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Signature:

Kenny Jones	Date

The Laplace and Heat Operators on Quantum Graphs

By

Kenny Jones
Doctor of Philosophy

Mathematics

David Borthwick
Advisor

Shanshuang Yang
Committee Member

Alessandro Veneziani
Committee Member

Accepted:

Kimberly Jacob Arriola
Dean of the James T. Laney School of Graduate Studies

Date

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By

Kenny Jones
B.B.A, Georgia State University, 2014
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Special thanks to Dr. David Borthwick, Dr. Evans Harrell, and Dr. Livia Corsi for their infinite patience and guidance.

Thanks to my mom, Carol Lucas, for her slightly less than infinite patience.

An abstract of
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Abstract

The Laplace and Heat Operators on Quantum Graphs
By Kenny Jones

This thesis analyzes the Laplace and heat operators on quantum graphs. The thesis is separated into four chapters,

- Chapter 1: Introduction to quantum graphs, the Laplace operator, and summary of the main results.
- Chapter 2: Strategies for bounding the spectral gap of a quantum graph, including a sharp upper bound for the spectral gap using the diameter and total number of vertices as parameters.
- Chapter 3: Bounds for the heat kernel of a quantum graph. The main results include a bound for small time and identifying a class of edges that can be bound by a Neumann interval.
- Chapter 4: Finds two mean value formulas for the heat equation on a quantum graph. Proves an additional bound for the mean value formula using the one dimensional free heat kernel.

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Contents

CHAPTER 1

Introduction

1. Motivation

Quantum graphs where first used in the 1930's to study free electrons in molecules. Since then quantum graphs have been used to understand a plethora of physical objects including crystal lattices, carbon-nanotubes, waveguides, and much more. They are also used to better understand other areas of mathematics and physics. Quantum graphs have been used to model quantum chaos, Anderson localization, and many dynamic systems.

Quantum graphs, or metric graphs as they are often called, can serve as a mathematical approximation for networks where there is a well defined distance function between nodes in the network. The implications of this are endless from understanding the dynamics of traffic on roads, to the spread of viruses, to electricity in robotics. This paper will mostly involve understanding the Laplace and heat operators on quantum graphs. The Laplace operator is often associated with the energy of a system. The eigenvalues of the laplace operator give the allowable energy states for a domain with no potential energy. The heat operator is used to understand diffusion of a system. Understanding these two operators on quantum graphs has many implications in nano-technology and quantum circuitry.

Although quantum graphs are often used to better understand physical systems the author would argue that they are interesting objects in and of themselves. They are a thought-provoking marriage of graphs and partial differential equations with many surprising and fascinating characteristics.

2. Introduction to Quantum Graphs

Let G be an arbitrary quantum graph, G is defined by a finite or countably infinite set of vertices $V(G)$ and edges $E(G)$, $G = \{V(G), E(G)\}$. We will use the simpler notation V and E, when there can be no confusion about G. Each edge $e \in E(G)$ is a one dimensional line segment connected to points $v_1, v_2 \in V(G)$, alternatively we can think of v_1 and v_2 as being the end points of e. The structure of G is determined by how edges are connected to vertices. Multiple edges can be connected to the same vertex and both end points of an edge can be connected to the same vertex, known as a loop. Below is an example of a quantum graph.

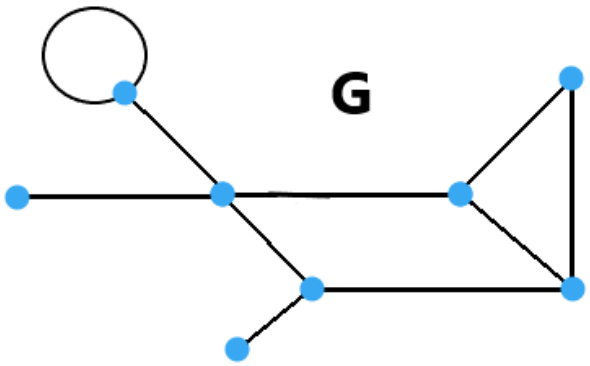


FIGURE 1. A quantum graph with edges in black and vertices in blue.

The cardinality of the sets V and E will be denoted $|V|$ and $|E|$, respectively. For $e \in E$ and $v \in V$, v and e are said to be *adjacent* if v is connected to e, expressed as $e \sim v$. Two edges $e_1, e_2 \in E$ are adjacent if e_1 and e_2 are connected to the same vertex, we use the same notation $e_1 \sim e_2$. All edges are adjacent to themselves.

DEFINITION 2.1. We call G a *metric graph* if for all $e \in E$, e can be assigned a positive length, $\ell(e)$, where $\ell(e) \in (0, \infty]$.

All quantum graphs in this paper are assumed to be metric graphs and $\ell(e)$ will always be the one dimensional lebesgue measure of e. Each edge e can be identified with the line segment $[0, \ell(e)]$, which introduces a coordinate system along e. When using a coordinate system, a point along e will be denoted x_e or simply x if e is clear. Edges have no direction, so the orientation of any coordinate system is arbitrary. Occasionally, it is useful to split an edge into two directed bonds. Let e be connected to v_1 and v_2. Then e can be split into two bonds $\vec{b}_{v_1,v_2}$ and $\vec{b}_{v_2,v_1}$, where $\vec{b}_{v_1,v_2}$ has the direction from v_1 to v_2 and $\vec{b}_{v_2,v_1}$ has the direction from v_2 to v_1. Two bonds $\vec{b}_{v,w}$ and $\vec{b}_{u,x}$ are consecutive if $w = u$, meaning $\vec{b}_{v,w}$ ends at the vertex $\vec{b}_{u,x}$ begins. This technique is fully explained in Chapter 3 section 2.

The total length of the graph G, or $L(G)$, can be found by summing all edge lengths for edges contained in G,

$$L(G) = \sum_{e \in G} \ell(e). \tag{2.1}$$

For all vertices $v \in V$, the number of edges connected to v is called the degree of v denoted d_v. If both endpoints of e are connected to v, i.e. e is a loop, then we count this edge twice in the degree. If $d_v = 2$, then v is called an artificial vertex. Artificial vertices do not affect the underlying topology of G and are often added or removed for convenience or as part of a technique to better understand the graph G. However, one must be careful when adding or deleting artificial vertices because G is defined by its set of edges and vertices, changing these sets technically changes the graph G to some new graph G'.

We will now introduce the metric used for all quantum graphs in this paper, first we must define a path along G.

DEFINITION 2.2. A *path* along a quantum graph is an ordered sequence of consecutive bonds, $\{\overrightarrow{b}_{1,2}, \overrightarrow{b}_{2,3}, ..., \overrightarrow{b}_{N-2,N-1}, \overrightarrow{b}_{N-1,N}\}$.

A bond can be repeated any multiple of times along a path. Let p be a path consisting of the bonds $\{\overrightarrow{b}_{1,2}, \overrightarrow{b}_{2,3}, ..., \overrightarrow{b}_{N-2,N-1}, \overrightarrow{b}_{N-1,N}\}$. The length of p, expressed $\ell(p)$, can be found by summing the lengths of all bonds along p.

DEFINITION 2.3. The *length of a path* can be calculated by

$$\ell(p) = \sum_{\overrightarrow{b} \in p} \ell(\overrightarrow{b}) \tag{2.2}$$

Let q_1 and q_2 be two points contained on edges of G, not necessarily the same edge. If $q_1, q_2 \notin V(G)$, then we can insert artificial vertices at q_1 and q_2, this creates a new graph G'. Note that $q_1, q_2 \in V(G')$. Using definition 2.2 we can define a path from q_1 to q_2 along G'.

We will define the distance function $d(q_1, q_2)$ to be the length of the shortest path between q_1 and q_2,

DEFINITION 2.4. Let $P(q_1, q_2)$ be the set of all paths between q_1 and q_2, then the *distance* between q_1 and q_2 is

$$d(q_1, q_2) = \min_{p \in P(q_1,q_2)} \ell(p) \tag{2.3}$$

The distance $d(q_1, q_2)$ on the new graph G' defines the distance between points q_1 and q_2 on the original graph G. This distance function defines a topology on the graph G, making G a topological space. Thus, we can define a function $f(q)$ for a point $q \in G$. For $q \notin V(G)$, $f(q)$ acts locally as if it is on a one dimension line segment. At vertices we impose vertex conditions, in this paper the standard Kirchoff-Neumann vertex conditions will be used,

$$\begin{cases} f \text{ is continuous on } G \\ \text{and} \\ \sum_{e \sim v} df(v)/dx_e = 0. \end{cases} \tag{2.4}$$

Where $df(v)/dx_e$ refers to the outward derivative of f away from the vertex v along the edge e. If $d_v = 1$, the second vertex condition becomes a Neumann boundary condition, $df(v)/dx_e = 0$. If $d_v = 2$, v is an artificial vertex, the second condition implies that the function is differentiable at v. We will sometimes refer to the first condition as the "continuity vertex condition" and the second condition as the "net flow vertex condition."

In order to be considered a *quantum* graph we equip G with a differential operator. This paper will focus on the Laplace operator $-\Delta$, or $-d^2/dx^2$, and the heat operator $\frac{\partial^2}{\partial x^2} - \partial_t$.

3. The Laplacian and Its Spectrum

A function f on a quantum graph can be thought of as existing on each edge e, $f_e := [0, \ell(e)] \to \mathbb{C}$. Using this we can define the following functional spaces for the set $E(G)$

$$L^2(E) = \bigoplus_{e \in E(G)} L^2([0, \ell(e)]), \tag{3.1}$$

$$H^k(E) = \bigoplus_{e \in E(G)} H^k([0, \ell(e)]). \tag{3.2}$$

Where

$$L^2([0,\ell(e)]) = \{f_e \mid \int_0^{\ell(e)} |f(x)|^2 dx < \infty\}, \tag{3.3}$$

$$H^k([0,\ell(e)]) = \{f_e \in L^2([0,\ell(e)]) \mid \int_0^{\ell(e)} (|f(x)|^2 + \sum_{n=1}^{k} |\frac{d^n f(x)}{dx^n}|^2) dx < \infty\}. \tag{3.4}$$

Along each edge, the Laplacian can be defined as

$$-\Delta f_e := f_e \to -\frac{d^2 f_e}{dx^2}. \tag{3.5}$$

On each edge the domain of the Laplacian is $H^2([0,\ell(e)])$. In order to make $-\Delta$ self-adjoint on G, we further restrict the domain to functions which satisfy the vertex conditions (2.4).

$$\mathcal{D}(-\Delta(G)) = \{f \in H^2(E) \mid \text{f satisfies the vertex conditions}\} \tag{3.6}$$

For a proof that $-\Delta(G)$ is self-adjoint acting on $\mathcal{D}(-\Delta(G))$ we refer the reader to *Theorem 1.4.4* of [**5**]. We can associate $-\Delta(G)$ with its quadratic form

$$h[f,f] := \sum_{e\in E} \int_e |\frac{df_e}{dx}|^2 dx, \tag{3.7}$$

the domain for h is defined as

$$\mathcal{D}(h) = H^1(G) = \{f \in H^1(E) \mid \text{f is continuous on } G\}. \tag{3.8}$$

Through out this paper we will assume all quantum graphs are compact and contain a finite number of edges and vertices. The spectrum of $-\Delta(G)$ will be referred to as $\sigma(-\Delta(G))$, or $\sigma(-\Delta)$ when G is clear. The following comes from [**5**], *Theorem 3.1.1.*

THEOREM 3.1. *If G is a compact quantum graph, then $\sigma(-\Delta)$ only contains isolated eigenvalues with finite multiplicity and as $j \to \infty$, $\lambda_j \to \infty$.*

PROOF. Restricting ourselves to $\mathcal{D}(-\Delta(G))$, $-\Delta(G)$ is self adjoint. This implies the resolvent $(-\Delta - i\mathbb{I})^{-1}$ continuously maps $L^2(E) \to \mathcal{D}(-\Delta(G)) \subset H^2(E)$. By the Sobolev embedding theorem the embedding of $H^2(E) \to L^2(E)$ is compact, which implies the resolvent is compact. □

The above theorem implies that for all $\lambda_j \in \sigma(-\Delta(G))$, there exists a function $\psi_j \in \mathcal{D}(-\Delta(G))$ such that

$$(-\Delta - \lambda_j)\psi_j = 0. \tag{3.9}$$

We will refer to λ_j and ψ_j as eigenvalue, eigenfunction pairs. Because $-\Delta(G)$ is self-adjoint on $D(-\Delta(G))$ all eigenvalues must be real. We order the eigenvalues such that $\lambda_j \leq \lambda_{j+1}$ for all $j \in \{0,1,2,...\}$. It is well known that all eigenfunctions are contained in $C^\infty(G)$ and for eigenvalues such that $\lambda_i \neq \lambda_j$, the eigenfunctions ψ_i and ψ_j are orthogonal, meaning

$$\int_G \psi_j \psi_i = 0. \tag{3.10}$$

We can ensure that all eigenfunctions are orthogonal. Let n be the dimension of the eigenspace associated with the eigenvalue λ_j, call this space S_j. By the Gram-Schmidt process we can choose n functions $\{\phi_1, \phi_2, ..., \phi_n\}$ in S_j such that each function ϕ_j is orthogonal

to ϕ_i, $i \neq j$. We then choose $\{\phi_1, \phi_2, ..., \phi_n\}$ to be the eigenfunctions associated with the eigenspace S_j.

Finding the values for eigenvalues, and bounding eigenvalues, frequently makes use of the Rayleigh quotient. The Rayleigh quotient on G is defined as

$$R(f) := \frac{\sum_{e\in E} \int_e |\frac{df_e}{dx}|^2 dx}{\sum_{e\in E} \int_e |f_e|^2 dx}. \tag{3.11}$$

Because all of the eigenfunctions can be made to be orthogonal and the set $\{\psi_j\}_{j=0}^{\infty}$ is a basis for $L^2(E)$, we can use the min-max formula to express all eigenvalues

$$\lambda_{j-1} = \min_{\substack{X\subset \mathcal{D}(-\Delta(G)) \\ dim(X)=j}} \{\max_{f\in X}\{R(f)\}\}. \tag{3.12}$$

The first non-trivial eigenvalue λ_1 is known as the spectral gap. In physics, the spectral gap has the interpretation as the smallest non-zero energy for a domain, or the first excited state. In the next chapter, we will further examine the spectral gap and provide common techniques and strategies for bounding the spectral gap.

4. Main Results

The topics in this paper can be separated into three main categories:

- Bounding the spectral gap
- Bounding the heat kernel
- Mean value formula for the heat equation

The main result for bounding the spectral gap is a sharp upper bound on the spectral gap using the diameter and $|V|$ for a graph. The diameter of a graph is defined as

$$D(G) = \max_{q,q_0\in G}\{d(q_0, q)\}, \tag{4.1}$$

where $d(q_0, q)$ is the distance between points $q_0, q \in G$. We also provide an algorithm for finding graphs with spectral gap arbitrarily close to our upper bound.

THEOREM 4.1. *Let G be a quantum graph with $|V|$ vertices and diameter D. Then the spectral gap is bounded by*

$$\lambda_1(G) \leq (\frac{\pi(|V|+2)}{2D})^2. \tag{4.2}$$

If the diameter can be realized at two vertices then

$$\lambda_1(G) \leq (\frac{\pi(|V|)}{2D})^2. \tag{4.3}$$

Furthermore, for all $\epsilon > 0$, there exists a quantum graph G^* such that $D(G^*) = D$ and $|V(G^*)| = |V|$ and

$$\lambda_1(G^*) \geq (\frac{\pi(|V|)}{2D})^2 - \epsilon. \tag{4.4}$$

In the next chapter, we focus on bounding the heat kernel. Let $K_G(t, q, q_0)$ be the heat kernel for G. There are two main results for bounding the heat kernel. The first is a short time estimate that utilizes the bond scattering matrix for G. The bound presented below is along the diagonal of the heat kernel, i.e. $q_0 = q$, however the theorem is extended to off

diagonal results.

PROPOSITION 4.2. *Let G be an arbitrary quantum graph with minimum edge length a_0. For $q \in G$, let v_0 be the closest non-artificial vertex with degree d_0. For $t < a_0^2/2log(m)$,*

$$K(t,q,q) = \frac{1}{\sqrt{4\pi t}}\Big[1 + (\frac{2}{d_0} - 1)e^{-d(v_0,q)^2/t} + O(me^{-a_0^2/t})\Big]. \tag{4.5}$$

The next bound involves identifing a class of edges called *direct path bounded* edges. For any edge in this class the heat kernel can be bounded by a Neumann interval with length $\ell(e)$, where q and q_0 have the same relative spacing on the Neumann interval as on e.

THEOREM 4.3. *Let $q, q_0 \in e$, where e is direct path bounded. Let e have vertices v_l and v_r with $\ell_1 := |v_l - q_0|$ and $\ell_2 := |v_r - q_0|$. If every path from q_0 to q_0 containing both v_r and v_l has length equal to or greater than $\max\{2\ell_1, 2\ell_2\}$. Then*

$$K_G(t,q,q_0) \le K_I(t,q,q_0), \tag{4.6}$$

for all $t > 0$. Where $K_I(t,q,q_0)$ is the heat kernel for a Neumann interval of length ℓ, and q, q_0 have the same relative positions as on e. If G is not the Neumann interval then the inequality is strict.

The last section finds two mean value formulas for the heat equation on a quantum graph and a bound for the mean value formula. The main result from the chapter is given below. Let $Q(q_0,t_0,C) := \{(x,t) \in G \times (0,t_0) \mid K(t_0 - t, q_0, q) \ge C\}$ for some $C > 0$, $q_0 \in G$, and $t_0 \in (0,\infty)$. We refer to $Q(q_0,t_0,C)$ as the heat ball.

THEOREM 4.4. *Let G be a compact quantum graph and let $u(q,t)$ satisfy the heat equation, then*

$$u(q_0,t_0) = \int_{\partial Q} -uK_x n_1 ds. \tag{4.7}$$

Where ∂Q is the boundary of the heat ball $Q(q_0,t_0,C)$ for some $C > 0$.

CHAPTER 2

The Spectral Gap

1. Introduction to the Spectral Gap

Let $-\Delta := -d^2/dx^2$ be the Laplace operator which acts on the L^2 space of functions on the edges of G. $-\Delta$ has the quadratic form

$$h[f,f] := \|f'\|^2. \tag{1.1}$$

The domain for h are functions which are H^1 along each edge of G and are continuous on G, we will refer to this space of functions as $H^1(G)$.

DEFINITION 1.1. The *spectral gap* is the first non-trivial eigenvalue of the Laplace operator, $-d^2/dx^2$, which we will call λ_1.

Using the Rayleigh quotient we can find an explicit expression for λ_1,

$$\lambda_1 = \inf\left\{\frac{\int_G |f'|^2}{\int_G |f|^2} : f \in \mathcal{D}(-\Delta(G)), \int_G f = 0\right\}. \tag{1.2}$$

For many simple graphs we can exploit symmetries of the graph to find the first eigenvalue. All quantum graphs can be thought of as being constructed by connecting simpler sub-graphs. For example, a star graph is a graph with a single central vertex of degree d_v and d_v edges connected to the central vertex; all graphs are the union of connected star graphs. Understanding simple graphs builds an understanding of how size and shape affect the spectral gap. It is also a common strategy to utilize simple graphs to bound the spectral gap.

Below is a list of several common graphs and there exact spectral gap.

