigenvalues: any λ which satisfies this expression is an eigenvalue. The sine and cosine terms give us regular integer eigenvalues, and the k terms zero eigenvalues; but the interesting term is the $(1 + 4 \cos(kL))^4$ term. This will give eigenvalues of the form

$$\lambda_m = \frac{(\pm \arccos(-\frac{1}{4}) + 2m\pi)^2}{L^2} : m = 0, 1, 2, \dots \quad (2.13)$$

These eigenvalues are, in a sense, “split” as there are two eigenvalues associated with each n . As this behavior is not seen in the other quantum graphs we have studied, then its appearance suggests that the highly connected nature of the complete graph has given rise to some strange behavior.

For comparison, lets look at the 4-complete graph. The characteristic equation is

$$24k^4 \cos^2\left(\frac{kL}{2}\right) (1 + 3 \cos(kL))^3 \sin^4\left(\frac{kL}{2}\right) = 0. \quad (2.14)$$

As before, the split eigenvalues return. They are of the form

$$\lambda_m = \frac{(\pm \arccos(-\frac{1}{3}) + 2m\pi)^2}{L^2} : m = 0, 1, 2, \dots \quad (2.15)$$

The first split eigenvalue, for $n = 0$, is actually just a single eigenvalue, since we obtain the same spectrum for both $\frac{(\pm \arccos(-\frac{1}{3}))^2}{L^2}$. However, for positive m , we find

two different eigenvalues, each with a different eigenfunction solution. Upon solution we find three linearly independent eigenfunctions. The solutions display interesting behavior: each eigenfunction corresponds to a different number of vertices being the same value. One eigenfunction has three vertices at the same value; another, two; and finally no vertices the same. These three solutions are shown in Figure 2.13.

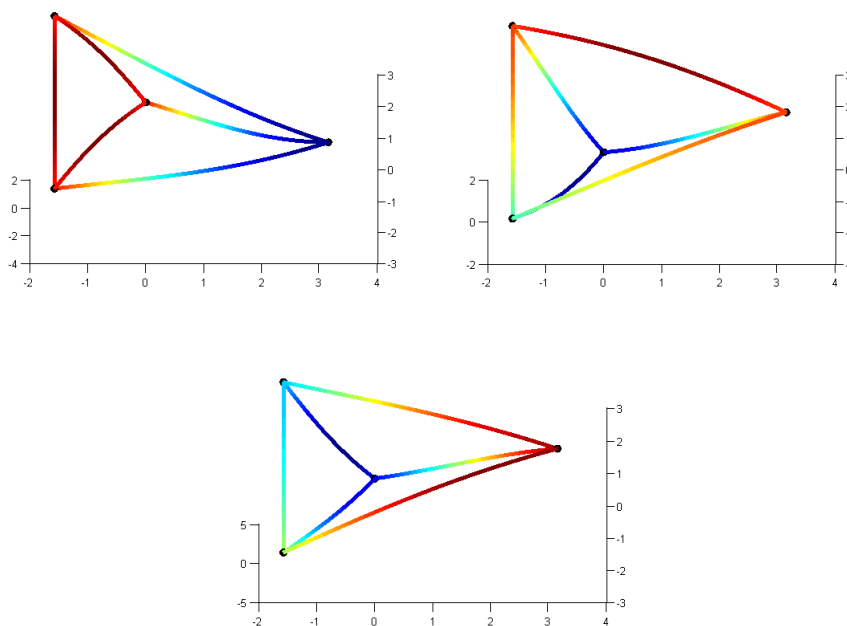


Figure 2.13: Solutions to the 4-Complete graph.

Obtaining the general form for all solutions to the complete graph for $n \geq 6$ remains an open problem, as their solution is dependent on the determinants of large matrices, even for small n . It is not clear whether other eigenvalues types will appear with even greater connectedness of high- n complete graphs. However, we can safely rest knowing that these eigenvalues do not appear in our previous cases; in fact, this method does indeed verify that the eigenvalues we found were all that exist for the star, path, and petal. While we cannot give a complete solution, we can formally state a theorem about the eigenvalues of these two complete graphs. (To determine the eigenfunctions for these

graphs, we simply substitute $k = \sqrt{\lambda}$ for the appropriate eigenvalue and then compute the null space. This will give the linearly independent eigenfunctions for that eigenvalue.)

Theorem 2.12. *Let Γ be an n -complete quantum graph. If $n = 4$ or $n = 5$, then the spectrum of Γ is given by the union of the sets $\Lambda_0 = \left\{ \frac{m^2 \pi^2}{L^2} : m \in \mathbb{N} \cup \{0\} \right\}$ and $\Xi_n = \left\{ \frac{(\pm \arccos(-\frac{1}{n}) + 2m\pi)^2}{L^2} : m \in \mathbb{N} \cup \{0\} \right\}$.*

The proof of this theorem is trivial, with most of the work already having been done above. One might ask why these types of eigenvalues occur. The answer may be that this type of eigenvalue is the result of a nontrivial emergent pattern that arises due to the highly connected nature of the complete graph. Suppose that you choose one vertex on the n -complete graph as the “center.” Fix the value at the vertex to be unity, and the eigenfunctions on every edge connected to the center can be $\cos(kx)$; this satisfies continuity and Kirchoff conditions. This resembles an $(n-1)$ -star, but the endpoints now have nontrivial connectedness.

