VACUUM ENERGY IN QUANTUM GRAPHS

A Senior Honors Thesis

by

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We calculate the vacuum energy in quantum graphs. Vacuum energy arose in quantum physics but has an independent mathematical interest as a functional carrying information about the eigenvalue spectrum of a system. A quantum graph is a metric graph with a Hamiltonian applied to it, and recent research in quantum graphs has been directed towards their eigenvalue statistics. Quantum graphs provide an interesting model, intermediate between one-dimensional and higher-dimensional systems, in which we can study aspects of vacuum energy. In order to find the expression for vacuum energy, we use two methods: direct computation with the trace formula and the method of images (i.e. multiple reflection). The latter method also directly gives the vacuum energy density. Both methods are done heuristically for star graphs then rigorously for general graphs. We also discuss some properties of the vacuum energy in quantum graphs including: repulsive Casimir forces, convergence and continuity in bond lengths.
To my parents.
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CHAPTER I

INTRODUCTION

In what is to follow, we discuss vacuum energy in the context of quantum graphs. In this chapter we discuss some of the motivation for our work and the general results. In chapter II, we discuss the definitions and notation that will be used. In chapter III, we concentrate our analysis on quantum star graphs using more heuristic arguments to obtain results expounded upon in later chapters. We also make some observations and make reference to the recent paper [1] for some consequences of vacuum energy in star graphs. In chapter IV, we make the trace formula approach given in section III.B rigorous. We also discuss how our vacuum energy expression converges and is continuous in the lengths of the bonds. In chapter V, we make the method of images first given in section III.C rigorous, and it derives the same expression for the vacuum energy as in chapter IV. In addition, it also provides an expression for the vacuum energy density.

A. Motivation

Vacuum energy has theoretical background in quantum field theory, and was first shown by Casimir [2] to have an observable effect on two perfectly conducting parallel plates, causing them to attract. Since then, different physical geometries have been suggested and various experiments have confirmed the effects of vacuum energy, and there have been various reviews of the literature on vacuum energy [3, 4, 5]. In our manuscript, we use quantum graphs as models for various mathematical aspects of vacuum energy.

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This thesis follows the style and format of the *New Journal of Physics*.
The equations of interest in the study of vacuum energy are those given by free space Hamiltonians with boundaries\(^1\):

\[
H \psi_n = \omega_n^2 \psi_n, \tag{1.1}
\]

where \(H\) is the Hamiltonian for the system (for example, it can be the negative Laplacian) and \(\omega_n\) is an eigenfrequency associated with the eigenfunction \(\psi_n\). Equation (1.1) is obtained by separation of variables from the time-dependent Schrödinger’s equation, \(i \frac{\partial}{\partial t} \Psi = H \Psi\), and a general solution to the latter has \(\Psi\) as a sum over the \(\psi_n\)'s. We can also obtain (1.1) by separation of variables in the cylinder equation, \(\frac{\partial^2}{\partial r^2} u = Hu\) as well as other partial differential equations.

The vacuum energy, formally defined, is

\[
E = \frac{1}{2} \sum_n \omega_n. \tag{1.2}
\]

The above expression (1.2) arises in quantum field theory in the context of cavities and cosmological models [4], and it is formally divergent. To get a meaningful result from this expression, the vacuum energies for two different configurations are subtracted from one another, and the behavior of this difference as the initial configuration expands to fill all of space gives the vacuum energy, \(E_c\) [3]. We call \(E_c\) the regularized vacuum energy and it can be expressed as the regular part of

\[
\frac{1}{2} \sum_n \omega_n e^{-\omega_n t}. \tag{1.3}
\]

This procedure is called “ultra-violet cutoff regularization”.

Solving the eigenvalue problem (1.1) directly gives all the information about the eigenvalues, but this is not always practical if even possible [6]. The cylinder equation,

\(^1\)We take \(\hbar = 1 = c\) throughout.
$Hu = \frac{\partial^2}{\partial t^2}u$, has a Green’s function for $t > 0$ which we shall call the cylinder kernel, $T(t; x, y)$. It has been shown in [7] that given a space $\Omega$ in which we are solving our eigenvalue problem and

$$\text{Tr } T(t) = \int_\Omega T(t; x, x) \, dx,$$  \hspace{1cm} (1.4)

the cylinder kernel is related to the vacuum energy by

$$-\frac{1}{2} \frac{\partial}{\partial t} \text{Tr } T(t) = \frac{1}{2} \sum_n \omega_n e^{-\omega_n t}. \hspace{1cm} (1.5)$$

This procedure also yields an expression that can be interpreted as the regularized vacuum energy density,

$$-\frac{1}{2} \frac{\partial}{\partial t} T(t; x, x) = \frac{1}{2} \sum_n \omega_n e^{-\omega_n t} |\psi_n(x)|^2. \hspace{1cm} (1.6)$$

Using a cylinder kernel approach, Liu and Fulling have found the vacuum energy between a plate with Robin boundary conditions and a plate with Dirichlet boundary conditions [8]. Their method uses the method of images (i.e. the method of multiple reflection) on the free space cylinder kernel to create the cylinder kernel for their parallel plate case. We use an analogue of this method in section III.C and chapter V to construct the cylinder kernel for a quantum graph.

In some of the calculations for energy, it simplifies the discussion to put movable pistons in place of stationary walls, so that the energy causes an attractive or repulsive force on the pistons. This has been investigated for a two dimensional box by Cavalcanti with the result that the force is attractive between the piston and the nearest wall [9]. Other attractive piston conditions have been investigated by Hertzberg, et al. [10]. Quantum graphs, on the other hand, provide one model where the vacuum energy actually gives a repulsive force on pistons [1] under certain conditions.