1) *Path Graph* $I(L)$: Consists of a single edge of length L and two degree 1 vertices. Because both vertices are degree one the second vertex condition forces the path graph to coincide with a Neumann interval of length L, as pointed out in (2.4). Hence,

$$\lambda_1(I(L)) = \frac{\pi^2}{L^2}. \tag{1.3}$$

2) *Symmetric Star Graph* S(L,E): The symmetric star graph has a single central vertex and $|E|$ edges of equal length $\frac{L}{|E|}$.

$$\lambda_1(S(L,E)) = \frac{\pi^2 E^2}{4L^2}. \tag{1.4}$$

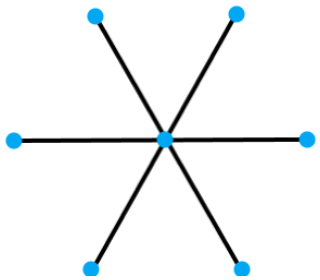


FIGURE 1. A symmetric star graph with 6 edges.

3) *Symmetric Flower Graph* F(L,E): A symmetric flower graph also has a single central vertex and $|E|$ edges of length $\frac{L}{|E|}$. However, all edges of a flower graph are loops, meaning both end points are attached to the central vertex.

$$\lambda_1(F(L,E)) = \frac{\pi^2 E^2}{L^2}. \tag{1.5}$$

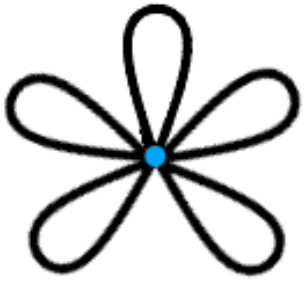


FIGURE 2. A symmetric flower graph with 5 edges.

3) *Symmetric Pumpkin Graph* K(L,E): A symmetric pumpkin graph has two vertices and $|E|$ edges. The vertices are the end points for each edge in $K(L,E)$, all edges have length $\frac{L}{|E|}$.

$$\lambda_1(F(L,E)) = \frac{\pi^2 E^2}{L^2}. \tag{1.6}$$

FIGURE 3. A symmetric pumpkin graph with 4 edges.

Our goal is to bound the spectral gap, λ_1. However, it is easy to show that for an arbitrary quantum graph one can not bound the spectral gap from above or below. Consider trying to bound the spectral gap from below. Let $\{I(n)\}_{n=1}^{\infty}$ be a sequence of path graphs with length $n \in \{1, 2, ...\}$, then

$$\lambda_1(I(n)) = \frac{\pi^2}{n^2}. \tag{1.7}$$

Clearly, the spectral gap of this sequence converges to zero.

Bounding the spectral gap from above is also impossible. Consider the sequence of symmetric star graphs $\{S(L,n)\}_{n=1}^{\infty}$, each graph in the sequence has the same total length L, and the number of edges increases for each graph in the sequence. We can compute the spectral gap for the n^{th} graph in the sequence as

$$\lambda_1(S(L,n)) = \frac{\pi^2 n^2}{L^2}. \tag{1.8}$$

The spectral gap for this sequence diverges.

These examples show that it is easy to find graphs with arbitrarily large spectral gaps or spectral gaps arbitrarily close to zero. However, if we fix a characteristic of the graph, i.e. L or $|E|$, it may be possible to create a bound. In the path graph sequence $\{I(n)\}_{n=1}^{\infty}$, fixing L would have excluded this sequence. In the second example, $\{S(L,n)\}_{n=1}^{\infty}$, fixing $|E|$ would have excluded the sequence. The most natural parameters to use to bound the spectral gap are:

(1) $L :=$ total length of G.
(2) $|V| :=$ total number of vertices of G.
(3) $|E| :=$ total number of edges of G.

(4) $D :=$ the diameter of G.

DEFINITION 1.2. The *diameter* of a graph G, denoted $D(G)$ or simply D if G is understood, is defined as the largest distance between two points in G,

$$D(G) := \sup\{d(q_1, q_2) : q_1, q_2 \in G\}. \tag{1.9}$$

Many results have been proven using one or several of the parameters above. Using only the length as a parameter the following lower bound for the spectral gap was first proven by Serge Nicaise [**17**],

$$\lambda_1 \geq \frac{\pi^2}{L^2}. \tag{1.10}$$

This makes intuitive sense as you would expect diffusion to be slowest on an interval. This result was extended by Leonid Friedlander [**9**] to be a lower bound for all eigenvalues of G,

$$\lambda_n(G) \geq (\frac{\pi(n+1)}{2L})^2, \tag{1.11}$$

for $n \geq 2$. No upper bound can be found fixing the total length of a graph, this follows from the sequence of symmetric star graphs, $\{S(L, n)\}_{n=1}^{\infty}$.

Other bounds rely on the procedure of graph *surgeries*, changes to the original graph G that monotonically affect the spectral gap. These surgeries are used in sequence to transform an arbitrary graph into a graph where the spectral gap is able to be calculated. If each surgery in the sequence monotonically increases the spectral gap, then the resulting graph must have a larger first eigenvalue and you can bound the spectral gap from above. If each surgery in the sequence decreases the spectral gap, then the first eigenvalue of the resulting graph is a lower bound.

In order to introduce these surgeries we need the following definitions:

DEFINITION 1.3. A *pendant sub-graph* is a sub-graph of G that is connected to the larger graph at a single vertex.

DEFINITION 1.4. We *identify* two vertices by joining them to make a single vertex. If v_1 and v_2 are identified to make a new vertex v_0, then any edge with either v_1 or v_2 as an endpoint now has v_0 as an endpoint. Any edge connecting v_1 and v_2 becomes a loop at v_0.

Let G be the original graph and G' the graph after performing a surgery. We will state each surgery such that $\lambda(G') \leq \lambda(G)$. We point out that the reverse action must increase the spectral gap. The following Lemma largely follows work found in [**13**], for a more in depth look at graph surgeries we point the reader to [**15**].

LEMMA 1.5. *Assume G and G' are compact, connected, and finite quantum graphs. Then for the following*

$$\lambda_1(G') \leq \lambda_1(G) \tag{1.12}$$

(1) *If G' is the result of connecting a pendant sub-graph to G.*
(2) *If G is the result of identifying two vertices of G'.*
(3) *If G' is the result of lengthening an edge of G*
(4) *If G' is the result of scaling G by $C \geq 1$, then*

$$C^{-2}\lambda_1(G') = \lambda_1(G) \tag{1.13}$$

PROOF. Results (1) and (3) rely on finding a test function on the new graph G' that is orthogonal to the constants and has a Rayleigh quotient smaller than $\lambda_1(G)$.

1) Attaching a pendant: Assume the pendant is attached at some vertex v. Let ψ_1 be the eigenfunction of G associated with the eigenvalue $\lambda_1(G)$. We can extend ψ_1 to a function $\widetilde{\psi} \in H^1(G')$ by setting $\widetilde{\psi} = \psi_1(v)$ on the pendant, which we label $G' \setminus G$. Let $\phi = \widetilde{\psi} - \int_{G'\setminus G} \psi_1(v)$, clearly, $\phi \in H^1(G')$ and it is easy to calculate that $\int_{G'} \phi = 0$. Using $\int_G \psi = 0$ and setting $\alpha = \int_{G'\setminus G} \psi_1(v)$, we calculate the Rayleigh quotient of ϕ as

$$\frac{\int_{G'} \|\phi'\|^2}{\int_{G'} \|\phi\|^2} = \frac{\int_G \|\psi_1'\|^2}{\int_G \|\widetilde{\psi} - \alpha\|^2 + \int_{G'\setminus G} \|\widetilde{\psi}(v) - \alpha\|^2}, \tag{1.14}$$

$$= \frac{\int_G \|\psi_1'\|^2}{\int_G \psi_1^2 - 2\psi_1\alpha + \alpha^2 + \int_{G'\setminus G} \|\widetilde{\psi}(v) - \alpha\|^2}, \tag{1.15}$$

$$= \frac{\int_G \|\psi_1'\|^2}{\int_G \psi_1^2 + \alpha^2 + \int_{G'\setminus G} \|\widetilde{\psi}(v) - \alpha\|^2}, \tag{1.16}$$

$$\leq \frac{\int_G \|\psi_1'\|^2}{\int_G \|\psi_1\|^2}, \tag{1.17}$$

$$= \lambda_1(G). \tag{1.18}$$

2) Identifying two vertices: Let G be the result of identifying two vertices of G'. If $f \in H^1(G)$ then there exists some function $\widetilde{f} \in H^1(G')$ such that for any edge $e \in G$ and its natural counterpart $\widetilde{e} \in G'$ we have $f(x_e) = \widetilde{f}(x_{\widetilde{e}})$. Where f and $\widetilde{f}$ have the same Rayleigh quotient. Thus, there is a natural identification between the functions in $H^1(G)$ and a subset of functions in $H^1(G')$. The result follows.

3)Lengthening an edge: This is solved in the same way as attaching a pendant, with the exception that $G' \setminus G$ represents the new added length of the edge.

4) Scaling the graph: Let G be an arbitrary quantum graph and construct G' by scaling G by $C \geq 1$. Let $f \in H^1(G')$ and $e \in G'$. Let $\widetilde{e} \in G$ be the natural counterpart of e. Then we can identify f with a function $\widetilde{f} \in H^1(G)$ by setting $\widetilde{f} = f(C^{-1}x_e)$ along $\widetilde{e}$. We can make the reverse identification by scaling by C. It is easy to calculate the Rayleigh quotient for the function $\widetilde{f} \in H^1(G)$ as

$$\frac{\int_G \|\widetilde{f}'\|^2}{\int_G \|\widetilde{f}^2\|} = \frac{\int_G \|f(C^{-1}x_e)'\|^2}{\int_G \|f(C^{-1}x_e)\|} = C^{-2}\frac{\int_{G'} \|f'\|^2}{\int_{G'} \|f^2\|}. \tag{1.19}$$

□

Using these graph surgeries we transform an arbitrary quantum graph into an *extremal graph*, a graph where the first eigenvalue is either maximized or minimized given a set of parameters. The next theorem is an example of this technique. We use the parameters $|L|$ and $|E|$ to derive an upper bound on the spectral gap, the theorem can be found in [**13**].

THEOREM 1.6. *Let G be a quantum graph with $L > 0$ and $|E| > 1$. Then,*

$$\lambda_1(G) \leq \frac{\pi^2|E|^2}{L^2}. \tag{1.20}$$

If $|E| = 1$, then G is either a loop or path graph, thus

$$\lambda_1(G) = \begin{cases} \frac{\pi^2}{L^2}, \ G \text{ is a path graph} \\ \frac{4\pi^2}{L^2}, \ G \text{ is a loop} \end{cases} \tag{1.21}$$

Proof. Let G be a quantum graph and let G_1 be the graph created by identifying all vertices of G, i.e. G_1 is a flower graph. Then by Lemma 1.5

$$\lambda_1(G) \leq \lambda_1(G_1). \tag{1.22}$$

Let F be a symmetric flower graph with total length L and $|E|$ edges. If $\lambda_1(G_1) \leq \lambda_1(F)$, then the proof is complete. Let e_1 and e_2 be the two longest edges of G_1 (if the two longest edges are not unique choose any two longest edges). Then $\ell(e_1)+\ell(e_2) \geq 2L/|E|$. Each petal of G_1 is a pendant, consider a new graph G_2 constructed from G_1 by removing all petals except for e_1 and e_2, then Lemma 1.5 implies

$$\lambda_1(G_1) \leq \lambda_1(G_2). \tag{1.23}$$

Let G_3 be a graph constructed from G_2 by un-identifying the central vertex, i.e. changing the two petals into a single loop of length $\ell(e_1) + \ell(e_2)$. Again, by Lemma 1.5 we have

$$\frac{4\pi^2}{(\ell(e_1) + \ell(e_2))^2} = \lambda_1(G_3) \leq \lambda_1(G_2). \tag{1.24}$$

However, since any eigenfunction on the circle G_3 can serve as a test function on the two petal graph G_2, as long as we insure that the eigenfunction is rotated in such a way as to satisfy the central vertex condition this proves

$$\lambda_1(G_2) \leq \lambda_1(G_3), \tag{1.25}$$

which implies

$$\lambda_1(G) \leq \lambda_1(G_3) = \frac{4\pi^2}{(\ell(e_1) + \ell(e_2))^2} \leq \frac{\pi^2|E|^2}{L^2}. \tag{1.26}$$

□

The following section introduces pumpkin chain graphs and a more involved sequence of surgeries that reduces any graph to a pumpkin chain while monotonically increasing the spectral gap, thus giving us an upper bound on the spectral gap.

2. Diameter Bounds and Pumpkin Chains

In this section we will discuss diameter bounds for quantum graphs. *Pumpkin chain* graphs play an important role in bounding the spectral gap using the diameter.

Definition 2.1. A *pumpkin chain* is a quantum graph constructed by placing symmetric pumpkin graphs end to end. Each vertex is either an end point of the chain or connects adjacent pumpkins.

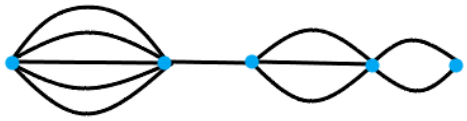


FIGURE 4. Pumpkin chain with 4 pumpkins and 5 vertices

Pumpkin chains are used when finding diameter bounds on the spectral gap for two reasons. First, given a graph G with diameter $D(G)$ there exists a sequence of surgeries from Lemma 1.5 that converts G into a pumpkin chain with diameter $D(G)$ such that each step in the sequence either increases the spectral gap or leaves it unchanged. This makes pumpkin chains a natural choice for creating upper bounds using the diameter as a parameter. The second reason is that finding the first eigenfunction on a pumpkin chain can be reduced to a Sturm-Liouville problem, making it possible to calculate the first eigenvalue.

The following pumpkin chain algorithm was first introduced by Kennedy et al, 2016 [**13**].

LEMMA 2.2 (Lemma 5.4 of [**13**]). *Given a compact, connected, non-empty metric graph G, there exists a pumpkin chain K such that*

(1) $D(G) = D(K)$, $\ell(G) \geq \ell(K)$, *and* $|V(G)| \geq |V(K)| - 2$.
(2) $\lambda_1(G) \leq \lambda_1(K)$.

If the combinatorial diameter is used, (1) is replaced by

(1′) $D(G) = D(K)$, $\ell(G) \geq \ell(K)$, *and* $|V(G)| \geq |V(K)|$.

PROOF. The pumpkin chain K can be constructed following the algorithm below, all steps in the algorithm either increase λ_1 or leave it unchanged by Lemma 1.5.

Step 1. Choose two points $q, q_0, \in G$ such that $d(q, q_0) = D(G)$. If q and q_0 are not vertices, insert artificial vertices at q and q_0 (these extra vertices produce the shift by -2 in (1)). If $d(q, q_0) = D$ can be achieved for $q, q_0 \in V$, then (1) is modified to (1′). Let $v_0 = q$ and $v_D = q_0$.

Step 2. Choose the shortest path between v_0 and v_D, if this path is not unique, choose any shortest path. Call this path Γ_1. Note, $\ell(\Gamma_1) = D$ and Γ_1 does not contain loops or any point twice. In the example below, Γ_1 is the central path.

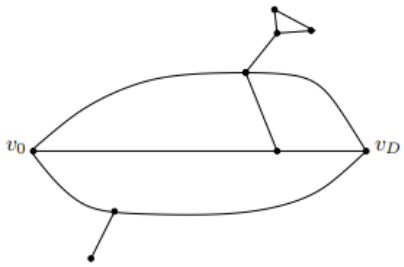


FIGURE 5. The initial graph G.

Step 3. Find the second shortest path, Γ_2, such that Γ_2 does not contain any point twice (edge or vertex) and $\Gamma_2 \nsubseteq \Gamma_1$. If two or more paths have the same length and satisfy the above conditions, choose one arbitrarily. If such a path does not exist, skip to Step 5.

Step 4. Continue to find the next shortest path connecting v_0 to v_D such that the path does not contain a point twice and

$$\Gamma_k \nsubseteq \bigcup_{i=1}^{k-1} \Gamma_i, \tag{2.1}$$

for each k. Because G is compact, this process must terminate after a finite number of steps. Let Γ_n be the last path, we have

$$D = \ell(\Gamma_1) \leq \ell(\Gamma_2) \leq \cdots \leq \ell(\Gamma_{n-1}) \leq \ell(\Gamma_n). \tag{2.2}$$

Step 5. Let $G_1 = \bigcup_{i=1}^{n} \Gamma_i$. Any connected component of $G \backslash G_1$ must be attached to G_1 by a single vertex (i.e., is a pendant of G). If this was not true, we could find a non-self-intersecting path Γ^* such that $\Gamma^* \nsubseteq G_1$, which would contradict step 4 terminating.

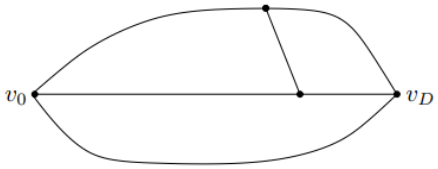


FIGURE 6. The graph G_1, created by removing pendants of G.

Step 6. We now construct a new graph G_2 by shortening edges of G_1 so that all paths connecting v_0 to v_D have length D. Starting with Γ_1, if $\ell(\Gamma_j) = D$ we do not change the path and rename the path Γ_j^*. If $\ell(\Gamma_j) > D$ then we shorten edges of Γ_j not contained in $\Gamma_j \bigcup_{i=1}^{j-1} \Gamma_i^*$ until $\ell(\Gamma_j) = D$, and rename the new path Γ_j^*. Note that some paths may have become subsets. The new graph $G_2 = \cup_{i=1}^{n} \Gamma_i^*$.

Step 7. Let $S = \{d(v_0, q) | q \in V(G_2)\}$. For each point q along Γ_j^*, $j \in \{1, 2, ..., n\}$, if $d(v_0, q) \in S$ we ensure there is a vertex at the point by adding an artificial vertex if needed.

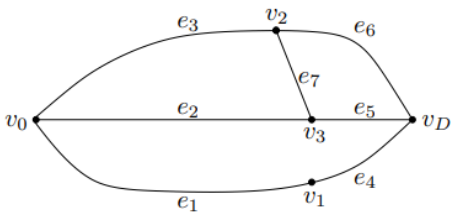


FIGURE 7. The graph G_2, created from G_1 by adding the artificial vertex v_1 and shortening edges such that $\ell(e_1) = \ell(e_2) = \ell(e_3)$ and $\ell(e_4) = \ell(e_5) = \ell(e_6)$.

Step 8. The final step is to identify all vertices with the same distance from v_0 i.e. if $d(v_0, v_i) = d(v_0, v_j)$ then we identify v_i and v_j.

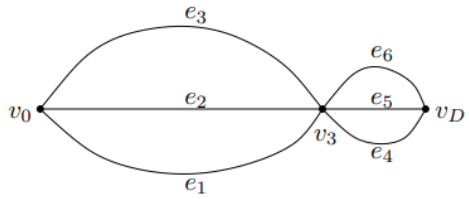


FIGURE 8. The pumpkin chain K created from G_2 by identifying vertices v_1, v_2, and v_3.

The construction of K involves cutting pendants, shortening edges, and identifying vertices. From Lemma 1.5, these operations can only increase the spectral gap. Therefore, $\lambda_1(G) \leq \lambda_1(K)$. □

Note that the algorithm used in Lemma 2.2 does not yield a unique result. For a pumpkin chain, finding the first eigenvalue reduces to a Sturm-Liouville problem. Let K be a pumpkin chain with diameter D and total number of vertices $|V|$. Let v_1 and $v_{|V|}$ be the end vertices of the pumpkin chain. Starting with the pumpkin with end point v_1, we label the k^{th} pumpkin in the chain G_k and its edge multiplicity m_k. We construct a function, $r(q) : G \to [0, D]$ such that for $q \in G$, $r(q) = d(v_1, q)$. And the function $w(x) : [0, D] \to \mathbb{Z}$, such that if $q \in G_k$ then $w(r(q)) = m_k$, the multiplicity of pumpkin G_k.