Now let the edge space of the vertices not connected to the center be $(-\frac{L}{2}, \frac{L}{2})$ instead of $(0, L)$; this is convenient because the cosine is even. Considering these edges, choosing the eigenfunctions to be $A \cos(kx)$ will also satisfy Kirchoff and continuity conditions. Then the equations at each non-center vertex are

$$\cos(kL) = A \cos\left(\frac{kL}{2}\right), \quad (2.16)$$

$$\sin(kL) + (n-2)A \sin\left(\frac{kL}{2}\right) = 0. \quad (2.17)$$

Eliminating A and utilizing half-angle formulae, one arrives at

$$1 + (n-1) \cos(kL) = 0. \quad (2.18)$$

This is a quantization condition giving us the eigenvalues we have seen before. The eigenvalues should have a multiplicity of $n-1$, since we can choose any vertex to be the

center but one case is not independent of the others. It is likely that with higher n , more nontrivial eigenvalues will emerge - multiple centers or even other phenomena. This is not a complete proof, but motivates a conjecture.

Conjecture 2.13. *Let Γ be an n -complete quantum graph. For some $n \geq 6$, then the spectrum of Γ contains eigenvalues not in the sets*

$$\Xi_n = \left\{ \frac{(\pm \arccos(-\frac{1}{n}) + 2m\pi)^2}{L^2} : m \in \mathbb{N} \cup \{0\} \right\} \text{ and } \Lambda_0 = \left\{ \frac{m^2\pi^2}{L^2} : m \in \mathbb{N} \cup \{0\} \right\}.$$

Chapter 3

Numerical Simulation and Applications

3.1 Tools for Visualization

When working with quantum graphs it helps to have a tool to visualize your results. Doing so is relatively straightforward if one knows the solutions; then it is a matter of simply specifying the solution and translating it to a graphical form. This was accomplished using the software package `Matlab`. `Matlab` contains a number of useful plotting tools that allow the user to create both three dimensional and color-scaled plots.

The general form of the algorithm consisted of three stages. The first is specifying the (x, y) coordinates of the graph itself, which is naturally unique to each individual graph. The second stage is the calculation of the quantum graph solution, which is represented as the z component of the three coordinate vector specifying each point on our graph. These are then plotted in the third stage. Each of these parts of the code are explained in further detail below.

3.1.1 Specifying the Graph

Determining the shape is primarily dictated by convenience or aesthetics. Every edge does not have to be straight, or any shape in general, as we showed earlier. It does not change the solution, only the way the solution looks. Provided that the edges and vertices have the requisite connectedness, any choice of the shape will be correct. With this in mind, we simply need to decide what curves to use and describe them in the (x, y) plane.

For example, for the n -star, we can choose the origin as the central vertex. For n vertices, we can choose to make the graph have equal angles between every edge. From here it is a simple problem in trigonometry: with specified lengths and specified angles, it is a simple matter to determine the x and y positions for each point.

The n -path offers a somewhat more challenging problem, but by no means a hard one. We pick two points to be the vertices. The goal is now to draw n edges between these points. We can draw one edge straight between them and then use the top and bottom halves of successively wider ellipses to get as many edges as we want. Simply taking the x coordinate as the same, we use a simple elliptic equation to determine y for each edge. Obviously here the edges will not be the same length, but linearly spacing the number of points the same achieves the same goal.

The n -petal can be drawn using rose graphs in polar coordinates. One can simply calculate the (r, θ) coordinates and use the native `Matlab` method `pol2cart` which will convert polar coordinates directly to cartesian ones. This is obviously quite useful, and simple knowledge of polar functions will allow you to determine what part of the graph corresponds to each edge.

Finally, we should consider how to plot the complete graphs. There is only one case where it is easy to represent the graph, and that is for $n = 4$. Otherwise the graphs will cross and this method does not offer a good representation. To achieve this we simply use the method to get a 3-star, and then draw 3 more edges connecting the endpoints together. The edges are, again, not the same length, but this is sufficient for plotting

purposes provided one uses the same number of points per edge.

The above simply specifies the graph shape in two dimensions, not the actual solutions. Once we have this (x, y) projection, we can simply let the z coordinate, or height, be the value of the solution at that point. The form of the solution on each edge can be referenced from the solutions we have calculated. With this in mind, we can calculate the solution and store it with the position of the graph as a point with coordinates (x, y, z) . It is important to remember what edges correspond to each solution, since the order of the solutions in the code is not necessarily the order of the solutions calculated analytically.

3.1.2 Plotting Tools

With our set of solution points, we need only to plot them and our graphical representation is complete. We can use native Matlab methods to plot the points, but this is difficult to visualize as it is only one color and is difficult to differentiate between height. Instead, we used the `clinep` method freely available on the Mathworks website to plot our solutions. This method will take a set of three dimensional points and plot them in three dimensions with a color scale corresponding to the height. This code is attributed to Daniel Ennis¹. The documentation can explain the use of the various parameters, which are used to specify the color scale.

It is also useful to emphasize the positions of the vertices. We can plot a black circle at the vertex to represent where the vertex is. Keep in mind that the (x, y) position of the vertex is fixed, but its height is not, since they are “free” to move. Simply calculate what the value of the vertex is for that specific solution and plot the point using the native `plot3` method, using whatever shape and color you desire.

As an example of these methods, we include a script which plots a solution of the 4-complete graph. This can be found in Appendix B.1.