LEMMA 2.3. *Let K be a pumpkin chain, then there exists an eigenfunction, ψ_1, of K with eigenvalue $\lambda_1(K)$ such that for $q \in G$, $\psi_1(q) = \phi(r(q))$, where $\phi(x) := [0, D] \to \mathbb{C}$.*

PROOF. Let ψ be an eigenfunction of K associated with eigenvalue λ_1. We construct a new eigenfunction ψ_1 by averaging the values of ψ along each pumpkin. Let $S(x) = \{q \in G \mid d(v_1, q) = x;\ x \in [0, D]\}$. The set $S(x)$ is a single point if $d(v_1, q) = x$ and q is a vertex. $S(x)$ has m_k points when $d(v_1, q) = x$ describes points belonging to the pumpkin G_k. Let $\psi_1(x) = \sum_{q \in S(x)} \psi(q)/|S(x)|$. It is easy to verify that ψ_1 is orthogonal to the constants with Rayleigh quotient $\lambda_1(K)$. □

This proves that for a pumpkin chain K, there exists an eigenfunction ψ_1 with eigenvalue $\lambda_1(K)$ such that $\psi_1(q)$ is only dependent on $d(v_1, q)$. We can use the coordinate system $x \in [0, D]$ to indicate the longitudinal position along the graph K, and use the function $w(x)$ to indicate the multiplicity of the pumpkin at position x. This reduces the problem to a one dimensional Sturm-Liouville problem of the form

$$\lambda_1 = \inf \left\{ \frac{\int_0^D |\phi'(x)|^2 w(x)}{\int_0^D |\phi(x)|^2 w(x)} : \phi \in H^1([0, D]), \int_0^D \phi(x) w(x) = 0 \right\}. \tag{2.3}$$

3. Sharp Diameter Bound for Quantum Graphs

Kennedy et al. [**13**] proved that by fixing the diameter and total number of vertices the spectral gap was bounded above by

$$\lambda_1(G) \leq \left(\frac{\pi(|V| + 1)}{D(G)}\right)^2. \tag{3.1}$$

If the diameter can be realized at two vertices then the estimate improves to

$$\lambda_1(G) \leq \left(\frac{\pi(|V| - 1)}{D(G)}\right)^2. \tag{3.2}$$

This estimate is sharp if $|V| = 2$. The following theorem extends their work, creating a smaller upper bound that is shown to be sharp for all $|V|$.

THEOREM 3.1. *Let G be a quantum graph with $|V|$ vertices and diameter D. Then the first non-zero eigenvalue satisfies*

$$\lambda_1(G) \leq \left(\frac{\pi(|V| + 2)}{2D}\right)^2. \tag{3.3}$$

If the diameter can be realized at two vertices then

$$\lambda_1(G) \leq \left(\frac{\pi(|V|)}{2D}\right)^2. \tag{3.4}$$

And for all $\epsilon > 0$, there exists a quantum graph G^* such that $D(G^*) = D$ and $|V(G^*)| = |V|$ with

$$\lambda_1(G^*) \geq \left(\frac{\pi(|V|)}{2D}\right)^2 - \epsilon. \tag{3.5}$$

PROOF. Let G have $|V(G)|$ vertices and diameter $D(G)$. Using the algorithm from Lemma 2.2 we can construct a pumpkin chain K such that

$$\lambda_1(G) \leq \lambda_1(K). \tag{3.6}$$

Where K has diameter D and at most $|V(G)| + 2$ vertices. We label the pumpkins $K_1, ..., K_{|V(K)|-1}$, where pumpkin K_j has length ℓ_j and multiplicity m_j.

As in Lemma 2.3, we construct a coordinate system along K. Let v_0 be an endpoint of K, then $d(v_0, q) = x$, $x \in [0, D]$ defines the coordinate system along each edge. As before in equation (2.3), $w(x)$ is a weight function that returns the multiplicity of the pumpkin at $d(v_0, q) = x \in [0, D]$. Then for any function $\psi \in H^1(G)$, where $\psi(q)$ is only dependent on $d(v_0, q)$ the Rayleigh quotient for ψ can be expressed

$$R(\psi) = \frac{\int_0^D |\psi'(x)|^2 w(x) dx}{\int_0^D |\psi(x)|^2 w(x) dx} \tag{3.7}$$

Let K_r be the longest pumpkin in K, i.e. $\ell_r \geq \ell_j$ for all $j \in \{1, 2, ..., |V(K)| - 1\}$, with endpoint v_1 where $d(v_0, v_1) = x_1$, and v_1 is the closest vertex of K_r to v_0. We construct the following test function along K,

$$\psi_1(x) := \begin{cases} b_1, & x \leq x_1, \\ b_1 \cos[\pi(x - x_1)/\ell_r], & x_1 \leq x \leq x_1 + \ell_r/2, \\ b_2 \cos[\pi(x - x_1)/\ell_r], & x_1 + \ell_r/2 \leq x \leq x_1 + \ell_1, \\ -b_2, & x \geq x_1 + \ell_r. \end{cases}$$

Choosing b_1 and b_2 such that

$$\int_0^D \psi_1(x) w(x) = 0. \tag{3.8}$$

The numerator of the Rayleigh quotient for ψ_1 is

$$\int_{x_1}^{x_2} |\psi_1'(x)|^2 m_r = \frac{\pi^2 m_r}{2 l_r}(b_1^2 + b_2^2), \tag{3.9}$$

and the denominator is bounded by

$$\int_{x_1}^{x_2} |\psi_1(x)| m_r \geq \frac{\ell_r m_r}{2}(b_1^2 + b_2^2). \tag{3.10}$$

This implies

$$\lambda_1(K) \leq \frac{\pi^2}{\ell_r^2}. \tag{3.11}$$

We construct a second test function $\psi_2(x)$, where ψ_2 is a quarter period cosine on the two longest pumpkins in K and constant on all other pumpkins. Let K_t be a pumpkin in K such that $\ell_t \geq \ell_j$ for all $j \in \{1, 2, ..., |V(K)| - 1\}, j \neq r$. Let K_t have endpoint v_2 where $d(v_0, v_2) = x_2$, and v_2 is the closest vertex of K_t to v_0. Without loss of generality let $x_1 < x_2$, and

$$\psi_2(x) := \begin{cases} b_3, & x \leq x_1, \\ b_3 \cos[\pi(x - x_1)/2\ell_2], & x_1 \leq x \leq x_1 + \ell_2, \\ 0, & x_1 + \ell_2 \leq x \leq x_2, \\ -b_4 \sin[\pi(x - x_2)/2\ell_2], & x_2 \leq x \leq x_2 + \ell_2, \\ -b_4, & x \geq x_2 + \ell_2. \end{cases}$$

Again, choosing b_3 and b_4 such that

$$\int_0^D \psi_2(x) w(x) = 0. \tag{3.12}$$

For ψ_2 the numerator is

$$\int_0^D |\psi_2'|^2 w(x) dx = \frac{\pi^2}{8\ell_t}(m_r b_3^2 + m_t b_4^2). \tag{3.13}$$

The denominator is bounded by

$$\int_0^D |\psi_2|^2 w(x) dx \geq \frac{\ell_t}{2}(m_r b_3^2 + m_t b_4^2). \tag{3.14}$$

Which implies

$$\lambda_1(K) \leq \frac{\pi^2}{4\ell_t^2}. \tag{3.15}$$

Given the constraints (3.11) and (3.15), we can find the maximum value for $\lambda_1(K)$. Since $\ell_t \geq \ell_j$ for $j \in \{1, 2, , ..., |V(K)| - 1\}$, $j \neq r$ we have

$$(|V(K)| - 2)\ell_t \geq D - \ell_r. \tag{3.16}$$

Combining this with (3.15) gives the bound

$$\lambda_1(K) \leq \frac{\pi^2(|V(K)| - 2)^2}{4(D - \ell_r)^2}. \tag{3.17}$$

Thus,

$$\lambda_1(K) \leq \pi^2(min\{1/\ell_r, \frac{(|V(K)| - 2)}{2(D - \ell_r)}\})^2. \tag{3.18}$$

The maximum is achieved when $\ell_r = 2D/(|V(K)| - 1)$ which proves 3.3, and 3.4 if no vertices were added in constructing K from the original graph G.

To prove the above estimate is sharp, given $\epsilon > 0$, D, and $|V|$ we must find a graph G^* such that $D(G^*) = D$, $V(G^*) = |V|$ with

$$\lambda_1(G^*) > (\frac{\pi|V|}{2D})^2 - \epsilon. \tag{3.19}$$

Based off the calculations in Theorem 3.1, G^* will be a pumpkin chain with $|V| - 1$ pumpkins. One of the pumpkins should have length $2D/(|V| - 1)$, and all other pumpkins will have length $D/(|V| - 1)$.

For arbitrarily small values of $\delta > 0$, to be specified later, we will choose edge multiplicities that produce the eigenvalue $\lambda_1(G^*) = \sigma_1^2$ where

$$\sigma_1 = \frac{\pi}{2(a + \delta)}.$$

If δ is small, an interval of length a will contain slightly less than a quarter period of $\cos(\sigma_1 x)$. Choosing an orientation and initial vertex v_0, let $d(v_0, v_j) = x_j$ where v_j is the first vertex of pumpkin K_j, for $j = 1, \ldots, (|V| - 1)$. One of the segments has length $2a$, which we label by j_0. (We do not assume the lengths are arranged in order.) The strategy is to splice together functions of the form

$$h_j(x) := \begin{cases} \cos(\sigma_1(x - x_j) + \eta_j), & 1 \leq j \leq j_0, \\ \sin(\sigma_1(x - x_j) + \eta_j), & j_0 < j \leq |V| - 1. \end{cases} \tag{3.20}$$

Each phase shift η_j will be an integer multiple of $\sigma_1\delta/2$. First, we determine the phase shift for given δ. Then multiply each h_j by an amplitude term b_j to satisfy the continuity condition. In order to satisfy the net flow vertex condition, our edge multiplicities m_j will be determined.

We start with specifying η_j If $j \neq j_0$, then

$$\eta_j := \begin{cases} 0, & \text{if } j = 1, \\ \sigma_1\delta/2, & \text{if } 1 < j < m, \\ \sigma_1\delta, & \text{if } j = m. \end{cases}$$

For the segment of length $2a$, $j = j_0$, the phase shifts,

$$\eta_{j_0} := \begin{cases} 0, & \text{if } j_0 = 1, \\ \sigma_1\delta, & \text{if } 1 < j_0 < m, \\ 2\sigma_1\delta, & \text{if } j_0 = m. \end{cases}$$

Let the edges of sub-pumpkin K_j have length ℓ_j. The full eigenfunction ϕ, is defined by setting

$$\phi(x) := b_j h_j(x), \quad \text{for } x \in [x_j, x_j + \ell_j],$$

with b_j defined by the continuity condition. The matching conditions at vertex x_j are

$$\begin{aligned} b_{j-1}h_{j-1}(x_j) &= b_j h_j(x_j), \\ b_{j-1}m_{j-1}h'_{j-1}(x_j) &= b_j m_j h'_j(x_j), \end{aligned} \tag{3.21}$$

for $j = 2, \dots, (|V| - 1)$. Hence the edge multiplicities satisfy the condition

$$m_{j-1}h'_{j-1}(x_j) = m_j h'_j(x_j), \quad 2 \le j \le m. \tag{3.22}$$

Choosing δ so that $\sin(\sigma_1\delta/2)$ and $\cos(\sigma_1\delta/2)$ are both rational, then by basic trigonometric identities all of the values of h and h'/σ appearing in (3.22) will be rational. Hence, we can find a set of integers $m_1, \dots, m_{|V|-1}$ satisfying 3.22.

We can find arbitrarily small values of δ satisfying the rational condition by choosing a large integer n and setting

$$\frac{\sigma_1\delta}{2} = \frac{\pi\delta}{4(a+\delta)} = \arctan\left(\frac{2n}{n^2-1}\right). \tag{3.23}$$

Let δ be small enough such that $\sigma_1\delta < \pi/8$, After choosing the corresponding integers $m_1, \dots, m_{|V|-1}$ satisfying ((3.22)), we can then solve the coefficient equations ((3.21)) to construct an eigenfunction ϕ with eigenvalue $\lambda = \sigma_1^2$. If $\sigma_1\delta < \pi/8$, ϕ will be strictly decreasing, with a single zero at the midpoint of K_{j_0}.

To show that ϕ corresponds to eigenvalue $\lambda_1(K)$, assume there exists an eigenfunction ψ associated to the eigenvalue $\lambda < \sigma_1^2$. On K_1, $\psi = b_1\cos(\sqrt{\lambda}x + \alpha_1)$ and since $\sqrt{\lambda} < \sigma_1$ on each K_j, $j \le j_0$, ψ must take the form $b_j\cos(\sqrt{\lambda}x + \alpha_j)$. If we re-scale such that $\psi(0) = \phi(0)$, for all $x \le x_{j_0} + a$ then $\psi(x) > \phi(x)$ i.e. ψ does not contain a zero on the interval $[0, x_j + a]$. We can apply the same logic in reverse starting from $\psi(D)$, and deduce ψ does not have a zero on the interval $[x_j + a, D]$. Clearly, this is a contradiction as ψ is continuous and orthogonal to the constants. Thus, ϕ must correspond to $\lambda_1(K)$. □

Given a delta, the multiplicities can be calculated using (3.23). For $|V| = 5$, $D = 1$ and choosing K_2 to be the pumpkin with double length we find the multiplicities $m_1 = 1$, $m_2 = 10^{10}$, $m_3 = 10^{20}$, and $m_4 = 2 \times 10^{10}$ correspond to the eigenvalue $\lambda_1(K) = (2.49998\pi)^2$ which is very close to our bound of $\lambda_1(K) \le (2.5\pi)^2$.

CHAPTER 3

The Heat Kernel

1. Introduction to the Heat Kernel

Let G be a compact connected quantum graph. Consider the initial value problem on G for $f(x) \in H^1(G)$, where along each edge $e \in G$

$$\begin{cases} \Delta u(x,t) = \frac{\partial u(x,t)}{\partial t}, \\ u(x,0) = f(x). \end{cases} \tag{1.1}$$

Where $u(x,t)$ must satisfy the vertex conditions,

$$\begin{cases} u(x,t) \text{ is continuous on } G \\ \text{and} \\ \sum_{e\sim v} \frac{\partial u(x,t)}{\partial x_e} = 0, \end{cases} \tag{1.2}$$

for all $t > 0$.

We can find a solution for $u(x,t)$ using the integral kernel,

$$u(x,t) = e^{t\Delta} f. \tag{1.3}$$

The eigenfunctions of $-\Delta$ form a basis for $L^2(G)$, Let $\{\psi_n\}_{n=0}^{\infty}$ be this basis of eigenfunctions where ψ_i is the eigenfunction with eigenvalue λ_i. In this basis, f can be expressed

$$f = \sum_{n=0}^{\infty} A_n \psi_n, \tag{1.4}$$

where

$$A_n = \int_G f(y)\psi_n(y)dy. \tag{1.5}$$

Then $e^{t\Delta} f$ is

$$e^{t\Delta} f = \sum_{n=0}^{\infty} A_n e^{-t\lambda_k} \psi_n(x), \tag{1.6}$$

$$= \sum_{n=0}^{\infty} [\int_G f(y)\psi_n(y)dy] e^{-t\lambda_k} \psi_n(x), \tag{1.7}$$

$$= \int_G [\sum_{n=0}^{\infty} e^{-t\lambda_k} \psi_n(x)\psi_n(y)] f(y)dy. \tag{1.8}$$

(1.9)

The bracketed summation inside the integral is the heat kernel on G and is the fundamental solution to the initial-boundary problem stated in 1.1 and 1.2. We will use the notation

$$K_G(t,q,q_0) = \sum_{n=0}^{\infty} e^{-t\lambda_k}\psi_n(q)\psi_n(q_0). \tag{1.10}$$

Where q and q_0 are points along edges of G. If the eigenfunctions for $-\Delta$ are known then the heat kernel can be represented explicitly. The eigenfunctions of $-\Delta$ on each edge of G have the form

$$\psi_n = B_n \cos(\sqrt{\lambda_n}x_e + C_n). \tag{1.11}$$

However, in general the constants in the above formula are unknown. In the next section we will introduce another representation of the heat kernel, which we will use to prove the main results for this chapter. For a more in depth introduction to heat kernels on Riemannian manifolds we point the reader to [**10**].

2. Bond Scattering Matrix and Heat Kernel Formula

Let G be a compact connected quantum graph. For any pair of vertices v, w (possibly coinciding) connected by an edge e, we call a *directed bond* either of the ordered sets $\overrightarrow{b}_{vw} := \{v,w\}$ and $\overleftarrow{b}_{vw} := \{w,v\} = \overrightarrow{b}_{wv}$. We say that a bond $\overrightarrow{b}_{vw}$ is incoming at w and outgoing from v. Two bonds $\overrightarrow{b}_{vw}$ and $\overrightarrow{b}_{uz}$ are *consecutive* if $w = u$, i.e. if $\overrightarrow{b}_{vw}$ is an incoming bond and $\overrightarrow{b}_{wz}$ is an outgoing bond for the same vertex w.

As in definition 2.2 from Chapter 1, we define a path along G as an ordered sequence of consecutive bonds $\{\overrightarrow{b}_{v_1v_2}, \overrightarrow{b}_{v_2v_3} \ldots, \overrightarrow{b}_{v_{n-1}v_n}\}$. For any path p, its length is denoted $\ell(p)$ which is calculated by summing the lengths of all bonds in p.

Fix two points q and q_0 along edges of G and insert artificial vertices v_q at q and v_{q_0} at q_0. Call $P(q,q_0)$ the collection of paths beginning at v_q and ending at v_{q_0}, this is clearly a countable set. If $q = q_0$ we include in $P(q,q)$ the *trivial path* i.e. the empty sequence $\{\}$, and we say that the trivial path has length zero.

Assume the graph G, including the artificial vertices v_q and v_{q_0}, has m edges (hence $2m$ bonds). We fix an ordering on the set of bonds in G so that given any $2m \times 2m$ matrix $A = \{a_{ik}\}$, we can uniquely associate each row and each column of A with a bond. According to the ordering on the bonds in G we can also identify any path p with an ordered sequence of integers $\{i_1, \ldots, i_q\} \in \{1, \ldots, 2m\}^q$, so that we can set

$$\alpha_A(p) := \begin{cases} 1 & \text{if } q = 0, 1, \\ \prod_{\ell=1}^{q-1} a_{i_\ell i_{\ell+1}} & \text{if } q \geq 2. \end{cases} \tag{2.1}$$

In particular the *bond scattering matrix* B is a $2m \times 2m$ orthogonal matrix with coefficients

$$\beta_{ik} := \begin{cases} 2/d_v - 1 & \text{if } k = \overrightarrow{b}_{wv} \text{ and } i = \overleftarrow{b}_{wv} \quad \text{(bounce)}, \\ 2/d_v & \text{if } k = \overrightarrow{b}_{wv} \text{ and } i = \overrightarrow{b}_{vu} \text{ with } \overrightarrow{b}_{wv} \neq \overrightarrow{b}_{vu} \quad \text{(transfer)}, \\ 0 & \text{otherwise.} \end{cases} \tag{2.2}$$

We will refer to β_{ik} as a *scattering component* of B.

Remark 2.1. Note that if a graph G' is obtained from G by adding an artificial vertex, then any path p in G corresponds to a path p' in G' and one has

$$\alpha_B(p) = \alpha_{B'}(p').$$

When the matrix B is understood, we will use the simpler notation $\alpha(p)$.

DEFINITION 2.2. We will call $K_G(t,q,q_0)$ a *rational heat kernel* if after inserting the artificial vertices v_q and v_{q_0} all edges have rational length.

From [**14**], we quote the following

PROPOSITION 2.3. *For a compact quantum graph G, if $\alpha_B(p)$ is defined as in* (2.1) *with B as in* (2.2)*, then the heat kernel for G is given by*

$$K_G(t,q,q_0) = \frac{1}{\sqrt{4\pi t}} \sum_{p\in P(q,q_0)} \alpha_B(p) e^{-\ell(p)^2/4t}. \tag{2.3}$$

In light of Proposition 2.3, we call the coefficients $\alpha_B(p)$ the *heat path coefficients* when B is the bond scattering matrix.

EXAMPLE 2.4. For a single interval I of length ℓ, with Neumann boundary conditions, the eigenfunction expansion of the heat kernel is

$$K_I(t,q,q_0) = \frac{1}{\ell} + \frac{2}{\ell}\sum_{j=1}^{\infty} e^{-(\frac{j\pi}{\ell})^2 t}\cos(\tfrac{j\pi}{\ell}q)\cos(\tfrac{j\pi}{\ell}q_0).$$

The alternative formula given by Proposition 2.3 is actually the result obtained by the method of images:

$$K_I(t,q,q_0) = \frac{1}{\sqrt{4\pi t}} \sum_{k\in\mathbb{Z}^+} \Big[e^{-(q-q_0+2k\ell)^2/4t} + e^{-(q+q_0+2k\ell)^2/4t}\Big]. \tag{2.4}$$

3. Heat Kernel for Small Time

From (2.3), it is clear that for small enough time the contributions from the shortest paths dominate the sum. The following proposition bounds the heat kernel for small time.

PROPOSITION 3.1. *Let G be an arbitrary quantum graph with minimum edge length a_0 and m edges. For a point $q \in G$, let v_0 be the closest non-artificial vertex with degree d_0. For $t < a_0^2/2log(m)$,*

$$K(t,q,q) = \frac{1}{\sqrt{4\pi t}}\Big[1 + (\frac{2}{d_{v_0}} - 1)e^{-d(v_0,q)^2/t} + O(me^{-a_0^2/t})\Big]. \tag{3.1}$$

PROOF. Let e have vertices v_0 and v_1 and $q \in e$, with $d(v_0,q) \le d(v_1,q)$. Let $|E(G)| = m$. The set $P(q,q)$ contains the trivial path, the path with a single reflection off of v_0, and the path with a single reflection off of v_1. All other paths in $P(q,q)$ contain a complete edge. Let $R(t,q)$ be the contribution to (2.3) from all paths containing a complete edge. We can re-write (2.3) as

$$K(t,q,q) = \frac{1}{\sqrt{4\pi t}}\Big[1 + (\frac{2}{d_{v_0}} - 1)e^{-d(v_0,q)^2/t} + (\frac{2}{d_{v_1}} - 1)e^{-d(v_1,q)^2/t} + R(t,q)\Big]. \tag{3.2}$$

Suppose that p is a path in $P(q,q)$ containing k complete edges, $k \ge 1$. Then, $\ell(p) \ge ka_0 + 2d(v_0,q)$, where a_0 is the shortest edge of G. The number of paths containing exactly k edges is bounded by m^k. Thus we can bound $R(t,q)$,

$$|R(t,q)| \le \sum_{k=1}^{\infty} m^k e^{-(2d(v_0,q)+ka_0)^2/4t}. \tag{3.3}$$

For $t < a_0^2/2log(m)$ and $k \ge 1$, we can bound each term in the sum above by

$$\frac{(ka_0)^2}{4t} + klog(m) \geq -\frac{a_0^2}{4t} + \frac{ka_0^2}{2t} + klog(m). \tag{3.4}$$

Creating a new bound for $R(t,q)$,

$$|R(t,q)| \leq \sum_{k=1}^{\infty} m^k e^{a_0^2/4t - ka_0^2/2t}, \tag{3.5}$$

$$= \sum_{k=1}^{\infty} e^{a_0^2/4t}(me^{-a_0^2/2t})^k, \tag{3.6}$$

$$= \frac{me^{-a_0^2/4t}}{1 - me^{-a_0^2/2t}}. \tag{3.7}$$

□

Using a similar strategy, for points $q_1 \neq q_2$

$$K(t,q_1,q_2) \sim \frac{c}{\sqrt{4\pi t}} e^{-d(q_1,q_2)^2/4t}. \tag{3.8}$$

Where c is the sum of $\alpha(p)$ coefficients for all minimum distance paths between q_1 and q_2,

$$c = \sum_{\substack{p \in P(q_1,q_2) \\ \ell(p) = d(q_1,q_2)}} \alpha(p). \tag{3.9}$$

We note that minimal paths can't contain reflections, so for all $\alpha(p)$ in the above sum

$$\alpha(p) = \prod_{v \in p} \frac{2}{d_v} > 0. \tag{3.10}$$

4. Construction of the Graph G_n^*

In the following sections our goal is to show that for particular edges we can bound the heat kernel coefficients associated with paths in $P(q,q_0)$. For these special edges, we can use the bound on the heat path coefficients to bound the heat kernel.

We start by partitioning the paths in $P(q,q)$ by

(1) The initial direction of the path (leaves q to the left or right).
(2) How many times the path returns to the point q.

We will need to control the sum of heat path coefficients for paths with less than M bonds. Every heat path coefficient $\alpha(p)$, can be associated with a path p via (2.1). To control the sum of coefficients in each partition we will construct directed bond graphs (DBG) G_n^* for $n \in \{1,2,...\}$. These DBG will allow us to control the sum of coefficients for the two partitions that return to q n-times, and are defined as follows.

Definition 4.1. A graph is a set of vertices connected by edges. With each edge we can associate two directed bonds. A directed bond graph is a set of vertices and bonds. Given a graph G, we define the directed bond graph (DBG) G^* associated to G as the set of vertices and bonds of G (i.e. G where the edges are all replaced by directed bonds).

We start by constructing a new graph G' by inserting two artificial vertices on either side of v_q along the same edge e, call these vertices v_1 and v_2. We also introduce the set

$\mathbb{P}(q)$, which is all paths along G' from v_q to v_q that do not bounce at artificial vertices (namely v_q, v_1, and v_2).

Note a subtle but important distinctions between the sets $\mathbb{P}(q)$ and $P(q,q)$. Every path in $\mathbb{P}(q)$ corresponds to a path in $P(q,q)$, but because of the inserted vertices v_1 and v_2 the path in $\mathbb{P}(q)$ will contain more bonds and hence more bond transfers.

We number the bonds of G' according to the following picture where only the edge e is included:

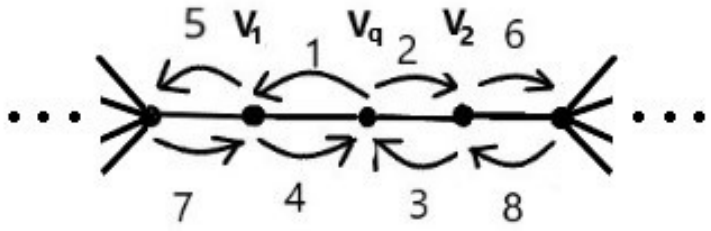


FIGURE 1. Outgoing bonds of v_q are labeled 1 and 2, incoming bonds of v_q are 3 and 4, and outgoing bonds of v_1 and v_2 oriented away from v_q are bonds 5 and 6 respectively

Note that we choose this numbering only for computational convenience, any alternate numbering would not change our result. Fix some numbering for all other bonds of G'. Let B' be the bond scattering matrix for the graph G'. By construction v_q, v_1, and v_2 are all artificial vertices. This implies the entries of columns 1 through 4 of B' are zeros except for a single entry equal to 1. Since the scattering component for bond transfers at artificial vertices is equal to 1, while it is zero for bounces. Moreover, if a path p bounces at a vertex of degree two, then by (2.1) we have $\alpha(p) = 0$, hence such a path does not contribute to the heat kernel formula. This means

$$K_G(t,q,q) = K_{G'}(t,q,q) = \frac{1}{\sqrt{4\pi t}} \sum_{p \in P(q,q)} \alpha_B(p) e^{-\ell(p)^2/4t} = \frac{1}{\sqrt{4\pi t}} \sum_{p' \in \mathbb{P}(q)} \alpha_{B'}(p') e^{-\ell(p')^2/4t}.$$

We insert the artificial vertices v_1 and v_2 because we will need to change the out-going bonds of v_q to loops. Inserting these vertices allows us to construct paths from v_1 or v_2 to v_q with the same heat path coefficients as paths in $\mathbb{P}(q)$.

Now consider the DBG $(G')^*$ associated with G' and construct the DBG G_1^* by changing the outgoing bonds of v_q (bond 1 and bond 2) to loops from v_q to v_q. We construct the matrix $\mathrm{B^*}_1$ from B' by changing columns 1 through 4 of B' to have a one in the first row and zeros elsewhere, keeping all other columns the same. Note that a path p containing bond 3 (respectively bond 4) has $\alpha_{\mathrm{B^*}_1}(p) = 0$ if the bond directly following bond 3 (respectively bond 4) is not bond 1 (respectively bond 2).

In Figure 2, we show the DBG $(G')^*$ and G_1^* for a 3 edged star graph.

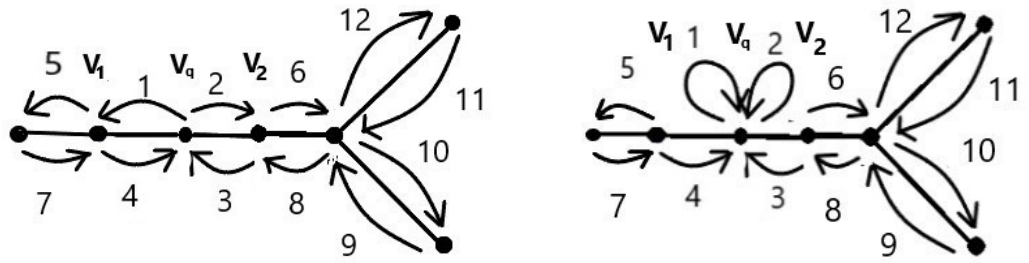


FIGURE 2. (a) The Graph $(G')^*$ for a 3 edged star graph and (b) the DBG G_1^* for the same 3 edged star graph

To construct the DBG G_n^*, we start with n copies of the DBG $(G')^*$. Assume $(G')^*$ has $2m$ bonds. Each copy of $(G')^*$ is ordered and relabeled such that bond i on copy k of $(G')^*$ is renumbered to be $i+(k-1)2m$. Each copy of v_q is relabeled such that v_q on copy k becomes v_{q_k}. Then we connect each copy of $(G')^*$ by having bond $4+(k-1)2m$ transfer to bond $6+2mk$ for $k \in \{1,2,...,n\}$, i.e bond 4 is connected to bond 6 of the next copy of $(G')^*$ and bond $3+(k-1)2m$ is connected to bond $5+2mk$, i.e. bond 3 transfers to bond 5 of the next copy of $(G')^*$. On the last copy of $(G')^*$, copy number n, $(G')^*$ is converted to G_1^*, i.e. bond $1+(n-1)2m$ and bond $2+(n-1)2m$ are changed to loops from v_{q_n} to v_{q_n}. We force the length of each bond in G_n^* to be the same length as the corresponding bond in $(G')^*$.

We now introduce a $2mn \times 2mn$ matrix B_n^* obtained from B' as follows. We start with a $2mn \times 2mn$ block diagonal matrix, containing n blocks of size $2m \times 2m$, where each block is the matrix B'. The matrix entries equal to one in the 3rd and 4th columns are moved down $2m+4$ rows for each block, excluding the last block where this is not possible. So, we change $b_{24} = 1$ to $b_{24} = 0$ and $b_{(6+2m)(4)} = 0$ to $b_{(6+2m)(4)} = 1$. Similarly, $b_{13} = 1$ is changed to $b_{13} = 0$ and $b_{(5+2m)(3)} = 0$ to $b_{(5+2m)(3)} = 1$. The last block is converted to the matrix $\mathrm{B^*}_1$.

Note that for each block, only entries associated with either incoming or outgoing bonds of v_q are changed. The DBG G_2^* for a three edged star graph is given in Figure 4.

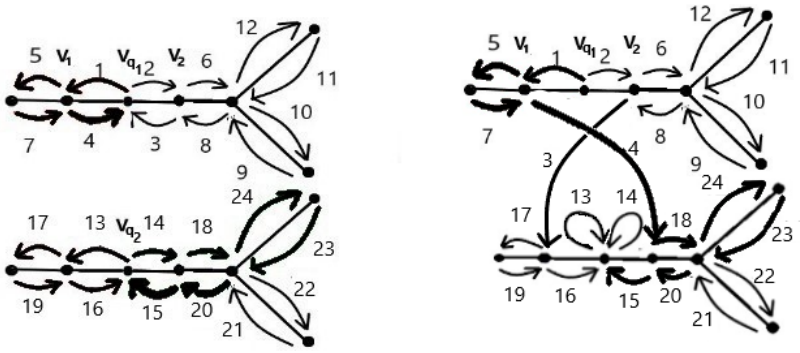


FIGURE 3. (a) Two copies of the DBG $(G')^*$ with renumbered bonds, and (b) G_2^*, bond 3 connects to bond 5+12=17 and bond 4 connects to bond 6+12=18. Bonds 1+12 and 2+12 are changed to loops

In the next section we will show there exists a bijection Ψ between non-trivial paths p along G' that return to v_q n-times and paths p^* along G_n^* from v_{q_1} to v_{q_n}. Furthermore, the bijection preserves the heat path coefficient for each path in the sense that

$$\alpha_{B'}(p) = \alpha_{\mathrm{B}^*{}_n}(\Psi(p)). \tag{4.1}$$

By investigating the heat path coefficients for paths from v_{q_1} to v_{q_n} along G_n^*, we can deduce information about the heat path coefficients for paths in $P(q,q)$ that return to v_q n-times. Investigating the non-zero heat path coefficients for the DBG G_n^* will be easier because the loops at v_{q_n} "trap" the heat path coefficients at the bond $1+2(n-1)m$ (first loop of v_{q_n}).

5. Identifying Paths along G' and G_n^*

We will show there is a bijection Ψ between non-trivial paths in $\mathbb{P}(q)$ that return to v_q n-times and paths p along G_n^* from bond 5 or bond 6 to v_{q_n} such that

$$\alpha_{B'}(p) = \alpha_{\mathrm{B}^*{}_n}(\Psi(p)). \tag{5.1}$$

We partition the paths of $\mathbb{P}(q)$ according to 2 criteria:

(1) Whether the first bond is bond 1 or bond 2 (initial direction).
(2) Number of outgoing bonds of v_q the path contains (number of returns to v_q).

It will also be convenient to work with paths of finite length. In order to do so we introduce the following sets:

DEFINITION 5.1. For $n \geq 1$ we denote by $P_{n,M}^i(G')$ the subset of $\mathbb{P}(q)$ of paths starting with bond $i \in \{1,2\}$, containing n outgoing bonds of v_q, and containing less than M bonds.

DEFINITION 5.2. For $n \geq 1$ we denote by $\widetilde{P_{n,M}^i}(G_n^*)$ the set of paths along G_n^* that start with bond $i \in \{5,6\}$ and end at bond $1+2m(n-1)$, i.e. the first loop bond of v_{q_n}, with exactly $M-n$ bonds.

REMARK 5.3. In Definition 5.1 (respectively 5.2) we wrote explicitly the dependence on G' (respectively 5.2) of the set $P^i_{n,M}$ (respectively $\widetilde{P^i_{n,M}}(G^*_n)$). We shall omit such dependence every time it is clear which graph (respectively DBG) we are referring to.

LEMMA 5.4. *For $n \geq 1$ there exists a bijective map $\Psi : P^i_{n,M} \to \widetilde{P^{i+4}_{n,M}}$ for all $i \in \{1,2\}$, and all M and n.*

PROOF. We will show the proof for $i = 1$, the proof for $i = 2$ follows the same strategy. First, we note that any path $p \in P^1_{n,M}$ is the concatenation of n sub-paths from v_q to v_q containing only one out-going bond of v_q, hence each sub-path starts and ends at v_q but never crosses-over v_q. Let $P_1 \subset \mathbb{P}(q)$, be the set of paths from v_q to v_q containing one out-going bond of v_q, and introduce the map

$$\phi_1 : P^1_{n,M} \longrightarrow \underbrace{P_1 \times \ldots \times P_1}_{n\text{–times}},$$

where we think of each P_1 to be on a separate copy of G'. We maintain the order of sub-paths with copies of G', i.e. the i^{th} sub-path is sent to the i^{th} copy of G'.
Assume p has $m < M$ bonds, $m \neq 1$ since any path in $\mathbb{P}(q)$ must contain at least two bonds, with the exception of the trivial path. Assume $m \geq 2$ and let $p = \{ \overrightarrow{b}_{w_1,w_2}, \overrightarrow{b}_{w_2,w_3}, ..., \overrightarrow{b}_{w_q,w_{q+1}} \}$. From the definition of $P^1_{n,M}$, $w_1 = w_{q+1} = v_q$ and $w_2 = v_1$. Moreover p contains n outgoing bonds of v_q, thus

$$\#\{\text{bond 1 in } p\} + \#\{\text{bond 2 in } p\} = n \tag{5.2}$$

Using each appearance of bond 1 or bond 2 as delimiters, we separate p into n shorter sub-paths. Where bond 1 or bond 2 mark the start of the next sub-path. By continuity of the path p, all sub-paths must end with either bond 3 or bond 4, i.e. if sub-path $k+1$ starts with bond 1, sub-path k must end with bond 3 and if sub-path $k+1$ starts with bond 2, sub-path k must end with bond 4. This implies each sub-path is contained in P_1. Thus, ϕ_1 is injective. We define the set ${P^1_{n,M}}'$ to be the image of $P^1_{n,M}$ under ϕ_1, so that $\phi_1 : P^1_{n,M} \to {P^1_{n,M}}'$, is bijective. The set ${P^1_{n,M}}'$ can be viewed as an ordered n-tuple of sub-paths. In Figure 4 is an example of a path in P^1_{2M} and its image under ϕ_1.