¹This code can be found, with documentation, at <http://www.mathworks.com/matlabcentral/fileexchange/8597-plot-3d-color-line/content/clinep.m>

3.1.3 Animation

Animation represents a slightly more challenging problem than representing a still image of a quantum graph. The essential principle behind creating an animation in `Matlab` is to make a series of frames, each of which is a stored image. To animate a quantum graph, we need a time dependence; we chose the simplest solution where on each edge the time dependence is sinusoidal and the same on each edge. Dividing up a time interval into the number of frames, we calculate the time dependence at each frame, use this as a coefficient on each solution for eigenfunctions, and generate a new plot for each frame.

Unfortunately, generating this animation is not as simple in the implementation phase. After much trial and error we succeeded both holding the image at the same position in the frame for all the frame and also successfully clearing the frame of the previous plot. Once this was done it was a relatively simple matter to generate the movie. The actual script implementation of this animation is given in Appendix B.2.

3.2 Computer Algebra

We used the computer algebra package `Mathematica` for large symbolic calculations. We originally developed these scripts when we were confronted with the large complex systems that even the simplest complete graphs generate. However, the algorithm can indeed be applied to any of our quantum graphs, which can be used to check results.

Our code is structured as follows. For each edge we introduce a solution; this solution has two undetermined constants. Then we specify the equations which are determined from the vertex conditions unique to the problem. This consists of continuity equations and Kirchoff conditions. Each edge contributes exactly one Kirchoff equation and $n - 2$ independent continuity equations. We arrange the equations in terms of the undetermined coefficients and arrange them such that they are equal to zero. We then place these in a

matrix and compute the determinant. This will give an expression for the determinant in terms of trigonometric functions of kL . Since this determinant must be zero if there is a nontrivial solution, equating this equation with zero gives us a quantization condition. All possibilities for k give the possible eigenvalues. Once the eigenvalues are determined, we can substitute this value for k into the matrix and compute its null space. This will give the vectors of coefficients corresponding to the independent eigenfunction solutions corresponding to this eigenvalue.

In addition to the algebraic methods, **Mathematica** contains powerful graph visualization tools, which we used to generate images of the graphs. An example of **Mathematica** code is given in Appendix C.

Chapter 4

Conclusion

We began our inquiry with the goal of specificity. Ultimately we wanted to determine the actual dynamics of quantum graphs - that is, what solutions look like and how they depend on graphical structure. To accomplish this we made several crucial assumptions. Rather than consider general operators, we only worked with the Laplacian. Rather than arbitrary graphs, we restricted our study to specific classes of isotropic graphs. Rather than consider all allowed varieties of joint boundary conditions, we used only Kirchoff joints. While these assumptions restrict our results, they also liberate us from the harsh restrictions of generality. In doing this, we were able to proceed to direct proofs and problem solving.

From this concrete foundation we were then able to obtain concrete results. We demonstrated several useful properties of all types of isotropic Laplacian quantum graphs, several of which are analogous to other classical results in applied analysis. We were able to determine complete solutions for several classes of isotropic graphs, each of which has an infinite number of permutations. Our study of the complete graph yielded results of a form unique to the combinatorial structure of graphs. In finding these solutions we have developed a general problem solving method and computational techniques for calculating results and displaying solutions.

As is traditional in research, we conclude by looking to the future. Our results are a good foundation for numerous lines of further inquiry. Along our current path, we have not yet characterized all different types of eigenvalues of complete graphs. Given our labeling and direction conventions, it is conceivable that we develop an inductive method for specifying the coefficient matrix for a complete graph. Using techniques from linear algebra involving block matrices, it might be possible to determine the form of the determinant for a complete graph with n vertices. This would allow us to determine all types of eigenvalues for complete graphs.

Another possibility is the possibility of common solutions to all Laplacian quantum graphs, regardless of class. Every class we investigated contains as eigenfunctions cosine solutions, including multigraphs (the n -path), self-looping graphs (the n -star), and highly connected graphs (the n -complete graph). We already proved that constant solutions always exist for any quantum graph; the cosine solutions could also be a “trivial” case in that regard.

We could also look at relaxing the requirement of isotropy on the graphs. It might be possible to determine the eigenfunctions of anisotropic graphs from the form of the isotropic forms, which contain the important algebraic structure. It is not possible to simply dilate the edge solutions, since the derivative conditions will fail. However, in certain circumstances, it might be possible to determine solutions - perhaps if the edge lengths are integer multiples of each other.

Given that we have been working with the Laplacian, it should be possible to determine solutions to certain applied problems - such as diffusion or waves - on the graph. Whether such a model on graphs accurately reflects physical structures, such as thin wires, is contingent on whether the solution of “fat” graphs converges to the one-dimensional quantum graph solutions. If this convergence occurs, then several classical applied problems could be applied to these results. Alternatively, nonhomogeneous boundary conditions on the vertices are also potentially interesting.

4.1 Acknowledgements

It goes without saying that my research and results would not have been possible without the extensive support provided to me. I would like to thank the Computational Training for Undergraduates in the Mathematical Sciences (CSUMS) program (NSF-DMS 0703532) for supporting my work during the spring and summer of 2011. I would like to thank the Department of Mathematics at the College of William and Mary for providing me with the resources I needed for my research. I would especially like to thank my advisors, Professor Junping Shi and Professor Daniel Vasiliu, for providing me with expert mentorship and contributing so much to this project. I could not have asked for better advisors and look forward to working with them in the future.