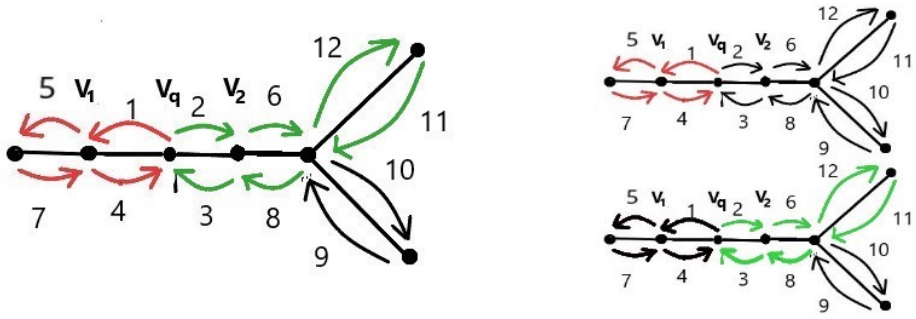


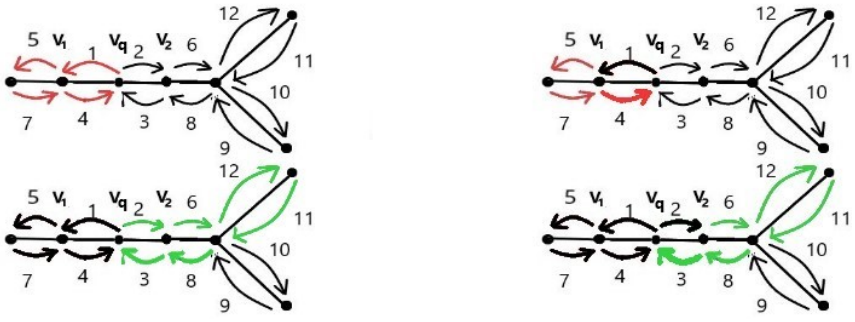
FIGURE 4. (a) Graph G' with path starting at v_q and containing two out-going bonds of v_q, and (b) two copies of G' containing the ordered P_1 sub-paths

Let P_1' be the set of paths on G' that start either at v_1 or v_2, end at v_q and have no out-going bond of v_q. We now introduce a map

$$\phi_2 : {P^1_{n,M}}' \longrightarrow \underbrace{P_1' \times \ldots \times P_1'}_{n\text{–times}},$$

which acts on each P_1 sub-path by removing the first bond. Note that for all paths in P_1, the first bond is uniquely specified by the second bond, since v_1 and v_2 are artificial vertices with a trivial bond transfer. For instance if the second bond for a path in P_1 is bond 6 this implies the first bond must be bond 2. Therefore ϕ_2 is injective, an example is in Figure 5.

We define ${P^1_{nM}}''$ to be the image of ${P^1_{nM}}'$ under ϕ_2, so that $\phi_2 : {P^1_{nM}}' \to {P^1_{nM}}''$ is bijective.



(a) An element of ${P^1_{2M}}'$ (b) The same elements image under ϕ_2

FIGURE 5. (a) An element of ${P^1_{2M}}'$, and (b) the same elements image under ϕ_2

As done when constructing G^*_n, we relabel the bond numbering for the n ordered copies of G' such that bond i along copy k of G' is relabeled bond $i + (k-1)2m$, $k \in \{1, 2, ..., n\}$. Thus, each bond on the n copies of G' can be naturally associated with a bond on G^*_n. Let

ϕ_3 represent this renumbering of bonds. Then, for $p \in {P^1_{n,M}}''$ clearly $\phi_3(p)$ is a continuous path on G^*_n, as any sub-path ending with bond $3+2m(k-1)$ the next sub-path must start with $5+2mk$.

Since, every path on G^*_n is uniquely determined by its order bond sequence we have for $p_a, p_b \in {P^1_{n,M}}''$, if $\phi_3(p_a) = \phi_3(p_b)$, then $p_b = p_a$. We let ${P^1_{nM}}'''$ be the image of ${P^1_{n,M}}''$ under ϕ_3. Thus, $\phi_3 : {P^1_{n,M}}'' \to {P^1_{n,M}}'''$ is bijective, see Figure 6.

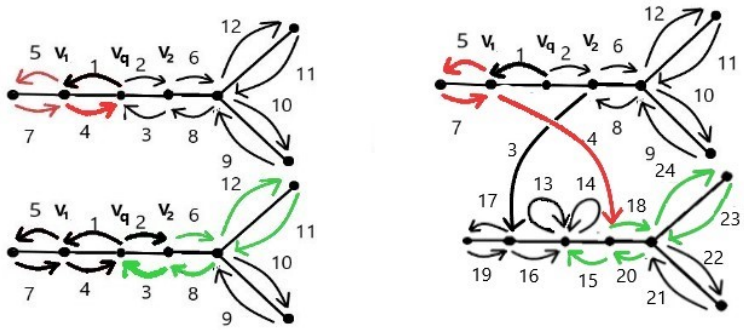


FIGURE 6. (a) An element in ${P^1_{2M}}''$, and (b) its image under ϕ_3

Finally, note that if $p'' \in {P^1_{n,M}}''$, and $\phi_3(p'') = p''' \in {P^1_{n,M}}'''$ then p''' has less than or equal to $M-(n-1)$ bonds, because we deleted a bond from each copy of G'. Since p has m bonds, then p''' must have $m-n$ bonds.

We introduce the last map ϕ_4,

$$\phi_4 : {P^1_{n,M}}''' \longrightarrow \widetilde{P^5_{n,M}}.$$

that adds $M-m$ loops, on bond $1+(n-1)2m$, to the path p'''. Thus, the path $\phi_4(p''')$ contains at least one loop and exactly $(m-n)+M-m = M-n$ bonds, an example is in Figure 7.

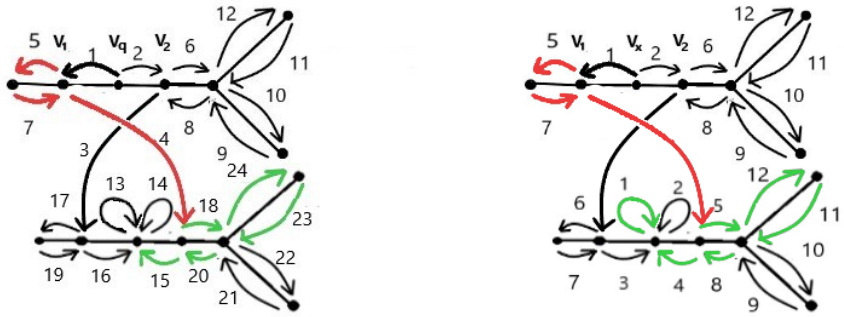


FIGURE 7. (a) Graph G^*_2 with path in ${P^1_{2,M}}'''$, and (b) image under ϕ_4 containing $M-10+1$ loops

Clearly, ϕ_4 is injective, and hence $\Psi := \phi_4 \circ \phi_3 \circ \phi_2 \circ \phi_1$ is injective. To complete the proof me must show that Ψ is onto $\widetilde{P^5_{n,M}}$. Let $\widetilde{p} \in \widetilde{P^5_{n,M}}$ and say it is given by the bond sequence $\{b_1^*, b_2^*, ..., b_t^*\}$. In particular $\widetilde{p}$ must start at bond 5 and end with bond $1 + 2(n-1)M$, containing exactly $M - n$ bonds by the definition of $\widetilde{P^5_{n,M}}$.

Let $p \in P^1_{n,M}$ obtained from $\widetilde{p}$ as follows:

(1) Delete the loops of $\widetilde{p}$.
(2) On the n copies of G' construct a sequence of paths having bond numbers equal to the bond numbers of $\widetilde{p}$ without the loops.
(3) To each path on each copy of G' add a bond starting at v_q as the first bond.
(4) Concatenate the paths on the copies of G' in a single path $p \in P^1_{n,M}$.

Then by construction $\Psi(p) = \widetilde{p}$, hence Ψ is onto.

□

LEMMA 5.5. *Let Ψ be the bijective map of Lemma 5.4. Let $\alpha_{G'}(p)$ be the heat path coefficient associated with path $p \in P^i_{n,M}$ and $\alpha_{G^*_n}(\phi(p))$ be the heat path coefficient for $\phi(p) \in \widetilde{P^{i+4}_{n,M}}$, $i \in \{1, 2\}$. Then*

$$\alpha_{B'}(p) = \alpha_{\mathrm{B^*}_n}(\Psi(p)), \tag{5.3}$$

for all M and n.

PROOF. We prove the result for $i = 1$; of course one can reason the same way for $i = 2$. The proof relies on the fact that $\Psi : P^1_{n,M} \to \widetilde{P^5_{n,M}}$ is bijective, and for each step in the mappings ϕ_1, ϕ_2, ϕ_3, and ϕ_4 we add or delete bond transfers with bond scattering matrix entries equal to one, thus the product of bond scattering matrix entries remains unchanged under the mappings.

Consider a path $p = \{i_1, \ldots, i_q\} \in P^i_{n,M}$, note that if $q = 0$ or $q = 1$, $\alpha_{B'}(p) = \alpha_{\mathrm{B^*}_n}(\Psi(p)) = 1$ and the result is trivial. Assume $q \geq 2$, then we can identify p with a sequence of elements of B', namely the sequence $\{\beta'_{i_1,i_2}, \beta'_{i_2,i_3}, \ldots, \beta'_{i_{q-1},i_q}\}$.

The map ϕ_1 acts on p by separating p into n sub-paths in $G' \times \ldots \times G' =: (G')^n$. Each sub-path of p as a path in G' is connected by either the bond transfer bond 3 to bond 1 or bond 4 to bond 2. Thus, applying ϕ_1 is equivalent to deleting all bond transfers from bond 3 to bond 1 and all bond transfers from bond 4 to bond 2. Note that $\beta'_{24} = \beta'_{13} = 1$, since v_q is an artificial vertex. If we denote the k-th sub-path of p as p_k we have

$$\alpha_{B'}(p) = \prod_{k=1}^{n} \alpha_{B'}(p_k). \tag{5.4}$$

Next, ϕ_2 acts on each copy of G' by deleting the first bond in each sub-path, we can write

$$\phi_2(p_1, \ldots, p_n) = (\phi_2(p_1), \ldots, \phi_2(p_n)). \tag{5.5}$$

Observe that ϕ_2 acts on p_k by deleting either bond 1 or bond 2 and thus deletes either the bond transfer from bond 1 to bond 5, β'_{51}, or bond 2 to bond 6, β'_{62}. Because v_1 and v_2 are artificial vertices, $\beta'_{51} = \beta'_{62} = 1$, and hence

$$\alpha_{B'}(p_k) = \alpha_{B'}(\phi_2(p_k)), \tag{5.6}$$

Combined with (5.4) implies

$$\alpha_{B'}(p) = \prod_{k=1}^{n} \alpha_{B'}(\phi_2(p_k)). \tag{5.7}$$

The map ϕ_3 concatenates all the sub-paths p_k onto a single path on G_n^*. The concatenation introduces bond transfers from bonds $4+(k-1)2m$ to $6+2km$ and from bonds $3+(k-1)2m$ to $5+2km$, $k \in \{1, 2, ..., n-1\}$. Moreover we note that $b^*_{6+2km,4+(k-1)2m} = b^*_{5+2km,3+(k-1)2m} = 1$ where $b^*_{i,k}$ are the elements of the matrix $\mathrm{B^*}_n$, so that

$$\prod_{k=1}^{n} \alpha_{B'}(\phi_2(p_k)) = \alpha_{\mathrm{B^*}_n}(\phi_3(\phi_2(p_1, \ldots, p_n))) = \alpha_{B'}(\phi_3(\phi_2(\phi_1(p))))). \tag{5.8}$$

Finally, ϕ_4 adds $M - m$ bond transfers to bond $1 + 2m(n-1)$, the loop bond of v_{q_n}. These bond transfers all correspond to an element of $\mathrm{B^*}_n$ equal to 1. Thus,

$$\alpha_{\mathrm{B^*}_n}(\phi_3(\phi_2(p_1, \ldots, p_n))) = \alpha_{\mathrm{B^*}_n}(\phi_4(\phi_3(\phi_2(p_1, \ldots, p_n))). \tag{5.9}$$

so that combining (5.9) with (5.8), (5.7) and the definition of Ψ the assertion follows. □

6. Bounding Coefficients in the Heat Kernel Formula

Lemma 6.1 below is a general fact about quantum graphs and their bond scattering matrices. Let e_s be the vector with components δ_{is} the Kronecker-delta.

LEMMA 6.1. *Let G be an arbitrary quantum graph with $2m$ directed bonds. Let B be the bond scattering matrix for G. Let $\mathcal{P}^m_{s,k}$ be the set of all paths starting with bond s and ending with bond k and having exactly $m+1$ bonds (hence m bond transfers). then*

$$(B^m e_s)_k = \sum_{p \in \mathcal{P}^m_{s,k}} \alpha_B(p).$$

PROOF. Let β_{ij} be the entry in row i, column j of B, defined as in (2.2). We know that $(B^m e_s)_k$ is a sum of products, we will show that all non-zero terms in the sum can be uniquely identified with a path along G from bond s to bond k with m bond transfers. Simple matrix multiplication shows

$$(B^m e_s)_k = \sum_{i=1}^{2m} \sum_{j=1}^{2m} \sum_{h=1}^{2m} \ldots \sum_{\ell=1}^{2m} (\beta_{is}) \beta_{ji} \beta_{hj} \cdot \ldots \cdot \beta_{k\ell}. \tag{6.1}$$

Let a be an arbitrary element in the above sum, and note that it has the form

$$a = \beta_{i_1,i_0} \beta_{i_2,i_1} \cdot \ldots \cdot \beta_{i_m,i_{m-1}}, \qquad i_0 = s,\ i_m = k. \tag{6.2}$$

We want to show that if the ordered sequence $\{i_0, i_1, \ldots, i_q\}$ is not a path $p \in \mathcal{P}^m_{s,k}$ then $a = 0$. In other words we need to show that i_d and i_{d+1} are consecutive bonds for $d \in \{0, 1, 2, ..., m-1\}$.

For a to be non-zero, each $\beta_{i_d j_d}$ must be non-zero. By the definition of B each non-zero β_{ij} is non-zero if i and j are consecutive bonds. Thus the assertion follows. □

COROLLARY 6.2. *One has*

$$((B^*_n)^{M-n-1} e_k)_{1+2m(n-1)} = \sum_{p \in P^i_{n,M}} \alpha(p), \tag{6.3}$$

for $i \in \{1, 2\}$, $k = i + 4$, and all M and n.

PROOF. From Lemma 5.5 it follows that

$$\sum_{p\in P^i_{n,M}} \alpha_{B'}(p) = \sum_{\widetilde{p}\in\widetilde{P^{i+4}_{n,M}}} \alpha_{\mathrm{B^*}_n}(\widetilde{p}). \tag{6.4}$$

where $P^i_{n,M}$ and $\widetilde{P^{i+4}_{n,M}}$ are defined in Definitions 5.1 and 5.2 respectively. Using Lemma 6.1 we have

$$\sum_{\widetilde{p}_\ell\in\widetilde{P^{i+4}_{n,M}}} \alpha_{\mathrm{B^*}_n}(\widetilde{p}) = ((B^*_n)^{M-n-1}e_5)_{1+2m(n-1)}, \tag{6.5}$$

so the assertion follows. □

DEFINITION 6.3. We say an edge is *direct path bounded* if for $i \in \{1,2\}$

$$1) \lim_{M\to\infty} \sum_{p\in P^i_{1,M}} \alpha(p) = 1, \tag{6.6}$$

$$2) \sum_{p\in P^i_{1,M_1}} \alpha(p) \le \sum_{p\in P^i_{1,M_2}} \alpha(p), \tag{6.7}$$

for all $M_0 \le M_1 \le M_2$, and $M_0 = \min_{p\in P^i_1}\{\#bonds(p)\}$.

Note, conditions 1) and 2) imply

$$|\sum_{p\in P^i_{1M}} \alpha(p)| \le 1. \tag{6.8}$$

DEFINITION 6.4. Let v_0, v_1 be the vertices for $e \in G$. We will say that e has no *loop paths* if for all $p \in P(v_0, v_1)$, p contains the edge e. In other words, the only way to get from v_0 to v_1 is to travel across e.

We will use the notation that $Be_i(j)$ is entry j in the vector Be_i.

LEMMA 6.5. *Let $e \in G$ be a direct path bounded edge with m edges, then for all $i \in \{1,2\}$*

$$|\sum_{n=1}^{N} (B^*_n)^M e_{i+4}(2m(n-1)+1)| \le N, \tag{6.9}$$

or equivalently

$$|\sum_{n=1}^{N}[\sum_{p\in P^i_{n,M}} \alpha(p)]| \le N. \tag{6.10}$$

PROOF. We will start with the assumption that e has no *loop paths*, defined in 6.4. For convenience, let

$$\alpha^i_j = \sum_{\substack{p\in P^i_{1,M}\\ \#bonds(p)=j}} \alpha(p). \tag{6.11}$$

Note that many α^i_j will be zero, these terms can be ignored. With the above notation we can rewrite

$$\sum_{p^i_{1,M}} \alpha(p) = \sum_{j=1}^{M} \alpha^i_j. \tag{6.12}$$

By assumption there are no loop paths, this implies any path $p \in P^1_{n,M}$ is the concatenation of n paths alternating between $P^1_{1,M}$ and $P^2_{1,M}$. Let $\#(p)$ represent the number of bonds along p. Since all paths in $P^i_{n,M}$ have less than or equal to M bonds

$$\sum_{p\in P^1_{n,M}} \alpha(p) = \sum_{p\in P^i_{(n-1),M}} [\alpha(p) \sum_{j=1}^{M-\#(p)} \alpha^k_j]. \tag{6.13}$$

Where $k = 1$ if n is odd and $k = 2$ if n is even. Without loss of generality assume n is even. The above formula gives a recursive relationship for finding the sum of heat kernel coefficients for paths in $P^i_{n,M}$,

$$\sum_{p\in P^1_{n,M}} \alpha(p) = \sum_{j_1=1}^{M} \sum_{j_2=1}^{M-j_1} ... \sum_{j_n=1}^{(M-j_1...-j_{n-1})} \alpha^1_{j_1}\alpha^2_{j_2}...\alpha^1_{j_{n-1}}\alpha^2_{j_n}. \tag{6.14}$$

Using the above equation, we can find the sum of heat kernel coefficients in both $P^1_{n,M}$ and $P^1_{(n-1),M}$ by

$$\sum_{p\in P^1_{n,M}} \alpha(p) + \sum_{p\in P^1_{(n-1),M}} \alpha(p) = \sum_{j_1=1}^{M} \sum_{j_2=1}^{M-j_1} ... \sum_{j_{n-1}=1}^{(M-j_1...-j_{n-2})} \alpha^1_{j_1}\alpha^2_{j_2}...\alpha^1_{j_{n-1}}(1 + \sum_{j_n=1}^{(M-j_1...-j_{n-1}} \alpha^2_{j_n}). \tag{6.15}$$

Extending this new recursive relation, we have

$$\sum_{n=1}^{N}(\sum_{p\in P^1_{n,M}} \alpha(p)) = \sum_{j_1=1}^{M} \alpha^1_{j_1}(1 + \sum_{j_2=1}^{M-j_1} \alpha^2_{j_2}(1 + ...(1 + \sum_{j_{n-1}=1}^{(M-j_1...-j_{n-2})} \alpha^1_{j_{n-1}}(1 + \sum_{j_n=1}^{(M-j_1...-j_{n-1})} \alpha^2_{j_n})...). \tag{6.16}$$

The assumption that e is direct path bounded implies for all Q,

$$|\sum_{j=1}^{Q} \alpha^i_j| \leq 1. \tag{6.17}$$

If $P^i_{1,M}$ contains at least one path than for all M

$$\sum_{j=1}^{M} \alpha^i_j \leq \sum_{j=1}^{(M+1)} \alpha^i_j. \tag{6.18}$$

Which implies if $P^i_{1,(M-j_1...-j_{n-1})}$ contains at least one path then

$$\sum_{j_n=1}^{(M-j_1...-j_{n-1})} \alpha^i_{j_n} \leq \sum_{j_n=1}^{(M-j_1...-1)} \alpha^i_{j_n}, \tag{6.19}$$

if $P^i_{1,(M-j_1...-j_{n-1})}$ does not contain a path then all $\alpha_{j_n} = 0$ and we can drop this term. This implies

$$(1 + \sum_{j_n=1}^{(M-j_1...-j_{n-1})} \alpha^i_{j_n}) \leq (1 + \sum_{j_n=1}^{(M-j_1...-1)} \alpha^i_{j_n}). \tag{6.20}$$

Where

$$0 \leq (1 + \sum_{j_n=1}^{(M-j_1\ldots-1)} \alpha_{j_n}^i) \leq 2, \tag{6.21}$$

and the sum is no longer dependent on j_{n-1}. Recall from the definition of direct path bounded that for $p \in P_{1,M}^i$, only the path with the least number of bonds can have a negative coefficient. We will call this coefficient $\alpha_{neg}^i < 0$. If α_{neg}^i is not less than zero, than the edge e must have a degree one vertex and $\alpha_{neg}^i = 1$ is the only non-zero coefficient. We can then replace $\sum_{j=1}^M \alpha_j^i$ with 1 and the result follows the steps below. Assume $\alpha_{neg}^i < 0$,

$$-2 \leq 2\alpha_{neg}^1 \leq \sum_{j_{n-1}=1}^{(M-j_1\ldots-j_{n-2})} \alpha_{j_{n-1}}^1 (1 + \sum_{j_n=1}^{(M-j_1\ldots-j_{n-2}-1)} \alpha_{j_n}^2) \leq 2 \sum_{j_{n-1}=1}^{(M-j_1\ldots-j_{n-2})} \alpha_{j_{n-1}}^1 \leq 2. \tag{6.22}$$

Repeating the process we have

$$-3 \leq 3\alpha_{neg}^{k_2} \leq \sum_{j_{n-2}=1}^{(M-j_1\ldots-j_{n-3})} \alpha_{j_{n-2}}^{k_1} (1 + \sum_{j_{n-1}=1}^{(M-j_1\ldots-j_{n-2}-1)} \alpha_{j_n}^k) \leq 3 \sum_{j_{n-2}=1}^{(M-j_1\ldots-j_{n-3})} \alpha_{j_{n-2}}^{k_1} \leq 3. \tag{6.23}$$

We continue the recursive process for the full sum,

(6.24)

$$|\sum_{n=1}^N [\sum_{p \in P_{n,M}^1} \alpha(p)]| = |\sum_{j_1=1}^M \alpha_{j_1}^1 (1 + \sum_{j_2=1}^{M-j_1} \alpha_{j_2}^2 (1 + \ldots (1 + \sum_{j_{n-1}=1}^{(M-j_1\ldots-j_{n-2})} \alpha_{j_{n-1}}^1 (1 + \sum_{j_n=1}^{(M-j_1\ldots-j_{n-1})} \alpha_{j_n}^k) \ldots)|$$

$$\leq |\sum_{j_1=1}^M \alpha_{j_1}^1 (1 + \sum_{j_2=1}^{M-j_1} \alpha_{j_2}^2 (1 + \ldots (1 + 2 \sum_{j_{n-1}=1}^{(M-j_1\ldots-j_{n-2})} \alpha_{j_{n-1}}^1) \ldots)| \tag{6.25}$$

$$\leq |\sum_{j_1=1}^M \alpha_{j_1}^1 (1 + \sum_{j_2=1}^{M-j_1} \alpha_{j_2}^2 (1 + \ldots (1 + 3 \sum_{j_{n-3}=1}^{(M-j_1\ldots-j_{n-2})} \alpha_{j_{n-1}}^1) \ldots)| \tag{6.26}$$

$$\vdots$$

$$\leq |\sum_{j_1=1}^M \alpha_{j_1}^1 (1 + (N-1) \sum_{j_2=1}^{M-j_1} \alpha_{j_2}^2| \tag{6.27}$$

$$\leq N \tag{6.28}$$

Now, we will show that dropping the assumption that e has no loop paths the above bound remains true. Let v_1 and v_2 be the vertices of e. Consider the sets $P_{1,M}^1$ and $P_{1,M}^2$. If there exists a path $p \in P_{1,M}^1$ where p is a loop path, i.e. the first vertex along p is v_1 and the last vertex is v_2, then by reversing the bond ordering of p, there exists some path p_{rev} such that $\ell(p) = \ell(p_{rev})$, $\#bonds(p) = \#bonds(p_{rev})$, $\alpha(p) = \alpha(p_{rev})$, and $p_{rev} \in P_{1M}^2$. We can separate $P_{1,M}^i$ into two sets, loop paths P_{loops}^i and paths that do not loop $P_{noloops}^i$,

$$P_{1,M}^i = P_{loops}^i \cup P_{noloops}^i. \tag{6.29}$$

Which implies

$$|\sum_{p \in P_{1,M}^i} \alpha(p)| = |\sum_{p \in P_{loops}^i} \alpha(p) + \sum_{p \in P_{noloops}^i} \alpha(p)| \leq 1. \tag{6.30}$$

Changing the indexing of the loop paths from $i \in \{1,2\}$ to $j \in \{1,2\}$, $j \neq i$, we have

$$|\sum_{p \in P_{1,M}^i} \alpha(p)| = |\sum_{p \in P_{loops}^j} \alpha(p) + \sum_{p \in P_{noloops}^i} \alpha(p)| \leq 1. \tag{6.31}$$

Hence, changing the indexing set for loop paths did not change the sum and all indexing paths return to q from the same direction. Thus, by changing the indexing set for loop paths we can repeat the above process.

□

For the definition of rational heat kernels, we refer the reader to definition 2.2. Rational heat kernels play a crucial role in bounding the heat kernel of a quantum graph. Recall the diagonal of the heat kernel on G can be expressed with the heat sum formula,

$$K_G(t,q,q) = \frac{1}{\sqrt{4\pi t}}\Big(\sum_{p\in P(q,q)} \alpha(p)e^{-\ell(p)^2/4t}\Big). \tag{6.32}$$

Up to this point, paths in $P^i_{n,M}$ are bounded by the number of bonds along the path, paths with less than $M+1$ bonds. For rational heat kernels, by inserting a finite number of artificial vertices all bonds can be made to have the same length. Hence, we can bound paths in $P^i_{n,M}$ by length. For rational heat kernels the matrix $(B^*_n)^M$ can be used to bound the $\alpha(p)$ coefficients and $\ell(p)$ in the exponential.

LEMMA 6.6. *Let G be a quantum graph with rational heat kernel $K_G(t,q,q)$. Then a graph G' can be constructed from G by inserting a finite number of artificial vertices such that for all $e \in G'$, $\ell(e) = C$. Let $P^{i,L}_n(G')$ be the set of all paths in $P^i_n(G')$ with length less than or equal to L, $i \in \{1,2\}$. Then*

$$\sum_{p\in P^{i,L}_n(G')} \alpha(p) = \sum_{p\in P^i_{n,M}(G')} \alpha(p), \tag{6.33}$$

for all n and M, where $L = C(M+1)$.

PROOF. Let $K_G(t,q,q)$ be a rational heat kernel, by definition after inserting the vertex v_q all bonds have rational length. Thus, there exists a C such that for all bonds $b_i \in G$, $\ell(b_i)/C = q_i$, where q_i is a positive integer. For all bonds b_i of G we insert $q_i - 1$ artificial vertices on b_i such that the distance between all adjacent vertices is exactly C. Let G' be the graph obtained from G by adding all such artificial vertices. Then, any path along G' containing $(M+1)$ bonds has length $(M+1)C$ and any path with less than $(M+1)$ bonds has length less than $(M+1)C$. □

LEMMA 6.7. *Let $e \in G$ and q be a point contained in e. For all $\epsilon, t > 0$, there exists a quantum graph R with edge e_r and point $q_r \in e_r$ such that $K_R(t,q_r,q_r)$ is a rational heat kernel satisfying*

$$|K_G(t,q,q) - K_R(t,q_r,q_r)| < \epsilon. \tag{6.34}$$

PROOF. Assume that after adding the artificial vertex v_q, G has m edges, where each edge is labeled e_i, $i \in \{1,2,...,m\}$. We construct the graph R, by adding length $\delta_i > 0$ to e_i in such a way that $\ell(e_i) + \delta_i$ is rational.

Let $e = e_1 \cup e_2$ where e_1 and e_2 are the two edges created after inserting the artificial vertex at $q \in e$. Let e_1' and e_2' be the edges in R obtained by adding δ_1 to e_1 and δ_2 to e_2, respectively. Call v_r the artificial vertex separating e_1' and e_2'.

Note that G and R have the same bond scattering matrix B. Let the N shortest paths in $P_G(q,q)$ and the corresponding paths in $P_R(q_r,q_r)$ as P_N and P_{rN}, respectively.

Then for all t, ϵ fixed, there exists $N = N(t, \epsilon)$ such that

$$\frac{1}{\sqrt{4\pi t}}|\sum_{p\in P_G(q,q)} \alpha_B(p)e^{-\ell(p)^2/4t} - \sum_{p\in P_N} \alpha_B(p)e^{-\ell(p)^2/4t}| < \epsilon/3, \tag{6.35}$$

and

$$\frac{1}{\sqrt{4\pi t}}|\sum_{p\in P_R(q_r,q_r)} \alpha_B(p)e^{-\ell(p)^2/4t} - \sum_{p\in P_{rN}} \alpha_B(p)e^{-\ell(p)^2/4t}| < \epsilon/3. \tag{6.36}$$

Each path $p \in P_N$ and its corresponding path $p_r \in P_{rN}$ must have finite length and hence contain a finite number of edges. Moreover $\alpha(p) = \alpha(p_r)$. Let

(1) Q^*:=maximum number of edges for any path in P_N.
(2) ℓ^*:= $min_{p_r\in P_{rN}}\{\ell(p_r)\}$.
(3) K^*:=$max_{p_r\in P_{rN}}\{|\alpha(p_r)e^{-(\ell(p)+\delta_i)^2/4t}|\}$.
(4) $\delta^* = \max_{i\in\{1,2,\ldots,M\}}\{\delta_i\}$.

Then for all $p \in P_N$ and the corresponding $p_r \in P_{rN}$

$$\begin{aligned}|\alpha(p)e^{-\ell(p)^2/4t} - \alpha(p_r)e^{-\ell(p_r)^2/4t}| &\le |\alpha(p)e^{-\ell(p)^2/4t} - \alpha(p)e^{-(\ell(p)+\delta^*Q^*)^2/4t}| \\ &\le |\alpha(p)e^{-\ell(p)^2/4t}(1 - e^{-(2(\ell^*\delta^*Q^*)+(\delta^*Q^*)^2))/4t})|.\end{aligned} \tag{6.37}$$

Summing the above bound for all $p \in P_N$ and $p_r \in P_{rN}$, we get

(6.38)

$$|\sum_{p\in P_N} \alpha_B(p)e^{-\ell(p)^2/4t} - \sum_{p\in P_{rN}} \alpha_B(p)e^{-\ell(p)^2/4t}| \le \sum_{p\in P_N} |\alpha(p)e^{-\ell(p)^2/4t}(1 - e^{-(2(\ell^*\delta^*Q^*)+(\delta^*Q^*)^2))/4t})|,$$

$$\le K^*N(1 - e^{-(2(\ell^*\delta^*Q^*)/4t+(\delta^*Q^*)^2/4t}). \tag{6.39}$$

Choosing $\delta^* = \delta^*(t, \epsilon)$ small enough implies

$$\frac{1}{\sqrt{4\pi t}}|\sum_{p\in P_N} \alpha_B(p)e^{-\ell(p)^2/4t} - \sum_{p\in P_{rN}} \alpha_B(p)e^{-\ell(p)^2/4t}| < \epsilon/3. \tag{6.40}$$

which together with (6.35) and (6.36) implies (6.34). □

7. Direct Path Bounded Edges

From definition 6.3, e is a direct path bounded edge if for all $i \in \{1, 2\}$

$$1) \lim_{M\to\infty} \sum_{p\in P^i_{1,M}} \alpha(p) = 1, \tag{7.1}$$

and

$$2) \sum_{p\in P^i_{1,M_1}} \alpha(p) \le \sum_{p\in P^i_{1,M_2}} \alpha(p), \tag{7.2}$$

for all $M_0 \le M_1 \le M_2$, where $M_0 = min_{p\in P^i_1}\{\#bonds(p)\}$.

Let $e \in G$ with endpoints $\{v_0, v_1\}$, and $q \in e$. As in section 4, Let $P_1(q, q)$ be all paths along G from q to q that contain one out-going bond of q, i.e. return to q a single time. Then, $P_1(q, q) = P^1_1 \cup P^2_1$, where P^1_1 is all paths in $P_1(q, q)$ that first touch v_0 and P^2_1 is all paths that first touch v_1. If both P^1_1 and P^2_1 are bounded by (7.1) and (7.2), then e is direct path bounded. We restrict our attention to paths that first touch v_0. The strategy

is to find sub-graphs connected to v_0 where P_1^1 is bounded by (7.1) and (7.2). We can then construct a class of edges, where if the sub-graphs connected to v_0 and v_1 satisfy (7.1) and (7.2) then e is direct path bounded.

The first sub-graph that bounds P_1^1 by (7.1) and (7.2) is a symmetric star sub-graph connected at v_0. Where all edges $e_i \sim v_0$, $e_i \neq e$, have the same length and contain a degree one vertex.

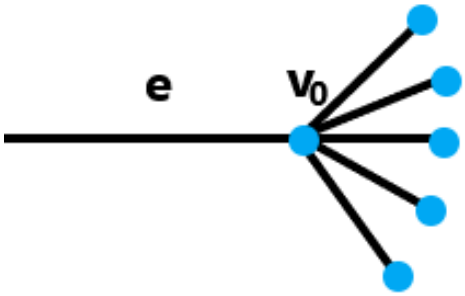


FIGURE 8. The above sub-graph shows endpoint v_0 connected to a symmetric star

LEMMA 7.1. *Let v_0 be a vertex of e, and v_0 is connected to a symmetric star sub-graph, for all $e_i \sim v_0$, $e_i \neq e$, $\ell(e_i) = L > 0$ and for $v_i \sim e_i$, $v_i \neq v_0$, $d_{v_i} = 1$. If P_1^1 is all paths that first touch v_0 and contain a single outgoing bond of q then*

$$1) \lim_{M\to\infty} \sum_{p\in P_{1,M}^1} \alpha(p) = 1, \tag{7.3}$$

and

$$2) \sum_{p\in P_{1,M_1}^1} \alpha(p) \leq \sum_{p\in P_{1,M_2}^1} \alpha(p), \tag{7.4}$$

for all $M_0 \leq M_1 \leq M_2$, where $M_0 = min_{p\in P_1^1}\{\#bonds(p)\}$.

PROOF. Let v_0 have degree d and P_1^1 be all paths that start toward v_0 and return to q a single time. We partition the paths in P_1^1 by the number of times they touch v_0. Let the paths that touch v_0 N times be R_N. Since all edges connected to v_0, with the exception of e, have the same length all paths in each partition have the same length. If $p_i \in R_N$ and $p_j \in R_{N+1}$ then $\#bonds(p_i) = \#bonds(p_j) - 2$. We can examine the $\alpha(p)$ coefficients for each R_N.

R_1 has a single path with heat path coefficient $(\frac{2}{d} - 1)$,

$$\sum_{p\in R_1} \alpha(p) = (\frac{2}{d} - 1). \tag{7.5}$$

R_2 has $d-1$ paths with two transmissions through v_0, with heat path coefficients $(\frac{2}{d})^2$,

$$\sum_{p\in R_2}\alpha(p) = (d-1)(\frac{2}{d})^2. \tag{7.6}$$

R_3 has $(d-1)^2$ paths, $(d-1)(d-2)$ containing 3 transmissions through v_0 with heat path coefficient $(\frac{2}{d})^3$ and $(d-1)$ paths with 2 transmissions and one reflection off v_0 with heat path coefficients $(\frac{2}{d})^2(\frac{2}{d}-1)$,

$$\sum_{p\in R_3}\alpha(p) = (d-1)(d-2)(\frac{2}{d})^3 + (d-1)(\frac{2}{d})^2(\frac{2}{d}-1). \tag{7.7}$$

Noticing each time a path returns to v_0 it has $(d-1)$ choices to transmit and one choice to reflect, the heat path coefficients for R_N follow a binomial distribution, $N > 2$.

$$\begin{aligned}\sum_{p\in R_N}\alpha(p) &= (2/d)^2(d-1)\sum_{k=0}^{N-2}\binom{N-2}{k}(2/d)^{N-k-2}(d-2)^{N-2-k}(2/d-1)^k,\\ &= (2/d)^2(d-1)(2/d(d-2)+(2/d-1))^{N-2},\\ &= (2/d)^2(d-1)(2-4/d+2/d-1)^{N-2},\\ &= (2/d)^2(d-1)(1-2/d)^{N-2}.\end{aligned} \tag{7.8}$$

Adding heat path coefficients from paths in $\cup_{i=1}^{N}R_i$,

$$\sum_{p\in\cup_{i=1}^{N}R_i}\alpha(p) = (2/d-1)+(2/d)^2(d-1)\sum_{k=0}^{N-2}(1-2/d)^k. \tag{7.9}$$

Which implies if $N_1 \le N_2$ then

$$\sum_{p\in\cup_{i=1}^{N_1}R_i}\alpha(p) \le \sum_{p\in\cup_{i=1}^{N_2}R_i}\alpha(p). \tag{7.10}$$

Hence, a symmetric star shaped sub-graph satisfies (7.2). To show (7.1) is satisfied, take the sum of heat path coefficients from all paths in $\cup_{i=1}^{\infty}R_i$.

$$\begin{aligned}\lim_{M\to\infty}\sum_{p\in P^1_{1,M}}\alpha(p) &= \sum_{p\in\cup_{i=1}^{\infty}R_i}\alpha(p)\\ &= (2/d-1)+(2/d)^2(d-1)\sum_{k=0}^{\infty}(1-2/d)^k\\ &= (1-2/d)+(2/d)^2(d-1)(\frac{1}{1-(1-2/d)})\\ &= 1\end{aligned} \tag{7.11}$$

□

The next sub-graph we consider is a symmetric flower sub-graph at v_0, i.e. for $e_i \sim v_0$, $e_i \neq e$, $\ell(e_i) = L$ and both endpoints of e_i are v_0.

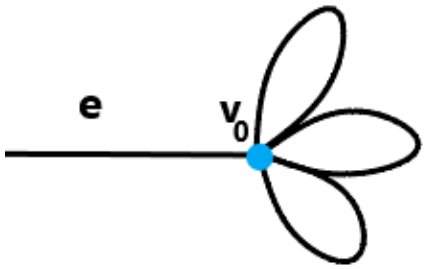


FIGURE 9. The above sub-graph shows endpoint v_0 connected to a symmetric flower

COROLLARY 7.2. *Let v_0 be a vertex of e, connected to a symmetric flower sub-graph. So, for all $e_i \sim v_0$, $e_i \neq e$, $\ell(e_i) = L$ and v_0 is both end points for e_i (i.e. e_i is a loop connected to v_0). Then*

$$1) \lim_{M\to\infty} \sum_{p\in P^1_{1,M}} \alpha(p) = 1, \tag{7.12}$$

and

$$2) \sum_{p\in p^1_{1,M_1}} \alpha(p) \leq \sum_{p\in P^1_{1,M_2}} \alpha(p), \tag{7.13}$$

for all $M_0 \leq M_1 \leq M_2$, where $M_0 = min_{p\in P^1_1}\{\#bonds(p)\}$.