Appendix A

General Solutions

A.1 n -Star

The n -star problem can be stated thus:

$$\left\{ \begin{array}{l} u_i''(x) = -\lambda u_i(x), \\ u_1(0) = u_2(0) = \dots = u_n(0), \\ \partial_n u_1(L) = \partial_n u_2(L) = \dots = \partial_n u_n(L) = 0, \\ \sum_{i=1}^n \partial_n u_i(0) = 0, \end{array} \right. \quad (\text{A.1})$$

Again we look for solutions of the form

$$u_i(x) = A_i \cos(kx) + B_i \sin(kx), \quad (\text{A.2})$$

$$u_i'(x) = -A_i k \sin(kx) + B_i k \cos(kx). \quad (\text{A.3})$$

Applying our first boundary condition, we find

$$u_i(0) = A_i \cos(0) + B_i \sin(0) = A_i. \quad (\text{A.4})$$

Equating them according to the condition, we find

$$A_1 = A_2 = \dots = A_n = A. \quad (\text{A.5})$$

Dropping the subscripts in favor of a general A , we next apply the second condition:

$$u'(L) = -Ak \sin(kL) + B_i k \cos(kL) = 0. \quad (\text{A.6})$$

We now consider cases of $\sin(kL)$.

Case 1: $\sin(kL) \neq 0$.

Then this condition (after dividing off the k) becomes

$$A \sin(kL) = B_i \cos(kL). \quad (\text{A.7})$$

This itself is split into cases based on the value of $\cos(kL)$.

Case 1a. $\cos(kL) \neq 0$.

Then we can divide by $\cos(kL)$, yielding

$$B_i = A \frac{\sin(kL)}{\cos(kL)}. \quad (\text{A.8})$$

Since this is true for all B_i , we drop the subscript. We next apply the third condition, obtaining

$$\sum_{i=1}^n B_i k = 0. \quad (\text{A.9})$$

Dividing off the k and noting the summation simply yields a multiplication by n , we find that B must be zero. This can be applied to our equation for B , and noting that neither $\sin(kL)$ nor $\cos(kL)$ can be zero, this implies that A is also zero. Hence, for this case there is only the trivial solution.

Case 1b: $\cos(kL) = 0$.

Then we find that

$$A \sin(kL) = 0. \quad (\text{A.10})$$

Since $\sin(kL) \neq 0$, this implies that A must be zero. Considering the last condition, we obtain that

$$\sum_{i=1}^n B_i k = 0. \quad (\text{A.11})$$

Dividing off the k , we find a constraint on our choice of B_i . Solutions for this case are then $u_i(x) = B_i \sin(kx)$, with half-integer eigenvalues.

Case 2: $\sin(kL) = 0$.

Then we obtain

$$B_i \cos(kL) = 0. \quad (\text{A.12})$$

Since $\cos(kL) \neq 0$ if $\sin(kL) = 0$, this implies that all $B_i = 0$. Applying our next condition, we find that

$$\sum_{i=1}^n -Ak \sin(0) = 0. \quad (\text{A.13})$$

This is true trivially. Thus, for this case we obtain integer eigenvalues with $A \cos(kx)$ solutions.

Having considered all cases, we have the following results. There are two types of eigenvalues, with corresponding solutions.

$$\lambda = \frac{m^2 \pi^2}{L^2}, \quad u_i(x) = A \cos\left(\frac{m\pi x}{L}\right) \quad (\text{A.14})$$

$$\lambda = \frac{(m - \frac{1}{2})^2 \pi^2}{L^2}, \quad u_i(x) = B_i \sin\left(\frac{(m - \frac{1}{2})\pi x}{L}\right) : \sum_{i=1}^n B_i = 0. \quad (\text{A.15})$$

A.2 n -Path

The n -path problem can be stated thus:

$$\left\{ \begin{array}{l} u_i''(x) = -\lambda u_i(x), \\ u_1(0) = u_2(0) = \dots = u_n(0), \\ u_1(L) = u_2(L) = \dots = u_n(L), \\ \sum_{i=1}^n \partial_n u_i(0) = 0, \\ \sum_{i=1}^n \partial_n u_i(L) = 0. \end{array} \right. \quad (\text{A.16})$$

Again, as we are solving the Laplacian on one dimensional edges, we look for solutions of the form

$$u_i(x) = A_i \cos(kx) + B_i \sin(kx), \quad (\text{A.17})$$

$$u_i'(x) = -A_i k \sin(kx) + B_i k \cos(kx). \quad (\text{A.18})$$

Applying the first condition, we obtain

$$u_i(0) = A_i \cos(0) + B_i \sin(0) = A_i. \quad (\text{A.19})$$

Equating them, we obtain

$$A_1 = A_2 = \dots = A_n = A. \quad (\text{A.20})$$

We drop the subscripts. Next, we apply the second condition.

$$u_i(L) = A \cos(kL) + B_i \sin(kL). \quad (\text{A.21})$$

Equating them, the $A \cos(kL)$ terms cancel, leaving

$$B_1 \sin(kL) = B_2 \sin(kL) = \dots = B_n \sin(kL). \quad (\text{A.22})$$

Again, at this point, we must split up our treatment into cases based on whether $\sin(kL) = 0$.

Case 1. $\sin(kL) \neq 0$.

Then we can divide $\sin(kL)$ off to obtain

$$B_1 = B_2 = \dots = B_n = B. \quad (\text{A.23})$$

Again, we drop the subscripts. Applying the third constraint, we have that

$$\sum_{i=1}^n Bk = 0. \quad (\text{A.24})$$

Dividing the k off, and noting that the summation simply multiplies by n , we find that $B = 0$. Applying the next condition,

$$\sum_{i=1}^n -Ak \sin(kL) = 0. \quad (\text{A.25})$$

Dividing by $-Ak$, we find that

$$\sum_{i=1}^n \sin(kL) = 0. \quad (\text{A.26})$$

Since $\sin(kL)$ is single valued, then this indicates that $\sin(kL) = 0$, which is a contradiction.

Case 2. $\sin(kL) = 0$.

Then of course the second constraint is trivial, so we move on to the third constraint.

$$\sum_{i=1}^n B_i k = 0. \quad (\text{A.27})$$

Dividing off the k , we find that this gives us the condition

$$\sum_i B_i = 0. \quad (\text{A.28})$$

Next considering the final condition, we find that

$$\sum_{i=1}^n -Ak \sin(kL) + B_i k \cos(kL) = 0. \quad (\text{A.29})$$

Again dividing off k , noting that $\sin(kL)$ is zero, and dividing off the $\cos(kL)$ term (which is not zero since $\sin(kL) = 0$), we find the equivalent condition

$$\sum_i B_i = 0. \quad (\text{A.30})$$

Having considered all cases, we find the following results. There are two types of solutions associated with the integer eigenvalues.

$$\lambda = \frac{m^2 \pi^2}{L^2}, \quad u_i(x) = A \cos\left(\frac{m\pi x}{L}\right); \quad (\text{A.31})$$

$$\lambda = \frac{m^2 \pi^2}{L^2}, \quad u_i(x) = B_i \sin\left(\frac{m\pi x}{L}\right) : \sum_{i=1}^n B_i = 0. \quad (\text{A.32})$$

A.3 n -Petal

The n -petal problem can be stated thus:

$$\left\{ \begin{array}{l} u_i''(x) = -\lambda u_i(x), \\ u_1(0) = u_2(0) = \dots = u_n(0), \\ u_1(L) = u_2(L) = \dots = u_n(L), \\ u_i(0) = u_i(L), \\ \sum_{i=1}^n \partial_n u_i(0) + \partial_n u_i(L) = 0. \end{array} \right. \quad (\text{A.33})$$

We must choose a definite direction convention in specifying this problem. We define the point 0 at the beginning of the loop and L at the end of the loop; while these points are technically the same, we choose the direction of positive flow to be out from the zero point and in from the L point. This gives rise to the sign in the summation in the last constraint.

As we are solving the Laplacian on one dimensional edges, we look for solutions of the form

$$u_i(x) = A_i \cos(kx) + B_i \sin(kx), \quad (\text{A.34})$$

$$u_i'(x) = -A_i k \sin(kx) + B_i k \cos(kx). \quad (\text{A.35})$$

If we utilize the first constraint, we evaluate each part of the solution at zero. Then we have

$$u_i(0) = A_i \cos(0) + B_i \sin(0) = A_i. \quad (\text{A.36})$$

Equating them all, we have that

$$A_1 = A_2 = \dots = A_n = A. \quad (\text{A.37})$$

Dropping the subscripts, we know that the coefficients of the cosines in the solutions are all the same.

Next we consider the second constraint.

$$u_i(L) = A \cos(kL) + B_i \sin(kL). \quad (\text{A.38})$$

Again equating them all, we find that the $A \cos(kL)$ terms cancel out, leaving

$$B_1 \sin(kL) = B_2 \sin(kL) = \dots = B_n \sin(kL). \quad (\text{A.39})$$

We now must split our treatment into two cases, based on if $\sin(kL) = 0$.

Case 1. $\sin(kL) \neq 0$.

In this case, we can divide off $\sin(kL)$ and obtain that

$$B_1 = B_2 = \dots = B_n = B. \quad (\text{A.40})$$

We again drop the subscripts of the constant. Next we consider the third constraint.

$$\begin{aligned} A &= A \cos(kL) + B \sin(kL), \\ A(1 - \cos(kL)) &= B \sin(kL). \end{aligned} \quad (\text{A.41})$$

Next, we consider the final constraint.

$$\sum_{i=1}^n k(B + A \sin(kL) - B \cos(kL)) = 0. \quad (\text{A.42})$$

The summation simply yields a multiplication by n ; dividing nk off the result, we are left with

$$B(1 - \cos(kL)) + A \sin(kL) = 0. \quad (\text{A.43})$$

This gives us these conditions:

$$\begin{aligned} A(1 - \cos(kL)) &= B \sin(kL) \\ B(1 - \cos(kL)) &= -A \sin(kL) \end{aligned} \quad (\text{A.44})$$

We obtain two possible solutions. Either $A = B = 0$, and $kL = \pi + 2\pi m$, or $kL = 2\pi m$, for $m \in \mathbb{Z}$. However, the second case is not possible, since $\sin(2\pi n) = 0$, which is specifically forbidden in this case. Thus, the only solution for case 1 is $u_i(x) = 0$.

Case 2. $\sin(kL) = 0$.

In this case the second condition is trivial. However we do know that $kL = m\pi$ for $m \in \mathbb{Z}$. The third condition gives us

$$A = A \cos(kL) + B_i \sin(kL). \quad (\text{A.45})$$

Since $\sin(kL) = 0$, this means that $A = A \cos(kL)$. We now have to split into two more cases, depending on if $\cos(kL) = 1$.

Case 2a. $\cos(kL) = 1$.