PROOF. Let $d_{v_0} = 2N + 1$, which implies v_0 is connected to N flower petals of length L. The heat path coefficients for those petals are the same as a symmetric star sub-graph with $2N$ edges (not including e_0) and each edge having length $L/2$. □

If the sub-graph at v_0 is a symmetric pumpkin, meaning for $e_i \sim v_0$, $e_i \neq e$, $\ell(e_i) = L$ and all e_i share the same endpoints.

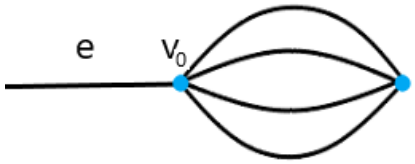


FIGURE 10. The above sub-graph shows endpoint v_0 connected to a symmetric pumpkin

COROLLARY 7.3. *Let v_0 be connected to a symmetric pumpkin sub-graph, $e_i \sim v_0$, $e_i \neq e$, $\ell(e_i) = L$ and $e_i \sim v_2 \neq v_0$. Then*

$$1) \lim_{M\to\infty} \sum_{p\in P^1_{1,M}} \alpha(p) = 1, \tag{7.14}$$

and

$$2) \sum_{p\in P^1_{1,M_1}} \alpha(p) \leq \sum_{p\in P^1_{1,M_2}} \alpha(p), \tag{7.15}$$

for all $M_0 \leq M_1 \leq M_2$, where $M_0 = min_{p\in P^1_1}\{\#bonds(p)\}$.

PROOF. Let v_0 be connected to a pumpkin sub-graph with multiplicity M and v_2 be the vertex of the pumpkin across from v_0. Then v_2 has degree M. Let p be a path along G ending at v_2 with heat path coefficient $\alpha(p)$, where the last edge along p is e_i. By the symmetry of the pumpkin there must be a corresponding path with heat path coefficient $\alpha(p)$ contained on each edge of the pumpkin not equal to e_i. All corresponding paths have the same length and same number of bonds, call these paths $\{p_1, ..., p_M\}$. Consider the scattering of each of these paths at v_2. Along each edge of the pumpkin sub-graph there will be $(M-1)$ equal transmissions through v_2 and a single reflection.

$$\alpha(p)(\frac{2}{M}(M-1) + (\frac{2}{M} - 1)) = \alpha(p). \tag{7.16}$$

This implies v_2 behaves like a degree one vertex for all paths from q. Which reduces the pumpkin argument to the symmetric star case.

□

8. Comparison Between Neumann Interval and Direct Path Bounded Edges

From Lemma 6.6, if $K_G(t,q,q)$ is a rational heat kernel we can construct a new graph G' by inserting a finite number of artificial vertices such that all edges of G' have the same length and

$$K_G(t,q,q) = K_{G'}(t,q,q), \tag{8.1}$$

for all $t > 0$.

When using the heat sum formula for rational heat kernels, the number of bonds in a path is equal to the total length of the path times a constant. So, the matrix $(B^*_n)^M$ can be used to bound the sum of heat path coefficients according to the length for paths in P^i_n. For example, let $K_G(t,q,q)$ be a rational heat kernel, after constructing G' from G by inserting a finite number of artificial vertices every edge in G' has length C. Then if G has m edges,

$$(B^*_n)^{(M-n-1)} e_5(2m(n-1)+1) = \sum_{p\in P^i_{n,M}} \alpha(p) = \sum_{p\in P^{i,L}_n} \alpha(p), \tag{8.2}$$

where $L = C(M+1)$.

We construct a new set of paths,

DEFINITION 8.1.

$$P(L,q,G) = \sum_{n=1}^{\infty} [\sum_{p\in P^{i,L}_n} \alpha(p)]. \tag{8.3}$$

$P(L,q,G)$ is all paths along G beginning and ending with q with length less than or equal to L.

THEOREM 8.2. *Let G and G' be compact connected quantum graphs, if*

$$\sum_{p\in P(L,q,G)} \alpha(p) \leq \sum_{p'\in P(L,q',G')} \alpha(p'), \tag{8.4}$$

for all $L \geq 0$. Then

$$K_G(t,q,q) \leq K_{G'}(t,q',q'), \tag{8.5}$$

for all $t > 0$.

PROOF. Let p be a path along G beginning and ending at q and p' be a path along G' beginning and ending at q'. We will proceed by contradiction, assume there exists some time t_0 such that

$$K_G(t_0,q,q) > K_{G'}(t_0,q',q') \tag{8.6}$$

Then for all $\epsilon > 0$, there exists N_1 and N_2 such that for all $L_1 > N_1$,

$$|K_G(t_0,q,q) - \sum_{p\in P(L_1,q,G)} \alpha(p) e^{-\ell(p)^2/4t_0}| < \frac{\epsilon}{2}, \tag{8.7}$$

and for all $L_2 > N_2$,

$$|K_G(t_0,q',q') - \sum_{p'\in P(L_2,q',G')} \alpha(p') e^{-\ell(p')^2/4t_0}| < \frac{\epsilon}{2}. \tag{8.8}$$

Let $L^* > \max\{N_1, N_2\}$, then for ϵ small enough

$$\sum_{p\in P(L^*,q,G)} \alpha(p) e^{-\ell(p)^2/4t_0} > \sum_{p'\in P(L^*,q',G')} \alpha(p') e^{-\ell(p')^2/4t_0}. \tag{8.9}$$

Which implies

$$\sum_{p\in P(L^*,q,G)} \alpha(p) e^{-\ell(p)^2/4t_0} - \sum_{p'\in P(L^*,q',G')} \alpha(p') e^{-\ell(p')^2/4t_0} > 0. \tag{8.10}$$

Let

$$K_{L^*} = \sum_{p\in P(L,q,G)} \alpha(p) e^{-\ell(p)^2/4t_0} - \sum_{p'\in P(L,q',G')} \alpha(p') e^{-\ell(p')^2/4t_0}. \tag{8.11}$$

Assume there are Q unique path lengths for paths in $P(L^*,q,G) \cup P(L^*,q',G')$. We will enumerate these path lengths, let ℓ_j correspond to the j^{th} shortest unique path length in $P(L^*,q,G) \cup P(L^*,q',G')$. We will combine terms in K_{L^*} by summing the coefficients from paths with the same length. Let

$$\alpha_j = \sum_{\substack{p\in P(L^*,q,G) \\ \ell(p)=\ell_j}} \alpha(p) - \sum_{\substack{p'\in P(L^*,q',G') \\ \ell(p)=\ell_j}} \alpha(p'). \tag{8.12}$$

Then K_{L^*} is equal to,

$$K_{L^*} = \sum_{i=1}^{Q} \alpha_i e^{\ell_i^2/4t_0} > 0. \tag{8.13}$$

By assumption (8.4),

$$\sum_{i=1}^{m} \alpha_i < 0. \tag{8.14}$$

for all $m \leq Q$.

If $\alpha_i < 0$, we can increase K_{L^*} by increasing ℓ_i. By assumption 8.4, $\alpha_1 \leq 0$, we increase the path length of ℓ_1 so that $\ell_1 = \ell_2$ and combine terms in K_{L^*} with coefficients α_1 and α_2,

$$\sum_{i=1}^{2} \alpha_i e^{-\ell_i^2/4t_0} \leq (\alpha_1 + \alpha_2) e^{-\ell_2^2/4t_0}. \tag{8.15}$$

Again by (8.4), $\alpha_1 + \alpha_2 \leq 0$. Which implies

$$(\alpha_1 + \alpha_2) e^{-\ell_2^2/4t_0} + \alpha_3 e^{-\ell_3^2/4t_0} \leq (\alpha_1 + \alpha_2 + \alpha_3) e^{-\ell_3^2/4t_0}. \tag{8.16}$$

We repeat the process for all $j \in \{1, 2, ..., M\}$, where at each step by assumption

$$\sum_{i=1}^{j} \alpha_i < 0. \tag{8.17}$$

and

$$(\sum_{i=1}^{j} \alpha_i) e^{-\ell_j^2/4t_0} + (\alpha_{j+1}) e^{-\ell_{j+1}^2/4t_0} \leq (\sum_{i=1}^{j+1} \alpha_i) e^{-\ell_{j+1}^2/4t_0} \tag{8.18}$$

When $j = M$, we have

$$K_{L^*} \leq (\sum_{i=1}^{M} \alpha_i) e^{-\ell_M^2/4t_0} \leq 0 \tag{8.19}$$

which contradicts (8.10) and completes the proof.

□

Corollary 8.3. *Let $e \in G$ be a direct bounded edge with vertices v_l and v_r, and length ℓ. For $q \in e$, where $|v_l - q| = \ell_1$ and $|v_r - q| = \ell_2$, if $K_G(t, q, q)$ is a rational heat kernel and any path in $P(q, q)$ containing both v_l and v_r has length equal to or greater than $\max\{2\ell_1, 2\ell_2\}$, then*

$$K_G(t, q, q) \leq K_I(t, q, q), \tag{8.20}$$

for all $t > 0$, where I is the Neumann interval of length ℓ and q has the same relative spacing along the interval as on e. If G is not the Neumann interval the inequality is strict.

Proof. Let $B(I)$ be the bond scattering matrix for I. For each path p on I we have $\alpha(p) = 1$. The heat path formula for the Neumann interval I reads

$$K_I(t, q, q) = \frac{1}{\sqrt{4\pi t}} (1 + \sum_{k=0}^{\infty} e^{-(2\ell_1 + 2k\ell)^2/4t} + e^{-(2\ell_2 + 2k\ell)^2/4t} + 2e^{-(2(k+1)\ell)^2/4t}). \tag{8.21}$$

where the first summand is the term corresponding to the trivial path; compare with (2.4).

If we partition the paths for the Neumann interval according to their initial direction and how many out-going bonds of v_q the path contains (as we did in Section 5), each partition contains exactly one path. The path length in $P_n^1(I)$ alternates between $2\ell_1 + (n-1)\ell$ for n odd and $n\ell$ for n even. Similarly, the paths in $P_n^2(I)$ alternate between $2\ell_2 + (n-1)\ell$ for n odd and $n\ell$ for n even.

By assumption $K_G(t,q,q)$ is a rational heat kernel, construct a new graph G' from G by inserting a finite number of artificial vertices such that all edges in G' have length C, as we did in (6.6). Constructing the matrices B_n^* from G' we can use (6.5) to get

$$\sum_{n=1}^{N}(B_n^*)^M e_{i+4}(2m(n-1)+1) \leq N, \tag{8.22}$$

for all $N, M \in \{1,2,...\}$, and $i \in \{1,2\}$.

Because all bonds of G' have the same length, $(B_n^*)^M e_5(2m(n-1)+1)$ is the sum of heat path coefficients from $P_n^{1,L}$, where $L = C(M+1)$. By assumption the shortest path in $P(q,q)$ containing both v_l and v_r must be greater than or equal to $\max\{2\ell_1, 2\ell_2\}$. This implies than any *loop path* in $P(q,q)$, has length greater than or equal to $\max\{2\ell_1, 2\ell_2\}$. Thus, the shortest path $p \in P(q,q)$ starting in the direction of v_l has length $2\ell_1$. Similarly the shortest path $p \in P(q,q)$ starting in the direction of v_r has length $2\ell_2$. This implies that the length of any path in $P_n^i(G)$ has a lower bound $2\ell_i + (n-1)\ell$ for n odd and $n\ell$ for n even, which are the lengths of paths in $P_n^i(I)$ for n odd or even, respectively.

We construct a new graph I' by inserting a finite number of artificial vertices on I and ensuring that all edges of I' have length C. Let I' have m^* edges. If $(M-1)$ is less than $(2\ell_i + (n-1)\ell)/C$ for n odd or $2\ell/C$ for n even then $P_{n,M}^i(G') = P_{n,M}^i(I') = \varnothing$, and

$$(B(I')_n^*)^M e_{(i+4)}(2m^*(n-1)+1) = (B_n^*(G'))^M e_{(i+4)}(2m(n-1)+1) = 0. \tag{8.23}$$

Summing the terms in the Neumann interval and using Lemma 6.5, if M is large enough to include the shortest path in each partition then

$$\sum_{n=1}^{N}(B(I')_n^*)^M e_{(i+4)}(2m^*(n-1)+1) = N \geq \sum_{n=1}^{N}(B_n^*)^M e_{(i+4)}(2m(n-1)+1). \tag{8.24}$$

If M is not large enough, the contribution from both sums in (8.24) is zero and the inequality remains true. The result follows from Theorem 8.2.

If G is not the Neumann interval then the inequality (8.20) becomes strict. Assume G is not the Neumann interval, then at least one of the end points of e must be a vertex of degree greater than 2. Equation (8.15) in Theorem 8.2 becomes a strict inequality as $\alpha_1 < 0$,

$$\sum_{i=1}^{2}\alpha_i e^{-\ell_i^2/4t_0} < (\alpha_1+\alpha_2)e^{-\ell_2^2/4t_0}. \tag{8.25}$$

Hence, (8.20) becomes a strict inequality.

□

9. Neumann Comparison: Off Diagonal Results

Corollary 8.3 can be adapted to the off diagonal heat kernel by showing that there is a bijection between paths along a quantum graph from q to q and paths from q to q_0, for any q_0 contained along the same edge as q.

LEMMA 9.1. *If q and q_0 belong to the same edge of a quantum graph there is a bijection between the sets $P(q,q)$ and $P(q,q_0)$.*

PROOF. We start by inserting two artificial vertices along G at q and q_0, call them v_q and v_{q_0}, respectively. Without loss of generality, assume v_{q_0} is to the right of v_q. As in Lemma 5.4 it is convenient to distinguish paths that start to the right or to the left. Let

$\mathbb{P}_r(q,q)$ and $\mathbb{P}_r(q_0,q)$ be the set of paths that start to the right in $P(q,q)$ and $P(q_0,q)$, respectively. Any path in $\mathbb{P}_r(q,q)$ can be obtained from a path in $\mathbb{P}_r(q_0,q)$ by adding the bond $\overrightarrow{b}_{v_q,v_{q_0}}$ as the first bond. Conversely, any path in $\mathbb{P}_r(q_0,q)$ can be obtained from a path in $\mathbb{P}_r(q,q)$ by deleting the first bond $\overrightarrow{b}_{v_q,v_{q_0}}$. Thus, there is a one to one correspondence between $\mathbb{P}_r(q,q)$ and $\mathbb{P}_r(q_0,q)$. We can use the same reasoning for paths that start towards the left. Then there is a one to one correspondence between $P(q,q)$ and $P(q_0,q)$ and of course the latter has a one to one correspondence with $P(q,q_0)$, so the assertion follows. □

LEMMA 9.2. *The bijection described in Lemma 9.1 preserves the heat path coefficients for all paths.*

PROOF. The bijection in Lemma 9.1 either adds or deletes the bond transfer at v_q which is an artificial vertex and hence has a bond scattering matrix entry equal to one. Thus, the bijection does not change the heat path coefficient. □

Thanks to Lemma 9.1 we can introduce a partition of $P(q,q_0)$ that bijectively corresponds to the partition of $P(q,q)$ in definition 5.1. We shall use the same notation for the partition of $P(q,q_0)$ as the one of $P(q,q)$. Thus, if we ensure that all paths in each partition of $P(q,q_0)$ have length longer than the single path in the corresponding Neumann interval partition, then for $q,q_0 \in e$ Lemma 8.3 extends to $q \neq q_0$.

THEOREM 9.3. *Let G be a quantum graph and $K_G(t,q,q_0)$ be the heat kernel on G, where q and q_0 belong to the same edge e with length ℓ and vertices v_l and v_r. Let $\ell_1 := |v_l - q_0|$ and $\ell_2 := |v_r - q_0|$. If every path from q_0 to q_0 containing both v_r and v_l has length equal to or greater than $\max\{2\ell_1, 2\ell_2\}$ and e is direct path bounded then*

$$K_G(t,q,q_0) \leq K_I(t,q,q_0), \tag{9.1}$$

for all $t > 0$, where $K_I(t,q,q_0)$ is the heat kernel for a Neumann interval of length ℓ with q and q_0 have the same relative positions as on e. If G is not the Neumann interval than the inequality is strict.

PROOF. Using the bijection of Lemma 9.1 both for G and the Neumann interval I, we either add or delete a bond which has the same length in G and in I, so we can confine ourselves to paths starting from q and returning to q. Then we simply apply Lemma 8.3. □

CHAPTER 4

Mean Value Theorem

1. Mean Value Formula

Let H be the heat operator in one dimension and H' its adjoint i.e.

$$Hf = f_{xx} - f_t \qquad H'v = v_{xx} + v_t. \tag{1.1}$$

Let D be a region in $\mathbb{R} \times (0, \infty)$, (ξ, τ) be our variables of integration, and $\vec{n} = (n_1, n_2)$ be the outward normal with respect to ∂D. By the divergence theorem, if $Hf = 0$ and $H'v = 0$, then

$$\int \int_D [fH'v - vHf]dA = \int_{\partial D} [(fv_\xi - f_\xi v)n_1 + fvn_2]ds = 0. \tag{1.2}$$

Choosing $v \equiv 1$, equation (1.2) becomes

$$\int_B [-f_\xi n_1 + fn_2]ds = \int_B -f_\xi d\tau + fd\xi = 0. \tag{1.3}$$

Recall the distance function along G,

$$d(q_0, q) = \min_{p \in P(q_0, q)} \{\ell(p)\}. \tag{1.4}$$

Fix a point $q_0 \in G$, where $q_0 \notin V(G)$. For all $q \in G$, if q is a singularity of $d(q_0, q)$ we insert an artificial vertex at q and add q to the set $V(G)$. Let q_0 belong to the edge e_0 and v_0 be the closest vertex to q_0, we construct the following coordinate system along each edge of G

$$x = \begin{cases} d(q_0, q) & e \neq e_0, \\ d(v_0, q) & e = e_0. \end{cases} \tag{1.5}$$

Let $h(t_0 - t, q_0, x)$ be the reverse time heat kernel on G. Then along each $e \in G$

$$h_{xx} + h_t = 0. \tag{1.6}$$

Definition 1.1. The *heat ball* on G is the set $Q(q_0, t_0, C) := \{(x, t) \in G \times (0, t_0) \mid h(t_0 - t, q_0, x) \geq C\}$ for some $C > 0$. When we fix q_0, t_0, and C we will refer to the *heat ball* as Q.

Theorem 1.2. *Let G be a compact quantum graph and let $u(q, t)$ satisfy the heat equation on G, then*

$$u(q_0, t_0) = \int_{\partial Q} -uh_x n_1 ds. \tag{1.7}$$

Where ∂Q is the boundary of the heat ball $Q(q_0, t_0, C)$ for $q_0 \in G$, $t_0 \in (0, \infty)$, and $C > 0$.

PROOF. Fix $q_0 \in G$, $t_0 \in (0,\infty)$, and $C > 0$. On each edge $e \in E(G)$, let $Q_e = \{(x,t) \in e \times (0,t_0) \mid h(t_0 - t, q_0, x) \geq C\}$, i.e. $Q_e = e \cap Q$. Let $R_e = Q_e \cap \{V(G)\}$, R_e is the boundary of Q_e at the vertices of e. On the edge e_0, we define the set $J_{t_1} = Q_{e_0} \cap \{t \leq t_1\}$ for some $t_1 < t_0$, with boundary ∂J_{t_1}.