This restricts our values of m to only even integers; that is, $kL = 2m\pi$. Finally we consider the final constraint.

$$\sum_{i=1}^n k(B_i + A \sin(kL) - B_i \cos(kL)) = 0. \quad (\text{A.46})$$

Since $\sin(kL) = 0$, and since we can divide off the k , this reduces to

$$\sum_{i=1}^n B_i(1 - \cos(kL)) = 0. \quad (\text{A.47})$$

However, $\cos(kL) = 1$, so this is trivial, leaving the B_i free; the coefficient on the sine part of the solution is free to be any constant, and can be a different constant on each edge. There are then two solution parts: one corresponding to all $B_i = 0$, leaving the cosine terms; and one corresponding to $A = 0$, leaving the sine terms.

We now consider continuity at the vertex: for the sine solutions, since $\sin(kL) = 0$, then no matter what choice of B_i continuity will be satisfied. The cosine solutions also

pass this test.

Case 2b. $\cos(kL) = -1$.

This forces our coefficient A to be zero. Applying the last constraint, we have

$$\sum_{i=1}^n k(B_i - B_i \cos(kL)) = 0. \quad (\text{A.48})$$

Dividing the k off, and noting that $\cos(kL) = -1$, we have that

$$\sum_{i=1}^n 2B_i = 0. \quad (\text{A.49})$$

This finally reduces to

$$\sum_{i=1}^n B_i = 0. \quad (\text{A.50})$$

This imposes on the B_i coefficients a constraint, which is notably absent from the previous case.

After considering all cases, we have the following results. There are two types of eigenfunctions associated with even eigenvalues and one type of solution associated with odd eigenvalues:

$$\lambda = \frac{(2m)^2 \pi^2}{L^2}, \quad u_i(x) = A \cos\left(\frac{2m\pi x}{L}\right); \quad (\text{A.51})$$

$$\lambda = \frac{(2m)^2 \pi^2}{L^2}, \quad u_i(x) = B_i \sin\left(\frac{2m\pi x}{L}\right) : B_i \text{ free}; \quad (\text{A.52})$$

$$\lambda = \frac{(2m-1)^2 \pi^2}{L^2}, \quad u_i(x) = B_i \sin\left(\frac{(2m-1)\pi x}{L}\right) : \sum_i B_i = 0. \quad (\text{A.53})$$

Appendix B

Matlab Code

We include two Matlab scripts as examples of the method of visualization described in 3.1. The first is a 4-complete graph plot and the second is an animation of a simple wave solution on a 6-star.

B.1 4-Complete Graph

```
\begin{sf}  
% Author: Patrick King, Date: 4/9/2012  
% This script plots one solution to a 4-complete quantum  
% graph, corresponding to an eigenvalue of  
%  $(\arcsin(-1/4))^2/L^2$ .  
  
% This is the reference variable used in calculating the  
% solution value. Every edge has 100 points.  
x = linspace(0,pi,100);  
  
% Control the value of  $k = \sqrt{\lambda}$ , where  $\lambda$  is  
% the eigenvalue.
```

```

k = (acos(-1/3))/pi;

% Calculation of each of the 100 points on each edge. The
% x and y coordinates are the graph coordinates and the
% z is the graph solution.
x1 = linspace(0,pi,100);
y1 = linspace(0,0,100);
z1 = (-5/(3*sqrt(2)))*cos(k*x) + (1/3)*sin(k*x);

x2 = linspace(0,-pi/2,100);
y2 = linspace(0,sqrt(3)*pi/2,100);
z2 = (-5/(3*sqrt(2)))*cos(k*x) + (1/3)*sin(k*x);

x3 = linspace(0,-pi/2,100);
y3 = linspace(0,-sqrt(3)*pi/2,100);
z3 = (-5/(3*sqrt(2)))*cos(k*x) - (2/3)*sin(k*x);

x4 = linspace(pi,-pi/2,100);
y4 = linspace(0,sqrt(3)*pi/2,100);
z4 = 1/sqrt(2)*cos(k*x)+ sin(k*x);

x5 = linspace(pi,-pi/2,100);
y5 = linspace(0,-sqrt(3)*pi/2,100);
z5 = 1/sqrt(2)*cos(k*x);

x6 = linspace(-pi/2,-pi/2,100);
y6 = linspace(sqrt(3)*pi/2,-sqrt(3)*pi/2,100);
z6 = 1/sqrt(2)*cos(k*x);

```

```

% Parameter for clinep
W = 3;

% plotted on the same image
hold on;

% color plot of the solution sets
clinep(x1,y1,z1,z1,W);
clinep(x2,y2,z2,z2,W);
clinep(x3,y3,z3,z3,W);
clinep(x4,y4,z4,z4,W);
clinep(x5,y5,z5,z5,W);
clinep(x6,y6,z6,z6,W);

% vertex plots
plot3(0,0,-5/(sqrt(2)*3),'k.','MarkerSize',25.0);
plot3(pi,0,1/sqrt(2),'k.','MarkerSize',25.0);
plot3(-pi/2,sqrt(3)*pi/2,1/sqrt(2),'k.','MarkerSize',25.0);
plot3(-pi/2,-sqrt(3)*pi/2,1,'k.','MarkerSize',25.0);
\end{sf}

```

B.2 6-Star Animation

```

% Author: Patrick King, Date: 4/9/2012
% Generates an animation of a simple wave solution to
% the 6-star quantum graph.

% Time variable: 100 points.
t = linspace(0,5*pi,100);

```

```

% Reference variable used in calculating the solution.
x = linspace(0,pi,100);

% Calculation of the 100 points on each edge.
x1 = linspace(0,pi,100);
y1 = linspace(0,0,100);

x2 = linspace(0,pi/2,100);
y2 = linspace(0,sqrt(3)*pi/2,100);

x3 = linspace(0,-pi/2,100);
y3 = linspace(0,sqrt(3)*pi/2,100);

x4 = linspace(0,-pi,100);
y4 = linspace(0,0,100);

x5 = linspace(0,-pi/2,100);
y5 = linspace(0,-sqrt(3)*pi/2,100);

x6 = linspace(0,pi/2,100);
y6 = linspace(0,-sqrt(3)*pi/2,100);

% clinep parameter.
W = 3;

% looped plotting. In each we clear the plot, hold the frame at
% the same reference for each image, generate the image, and then
% store the image in a frame.

```



```

for(i = 1:100)

    z=cos(2*x)*cos(2*t(i));
    center = z(1);
    endpoint = z(100);

    close(gcf);
    figure;

    view([0 60]);

    xlim([-4,4]);
    ylim([-4,4]);
    zlim([-1,1]);

    axis manual;
    set(gca,'nextplot','replacechildren');
    set(gcf, 'Renderer', 'painters');

    hold on;

    plot3(0,0,center,'k.','MarkerSize',25.0);
    plot3(pi,0,endpoint,'k.','MarkerSize',25.0);
    plot3(-pi,0,endpoint,'k.','MarkerSize',25.0);
    plot3(pi/2,sqrt(3)*pi/2,endpoint,'k.','MarkerSize',25.0);
    plot3(pi/2,-sqrt(3)*pi/2,endpoint,'k.','MarkerSize',25.0);
    plot3(-pi/2,sqrt(3)*pi/2,endpoint,'k.','MarkerSize',25.0);
    plot3(-pi/2,-sqrt(3)*pi/2,endpoint,'k.','MarkerSize',25.0);

```

```
    clinep(x1,y1,z,z,W);
    clinep(x2,y2,z,z,W);
    clinep(x3,y3,z,z,W);
    clinep(x4,y4,z,z,W);
    clinep(x5,y5,z,z,W);
    clinep(x6,y6,z,z,W);
    h =(gcf);
    M(i) = getframe(h,[80 60 410 355]);
end

% code to generate the animation file
myVideo = VideoWriter('starwave.avi', 'Uncompressed AVI');

open(myVideo);
writeVideo(myVideo, M);
close(myVideo);
```

Appendix C

Mathematica Code

```
GraphPlot[{A → B, A → C, A → D, A → F, B → C, B → D, B → F, C → D, C → F,  
D → F}, DirectedEdges → True, VertexLabeling → True]
```

```
graf = Graph[{A → B, A → C, A → D, A → F, B → C, B → D, B → F, C → D, C → F,  
D → F}, DirectedEdges → True, VertexLabels → "Name", ImagePadding → 50]
```

```
MatrixForm[AdjacencyMatrix[graf], TableHeadings → {{A, B, C, D, F}, {A, B, C, D, F}}]
```

$$\begin{pmatrix} & \begin{array}{c|cccc} & A & B & C & D & F \\ \hline A & 0 & 1 & 1 & 1 & 1 \\ \hline B & 0 & 0 & 1 & 1 & 1 \\ C & 0 & 0 & 0 & 1 & 1 \\ D & 0 & 0 & 0 & 0 & 1 \\ F & 0 & 0 & 0 & 0 & 0 \end{array} \\ \hline \end{pmatrix}$$

AD:=AdjacencyMatrix[graf]

AD//MatrixForm

$$\begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

For [$i = 1, i < 11, i++$, $u_i[x_-] = C_{1,i}\text{Cos}[k * x] + C_{2,i}\text{Sin}[k * x]$]

$$\text{eqnsA} = \{u_1[0] - u_2[0] == 0, u_1[0] - u_3[0] == 0, u_1[0] - u_4[0] == 0, \\ u'_1[0] + u'_2[0] + u'_3[0] + u'_4[0] == 0\}$$

$$\{C_{1,1} - C_{1,2} == 0, C_{1,1} - C_{1,3} == 0, C_{1,1} - C_{1,4} == 0, \\ kC_{2,1} + kC_{2,2} + kC_{2,3} + kC_{2,4} == 0\}$$

$$\text{eqnsB} = \{u_1[L] - u_5[0] == 0, u_1[L] - u_6[0] == 0, u_1[L] - u_7[0] == 0, \\ -u'_1[L] + u'_5[0] + u'_6[0] + u'_7[0] == 0\}$$

$$\{\text{Cos}[kL]C_{1,1} - C_{1,5} + \text{Sin}[kL]C_{2,1} == 0, \text{Cos}[kL]C_{1,1} - C_{1,6} + \text{Sin}[kL]C_{2,1} == 0, \\ \text{Cos}[kL]C_{1,1} - C_{1,7} + \text{Sin}[kL]C_{2,1} == 0, k\text{Sin}[kL]C_{1,1} - k\text{Cos}[kL]C_{2,1} + kC_{2,5} \\ + kC_{2,6} + kC_{2,7} == 0\}$$

$$\text{eqnsC} = \{u_2[L] - u_5[L] == 0, u_2[L] - u_8[0] == 0, u_2[L] - u_9[0] == 0, \\ -u'_2[L] - u'_5[L] + u'_8[0] + u'_9[0] == 0\}$$