The boundary ∂J_{t_1} can be split into two sub-sets $\partial J_1 = \partial Q_{e_0} \cap \partial J_{t_1}$ and $\partial J_2 = Q_{e_0} \cap \{t = t_1\}$. If $\vec{n}_J = (n_{J,1}, n_{J,2})$ is the outward normal with respect to ∂J_{t_1}, then for ∂J_2 we have $n_1 = 0$. If $|t_1 - t_0| < \epsilon$, for ϵ small enough $\partial J_2 \cap V(G) = \varnothing$. Let $u(q,t)$ solve the heat equation on G. Using the coordinate system described in (1.5) and the divergence theorem,

(1.8)
$$0 = \int_{J_{t_1}} [u(h_{xx} + h_t) - h(u_{xx} - u_t)]dA = \int_{\partial J_{t_1}} [uh_x n_{J,1} - hu_x n_{J,1} + hun_{J,2}]ds,$$

(1.9)
$$= \int_{\partial J_1} [uh_x n_{J,1} - hu_x n_{J,1} + hun_{J,2}]ds + \int_{\partial J_2} [uh_x n_{J,1} - hu_x n_{J,1} + hun_{J,2}]ds,$$

(1.10)
$$= \int_{\partial J_1} [uh_x n_{J,1} - hu_x n_{J,1} + hun_{J,2}]ds + \int_{\partial J_2} hun_{J,2} ds.$$

Letting $t_1 \to t_0$ and using the delta function property of $h(t_0 - t, q_0, x)$, we have

(1.11)
$$u(q_0,t_0) = \lim_{t_1 \to t_0} \int_{J_2} uhn_{J,2} ds = \int_{\partial Q_{e_0}} [-uh_x n_{J,1} + hu_x n_{J,1} - hun_{J,2}]ds,$$
$$= \int_{\partial Q_{e_0} \setminus R_{e_0}} [-uh_x n_{J,1} + hu_x n_{J,1} - hun_{J,2}]ds + \int_{R_{e_0}} [-uh_x n_{J,1} + hu_x n_{J,1}]ds.$$

Let $\vec{n_e} = (n_{e,1}, n_{e,2})$ be the outward normal with respect to ∂Q_e. We note that $n_{e,2} = 0$ with respect to the boundary R_e. For all $e \neq e_0$, by the divergence theorem

(1.12)
$$0 = \int_{\partial Q_e} [-uh_x n_{e,1} + hu_x n_{e,1} - hun_{e,2}]ds,$$
$$= \int_{\partial Q_e \setminus R_e} [-uh_x n_{e,1} + hu_x n_{e,1} - hun_{e,2}]ds + \int_{R_e} [-uh_x n_{e,1} + hu_x n_{e,1}]ds.$$

Summing equations 1.11 and 1.12 for all $\{e_0, e_1, ..., e_N\}$, where for $i \in \{0,1,...,N\}$, $Q_{e_i} \neq \varnothing$, we get

(1.13) $$u(q_0,t_0) = \sum_{i=0}^{N} [\int_{\partial Q_e \setminus R_e} [-uh_x n_{e,1} + hu_x n_{e,1} - hun_{e,2}]ds + \int_{R_e} [-uh_x n_{e,1} + hu_x n_{e,1}]ds].$$

From the vertex conditions for h and u, we have $\sum_{e \sim v} u_x n_{e,1} = 0$ and $\sum_{e \sim v} h_x n_{e,1} = 0$ for all $v \in V$. This implies

(1.14)
$$\sum_{i=0}^{N} \int_{R_e} [-uh_x n_{e,1} + hu_x n_{e,1}]ds = \sum_{v \in V(G) \cap Q} [\sum_{e \sim v} \int_{R_e} [-uh_x n_{e,1} + hu_x n_{e,1}]ds],$$

(1.15)
$$= \sum_{v \in V(G) \cap Q} [\int_{R_e} [-u[\sum_{e \sim v} h_x n_{e,1}] + h[\sum_{e \sim v} u_x n_{e,1}]ds],$$

(1.16)
$$= 0.$$

Equation 1.13 becomes

(1.17)
$$u(q_0,t_0) = \sum_{i=0}^{N} [\int_{\partial Q_e \setminus R_e} [-uh_x n_{e,1} + hu_x n_{e,1} - hun_{e,2}]ds.$$

By construction of ∂Q_e, $h \equiv C$ on $\partial Q_e \setminus R_e$. Which implies,

$$u(q_0,t_0) = \sum_{i=0}^{N}[\int_{\partial Q_e \setminus R_e}[-uh_x n_{e,1} + C(u_x n_{e,1} - un_{e,2})]ds. \tag{1.18}$$

Using (1.3),

$$\begin{aligned} u(q_0,t_0) &= \sum_{i=0}^{N}[\int_{\partial Q_e \setminus R_e}[-uh_x n_{e,1} + C(u_x n_{e,1} - un_{e,2})]ds, \\ &= \sum_{i=0}^{N}[\int_{\partial Q_e \setminus R_e}[-uh_x n_{e,1}]ds, \\ &= \int_{\partial Q} -uh_x n_1 ds. \end{aligned} \tag{1.19}$$

□

2. Bounding the Mean Value Formula

In the previous section we found an expression for the mean value formula for the heat equation on a quantum graph using the heat kernel of G. We will now find an alternate representation for the mean value formula using the free heat kernel on $\mathbb{R}$. This new version can be used to bound the mean value formula on G. The free heat kernel on $\mathbb{R}$ can be expressed

$$K_{\mathbb{R}}(t,x,y) = \frac{1}{\sqrt{4\pi t}} e^{-|x-y|^2/4t}. \tag{2.1}$$

Using the coordinate system described in (1.5), we define the function $k(t_0 - t, q_0, x)$ on G as

$$k(t_0 - t, q_0, x) = \frac{1}{\sqrt{4\pi(t_0 - t)}} e^{-x^2/4(t_0-t)}. \tag{2.2}$$

For all $x \notin V$,

$$k_{xx} + k_t = 0. \tag{2.3}$$

For the next theorem, we define the following sets:

- $B(q_0,t_0,C) := \{(x,t) \in G \times (0,t_0) \mid k(t_0 - t, q_0, x) \geq C\}$, for some $C > 0$. When we fix $t_0 \in (0,\infty)$, $q_0 \in G \setminus V(G)$, and $C > 0$ we will refer to this set as B.
- $B_e(q_0,t_0,C) = B(q_0,t_0,C) \cap e$ for some $e \in E(G)$, when q_0, t_0, and C are clear we use the simpler notation B_e.
- $\vec{n_e} = (n_{e,1}, n_{e,2})$ is the outward normal with respect to B_e, using the coordinate system described in (1.5).

- d_v^+ and d_v^- are the number of edges $e \sim v$, such that on $B_e \cap v$, $\vec{n_e} = (-1, 0)$ and $\vec{n_e} = (1, 0)$, respectively. $B_e \cap v$ is the boundary of B_e at v. To account for our coordinate system, for v_0 we subtract one from $d_{v_0}^+$ and add one to $d_{v_0}^-$.

THEOREM 2.1. *Let G be a compact quantum graph. Using the sets described above if $u(q,t)$ solves the heat equation on G then*

$$u(q_0, t_0) = \int_{\partial B} -uk_x n_1 ds + \sum_{v \in V} (d_v^+ - d_v^-) \int_{B \cap v} uk_x ds. \tag{2.4}$$

PROOF. Through out this proof we will fix q_0, t_0, and $C > 0$. Using the sets described above and the coordinate system descirbed in (1.5), if

$$k(t_0 - t, q_0, x) = \frac{1}{\sqrt{4\pi(t_0 - t)}} e^{-x^2/4(t_0 - t)}, \tag{2.5}$$

then for all edges $e \neq e_0$, we have $x = d(q_0, q) > 0$, which implies for all $e \neq e_0$

$$k_x = \frac{-x}{2(t_0 - t)} k < 0. \tag{2.6}$$

For $e \in E(G)$, the boundary of B_e, denoted ∂B_e, consists of two sets. The first is $\{(x,t) \in e \times (0, t_0) \mid k(t_0 - t, q_0, x) = C,\ x \notin V\}$. The second is the boundary at the vertices of e, $T_e = B_e \cap \{V\}$. Let $\vec{n_e} = (n_{e,1}, n_{e,2})$ be the outward normal with respect to ∂B_e. Along the boundary T_e, we have $n_{e,2} = 0$.

On the edge e_0, we define the set $I_{t_1} := B_{e_0} \cap \{t \leq t_1\}$ for some $t_1 < t_0$. We separate the boundary of I_{t_1} into two sets $\partial I_1 = \partial B_{e_0} \cap \partial I_{t_1}$ and $\partial I_2 = B_{e_0} \cap \{t = t_1\}$. On ∂I_2 we have $n_{e_0,1} = 0$. If $|t_1 - t_0| < \epsilon$, then for ϵ small enough $\partial I_2 \cap V(G) = \varnothing$. Let u solve the heat equation on G. Let $\vec{n_I} = (n_{I,1}, n_{I,2})$ be the outward normal with respect to I_{t_1}. By the divergence theorem, on e_0

(2.7)

$$\begin{aligned}
0 = \int_{I_{t_1}} [u(k_{xx} + k_t) - k(u_{xx} - u_t)] dA &= \int_{\partial I_{t_1}} [uk_x n_{I,1} - ku_x n_{I,1} + kun_{I,2}] ds, \\
&= \int_{\partial I_{I,1}} [uk_x n_{I,1} - ku_x n_{I,1} + kun_{I,2}] ds + \int_{\partial I_2} [uk_x n_{I,1} - ku_x n_{I,1} + kun_{I,2}] ds, \qquad (2.8) \\
&= \int_{\partial I_1} [uk_x n_{I,1} - ku_x n_{I,1} + kun_{I,2}] ds + \int_{\partial I_2} kun_{I,2} ds. \qquad (2.9)
\end{aligned}$$

Letting $t_1 \to t_0$ implies $\partial I_{t_1} \to \partial B_{e_0}$. Using the delta function property of $k(t_0 - t, q_0, x)$,

$$u(q_0, t_0) = \lim_{t_1 \to t_0} \int_{\partial I_2} ukn_{I,2} ds = \int_{\partial B_{e_0}} [-uk_x n_{I,1} + ku_x n_{I,1} - kun_{I,2}] ds. \tag{2.10}$$

If $e \neq e_0$ then

$$\begin{aligned}
0 &= \int_{\partial B_e} [-uk_x n_{e,1} + ku_x n_{e,1} - kun_{e,2}] ds, \\
&= \int_{\partial B_e \setminus T_e} [-uk_x n_{e,1} + ku_x n_{e,1} - kun_{e,2}] ds + \int_{T_e} [-uk_x + ku_x] n_{e,1} ds.
\end{aligned} \tag{2.11}$$

Let $\{e_0, e_1, ..., e_N\}$ be edges such that $B_{e_i} \neq \varnothing$. Summing equations 2.10 and 2.11,

$$u(q_0,t_0) = \sum_{i=1}^{N}[\int_{\partial B_{e_i} \setminus T_{e_i}} [-uk_x n_{e_i,1} + ku_x n_{e_i,1} - kun_{e_i,2}]ds + \int_{T_{e_i}} [-uk_x + ku_x]n_{e_i,1}ds]. \tag{2.12}$$

If $v \cap B = \varnothing$, then for all $e \sim v$, $v \cap \partial B_e = \varnothing$. Otherwise, we will integrate over v, d_v times. Note that for all e, on T_e the outward normal $n_{e,1} = \pm 1$, however the sign is dependent on the coordinate system described in (1.5). If v_1 and v_2 are the vertices of e, then $T_e = (\partial B_e \cap v_1) \cup (\partial B_e \cap v_2)$. From the vertex condition that $\sum_{e\sim v} u_x n_{e,1} = 0$ and the continuity of k,

$$\sum_{e\sim v} \int_{\partial B_e \cap v} k u_x n_{e,1} ds = \int_{\partial B_e \cap v} k(\sum_{e\sim v} u_x n_{e,1}) ds = 0. \tag{2.13}$$

Which implies

$$u(q_0,t_0) = \sum_{i=1}^{N}[\int_{\partial B_{e_i} \setminus T_{e_i}} [-uk_x n_{e_i,1} + ku_x n_{e_i,1} - kun_{e_i,2}]ds + \int_{T_{e_i}} [-uk_x n_{e_i,1} ds]. \tag{2.14}$$

For each $v \neq v_0$, let d_v^+ be the number of edges adjacent to v such that on $\partial B_e \cap v$, $n_{e,1} = -1$. Similarly, let d_v^- be the number of edges adjacent to v such that on $\partial B_e \cap v$, $n_{e,1} = 1$. For $v = v_0$, to account for our coordinate system, we subtract one from $d_{v_0}^+$ and add one to $d_{v_0}^-$. For each $v \neq v_0$, select some $e \sim v$ call this edge e_v^*, selecting a single edge stops us from integrating over the boundary $\partial B_e \cap v$ multiple times. For all $e \sim v \neq v_0$, $k_x < 0$. Then

$$\sum_{e\sim v} \int_{B_e \cap v} -uk_x n_1 ds = (d_v^+ - d_v^-) \int_{B_{e_v^*} \cap v} uk_x ds. \tag{2.15}$$

Which implies

$$\sum_{i=1}^{N}[\int_{T_{e_i}} [-uk_x n_1 ds] = \sum_{v\in V} (d_v^+ - d_v^-) \int_{B_{e_v^*} \cap v} uk_x ds. \tag{2.16}$$

We note that if $B \cap v = \varnothing$, then the contribution to the sum from this vertex is zero. For the vertex v_0, the boundary $B_{e_0} \cap v_0$, $n_{e_0,1} = -1$ and $k_x > 0$. For all edges $e \sim v_0$, $e \neq e_0$, we have along the boundary $B_e \cap v_0$, $k_x < 0$ and $n_{e,1} = -1$. This implies

$$\sum_{e\sim v_0, e\neq e_0} \int_{B_e \cap v_0} -uk_x n_1 ds = (d_{v_0} - 1) \int_{B_{e_0} \cap v_0} uk_x ds, \tag{2.17}$$

and for $\partial B_{e_0} \cap v_0$, $k_x > 0$ and $n_{e_0,1} = -1$, so

$$\int_{B_{e_0} \cap v_0} -uk_x n_1 ds = \int_{B_{e_0} \cap v_0} uk_x ds = -\int_{B_{e_0} \cap v_0} u(-k_x) ds. \tag{2.18}$$

Where in (2.17), $k_x < 0$ and in (2.18), $k_x > 0$. For v_0, we choose the edge $e_{v_0}^*$ to be some $e \sim v$, $e \neq e_0$. If no such edge exists, then we choose $e_0 = e_{v_0}^*$ but we change the sign of k_x along $\partial B_{e_0} \cap v_0$. This change in sign is to account for our coordinate system being "backwards" with respect to k_x along e_0 near v_0. Summing (2.17) and (2.18),

$$\sum_{e\sim v_0, e\neq e_0} \int_{B_e \cap v_0} uk_x n_{e,1} ds - \int_{B_{e_0} \cap v_0} u(-k_x) n_{e_0,1} ds = (d_{v_0} - 2) \int_{B_{e_0} \cap v_0} u(k_x) ds. \tag{2.19}$$

Finally, we examine $\partial B_e \setminus T_e$. By construction, $k(t_0 - t, q_0, x) \equiv C$ on $\partial B_e \setminus T_e$. Summing over each ∂B_e, and choosing $w \equiv 1$ we have

(2.20)

$$\begin{aligned}\sum_{i=0}^{N}\int_{\partial B_{e_i}}[(-uw_x+wu_x)n_{e_i,1}-wun_2]ds &= \sum_{i=0}^{N}[\int_{\partial B_{e_i}\setminus T_{e_i}}[(-uw_x+wu_x)n_{e_i,1}-wun_{e_i,2}]ds\\ &+\int_{T_{e_i}}[(-uw_x+wu_x)n_{e_i,1}-wun_{e_i,2}]ds],\\ &=\sum_{i=0}^{N}[\int_{\partial B_{e_i}\setminus T_{e_i}}[u_xn_{e_i,1}-un_{e_i,2}]ds+\int_{T_{e_i}}u_xn_{e_i,1}ds,\\ &=\sum_{i=0}^{N}\int_{\partial B_{e_i}\setminus T_{e_i}}[u_xn_{e_i,1}-un_{e_i,2}]ds,\\ &=0.\end{aligned}$$

Where the third equality comes from the vertex condition $\sum_{e\sim v}u_xn_{e,1}=0$, and the final equality follows the same logic as (1.3). This implies

(2.21)

$$\begin{aligned}\sum_{i=1}^{N}\int_{\partial B_{e_i}\setminus T_{e_i}}[-uk_xn_{e_i,1}+ku_xn_{e_i,1}-kun_{e_i,2}]ds &= \sum_{i=1}^{N}\int_{\partial B_{e_i}\setminus T_{e_i}}uk_xn_{e_i,1}ds-C[-u_xn_{e_i,1}+un_{e_i,2}]ds,\\ &=\sum_{i=1}^{N}\int_{\partial B_{e_i}\setminus T_{e_i}}-uk_xn_{e_i,1}ds,\\ &=\int_{\partial B}-uk_xn_1ds.\end{aligned}$$

Thus, we have

$$u(q_0,t_0)=\int_{\partial B}-uk_xn_1ds+\sum_{v\in V}(d_v^+-d_v^-)\int_{B\cap v}uk_xds. \tag{2.22}$$

□

Definition 2.2. Let $V_1(G,q_0)=\{v\in V(G)\mid d_v=1 \text{ or } d(q_0,v) \text{ is a singularity of } d(q_0,\cdot)\}$, for $q_0\in G$.

Corollary 2.3. *Let G be a quantum graph and define $V_1(G,q_0)$ as in definition 2.2. If $B(q_0,t_0,C)\cap V_1(G,q_0)=\varnothing$ and $u(q,t)\geq 0$ solves the heat equation on G, then*

$$u(q_0,t_0)\leq\int_{\partial B}-uk_xn_1ds. \tag{2.23}$$

Proof. From theorem 2.1, we have

$$u(q_0,t_0)=\int_{\partial B}-uk_xn_1ds+\sum_{v\in V}(d_v^+-d_v^-)\int_{B\cap v}uk_xds \tag{2.24}$$

If v is not a singularity of $d(q_0,\cdot)$ and $v\neq v_0$, then for $v\neq v_0$, $d(q_0,v)$ is decreasing away from v for one edge adjacent to v, and increasing away from v for d_v-1 edges. This implies $d_v^+=d_v-1$ and $d_v^-=1$, which implies if $d_v>1$ then $d_v^+-d_v^-\geq 0$. Because $k_x<0$ for all $v\neq v_0$ and $u(q,t)\geq 0$

$$(d_v^+-d_v^-)\int_{B\cap v}uk_xds\leq 0. \tag{2.25}$$

For v_0, if v_0 is not a singularity of $d(q_0,\cdot)$ then for all edges adjacent to v_0 the coordinate system in increasing traveling away from v_0. This implies there are d_{v_0} edges adjacent to v_0

with $n_{e,1} = -1$ along $\partial B_e \cap v_0$. By the definition of d_v^+ and d_v^- for v_0, we subtract one from d_v^+ and add one to d_v^-. Hence, if $d_{v_0} > 1$ then $d_{v_0}^+ - d_{v_0}^- \geq 0$. This implies

$$(d_{v_0}^+ - d_{v_0}^-) \int_{B \cap v_0} u k_x ds \leq 0. \tag{2.26}$$

□

Note that for trees, the set $V_1(G, q_0) = \{v \in V \mid d_v = 1\}$.

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