$$\{\text{Cos}[kL]C_{1,2} - \text{Cos}[kL]C_{1,5} + \text{Sin}[kL]C_{2,2} - \text{Sin}[kL]C_{2,5} == 0, \\ \text{Cos}[kL]C_{1,2} - C_{1,8} + \text{Sin}[kL]C_{2,2} == 0, \text{Cos}[kL]C_{1,2} - C_{1,9} + \text{Sin}[kL]C_{2,2} == 0, \\ k\text{Sin}[kL]C_{1,2} + k\text{Sin}[kL]C_{1,5} - k\text{Cos}[kL]C_{2,2} - k\text{Cos}[kL]C_{2,5} + kC_{2,8} + kC_{2,9} == 0\}$$

$$\text{eqnsD} = \{u_3[L] - u_6[L] == 0, u_3[L] - u_8[L] == 0, u_3[L] - u_{10}[0] == 0, \\ -u'_3[L] - u'_6[L] - u'_8[L] + u'_{10}[0] == 0\}$$

$$\{\text{Cos}[kL]C_{1,3} - \text{Cos}[kL]C_{1,6} + \text{Sin}[kL]C_{2,3} - \text{Sin}[kL]C_{2,6} == 0, \\ \text{Cos}[kL]C_{1,3} - \text{Cos}[kL]C_{1,8} + \text{Sin}[kL]C_{2,3} - \text{Sin}[kL]C_{2,8} == 0, \text{Cos}[kL]C_{1,3} - C_{1,10} + \\ \text{Sin}[kL]C_{2,3} == 0, k\text{Sin}[kL]C_{1,3} + k\text{Sin}[kL]C_{1,6} + k\text{Sin}[kL]C_{1,8} - k\text{Cos}[kL]C_{2,3} \\ - k\text{Cos}[kL]C_{2,6} - k\text{Cos}[kL]C_{2,8} + kC_{2,10} == 0\}$$

$$\text{eqnsF} = \{u_4[L] - u_7[L] == 0, u_4[L] - u_9[L] == 0, u_4[L] - u_{10}[L] == 0, \\ -u'_4[L] - u'_7[L] - u'_9[L] - u'_{10}[L] == 0\}$$

$$\{\text{Cos}[kL]C_{1,4} - \text{Cos}[kL]C_{1,7} + \text{Sin}[kL]C_{2,4} - \text{Sin}[kL]C_{2,7} == 0, \text{Cos}[kL]C_{1,4} \\ - \text{Cos}[kL]C_{1,9} + \text{Sin}[kL]C_{2,4} - \text{Sin}[kL]C_{2,9} == 0, \text{Cos}[kL]C_{1,4} - \text{Cos}[kL]C_{1,10} \\ + \text{Sin}[kL]C_{2,4} - \text{Sin}[kL]C_{2,10} == 0, k\text{Sin}[kL]C_{1,4} + k\text{Sin}[kL]C_{1,7} + k\text{Sin}[kL]C_{1,9} \\ + k\text{Sin}[kL]C_{1,10} - k\text{Cos}[kL]C_{2,4} - k\text{Cos}[kL]C_{2,7} - k\text{Cos}[kL]C_{2,9} - k\text{Cos}[kL]C_{2,10} == 0\}$$

$$\text{eqns} = \text{Union}[\text{eqnsA}, \text{eqnsB}, \text{eqnsC}, \text{eqnsD}, \text{eqnsF}]/.k \rightarrow \text{Pi}/.L \rightarrow 3$$

$$\{C_{1,1} - C_{1,2} == 0, C_{1,1} - C_{1,3} == 0, C_{1,1} - C_{1,4} == 0, -C_{1,1} - C_{1,5} == 0, \\ -C_{1,1} - C_{1,6} == 0, -C_{1,1} - C_{1,7} == 0, -C_{1,2} - C_{1,8} == 0, -C_{1,2} - C_{1,9} == 0, \\ -C_{1,3} - C_{1,10} == 0, \pi C_{2,1} + \pi C_{2,2} + \pi C_{2,3} + \pi C_{2,4} == 0, -C_{1,2} + C_{1,5} == 0, \\ -C_{1,3} + C_{1,6} == 0, \pi C_{2,1} + \pi C_{2,5} + \pi C_{2,6} + \pi C_{2,7} == 0, -C_{1,4} + C_{1,7} == 0, \\ -C_{1,3} + C_{1,8} == 0, \pi C_{2,2} + \pi C_{2,5} + \pi C_{2,8} + \pi C_{2,9} == 0, -C_{1,4} + C_{1,9} == 0, \\ \pi C_{2,3} + \pi C_{2,6} + \pi C_{2,8} + \pi C_{2,10} == 0, \pi C_{2,4} + \pi C_{2,7} + \pi C_{2,9} + \pi C_{2,10} == 0, \\ -C_{1,4} + C_{1,10} == 0\}$$

$$\{b, m\} = \text{CoefficientArrays}[\text{eqns}, \{C_{1,1}, C_{1,2}, C_{1,3}, C_{1,4}, C_{1,5}, C_{1,6}, C_{1,7}, C_{1,8}, C_{1,9}, \\ C_{1,10}, C_{2,1}, C_{2,2}, C_{2,3}, C_{2,4}, C_{2,5}, C_{2,6}, C_{2,7}, C_{2,8}, C_{2,9}, C_{2,10}\}]$$

$$\{\text{SparseArray}[\langle 0 \rangle, \{20\}], \text{SparseArray}[\langle 50 \rangle, \{20, 20\}]\}$$

***m*//MatrixForm**

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