Quantum chaos is related to the semi-classics of the system and to the eigenvalue
statistics. A plausible initial conjecture was that chaos, by spreading eigenvalues apart, reduces the magnitude of the vacuum energy and hence of the Casimir effect. Following up this idea was one motivation of the work of [7] on vacuum energy in a twisted line bundle; they found that the twisting did indeed spread the eigenvalues and reduce the size of the vacuum energy (and even change its sign). However, that model does not exhibit chaos, so chaos is not a necessary condition for damping vacuum energy. Because of calculational complexity, there are no explicit calculations addressing sufficiency, and the consensus seems to be that chaos and vacuum energy are not closely related. Nevertheless, Federico Capasso, a well-known experimentalist in the field, has suggested that a connection between vacuum energy and eigenvalue statistics still deserves investigation [11], and that remark was an important influence on the choice of the topic of this research project. Thus, in order to investigate vacuum energy in the context of eigenvalue statistics, we look at quantum graphs.

In the past decade, a great body of research has developed in quantum graphs in eigenvalue statistics and consequently, in quantum chaos. For a detailed discussion of quantum chaos and how it relates to classical chaos see [6] and [12].

Informally, a quantum graph is just a network of wires attached at the nodes. Mathematically, it is a metric graph with a differential operator applied to it (i.e. a Hamiltonian). Quantum graphs are well suited for analysis since they are a one-dimensional system, and as a result, the semi-classical approach is exact. For a review of the literature on quantum graphs see [13]. Since a quantum graph is a ‘physical system’ in the sense that we have a Hamiltonian on it, we can theoretically find the vacuum energy contained within it.

In chapter II, we define quantum graphs. We define an equation similar to (1.1) to obtain a spectrum, \( \{ \omega_n \} \), on a quantum graph. Each vertex in a quantum graph must have boundary conditions to define the self-adjoint operator on the graph. A
full analysis of what boundary conditions apply has been done by Kostrykin and Schrader [14, 15, 16] and is given in a different form in [17]. The spectrum we find can be analyzed with periodic orbits on the graph as described by the trace formula first found by Roth [18]. Subsequent versions of it have been discussed and derived by Kottos and Smilansky [19], Kostrykin, Potthoff, and Schrader [20], and others (such as [21]). While Kottos and Smilansky derived it from a secular determinant, Roth and Kostrykin, Potthoff, and Schrader derived it in the context of multiple reflections. The derivation given for the trace formula in these texts assumes that the $S$ matrix (see section II.C) is independent of the wave number, $k$.

Quantum graphs exhibit statistics characteristic of a chaotic system (see [22] for more details), so in the context of quantum graphs, we can study how the vacuum energy may depend on the chaos of a system. Berkolaiko has discussed in [23] how the spectral statistics for quantum star graphs (see definition II.8) when the number of vertices tends to infinity, are the same as those found for Šeba billiards. Winn has discussed in [24] the relationship between quantum graphs and quantum chaos with emphasis also on quantum star graphs. In the end, Winn relates the results he obtains to families of billiards. Furthermore, it has been shown that star graphs have intermediate wave function statistics [25] and they do not have quantum ergodic wave functions [26]. Thus, while quantum star graphs are a relatively simple system to find the vacuum energy on (see chapter 3), more general graphs must be considered to discover how vacuum energy is affected by the spectral statistics.

Fulling in [27] has looked at the effect of the energy density near a quantum graph vertex by construction of the cylinder kernel for an infinite star graph (a graph with one vertex and $B$ bonds extending to infinity). The quantum field theory origins of this (in a graph context) were given by Bellazzini and Mintchev [28]. The construction of the cylinder kernel for an infinite star graph provides the ground work for the
method of images in section III.C and chapter V.

The classic example of the method of images (i.e. multiple reflection) is a charge between two parallel conduction plates, as can be found in most books on electricity and magnetism. For two plates the method of images can be thought of as tracing out the path of a photon between them and defining a transformation on some free space function everytime the photon hits a plate. There have been various paper written on finding vacuum energy with optical paths in different geometries (see for instance [29, 30, 31, 32, 8]).

B. General Results

In later chapters, through both the trace formula and the method of images, the vacuum energy in a quantum graph, $E_c$, is found to be,

$$E_c = -\frac{1}{2\pi} \sum_p \frac{A_p}{L_p r_p}.$$  \hspace{1cm} (1.7)

In this expression the sum is over periodic orbits on our graph, $A_p$ is the amplitude of the orbit (as determined by the boundary conditions at the vertices it visits), $L_p$ is the (metric) length of the orbit, and $r_p$ is the repetition number of the orbit (see section II.B for an explanation of $r_p$). The concise formula (1.7) is convergent and continuous in the lengths of the bonds. It still remains an open problem to relate (1.7) to the spectral statistics, but the fact that it is continuous in the lengths of the bonds hints that there is not a strong connection between vacuum energy and the chaos of a system.

In the context of star graphs, we can obtain repulsive forces from this expression for a large number of bonds as discussed in chapter III and in [1]. In that paper, our coauthor L. Kaplan finds that the vacuum energy expression converges numerically.
The method of images given in chapter V derives the trace of an arbitrary integral kernel on the graph and with application of the resolvent kernel, provides another derivation of the trace formula. More directly though, application of the free space cylinder kernel to the method of images provides the vacuum energy, and it reproduces the result obtained by using the trace formula.

Furthermore, the method of images gives an expression for the vacuum energy density. The trace formula, on the other hand, does not give directly a method to find the vacuum energy density.

The expression in (1.7) and the two methods provided here to obtain it should provide insight into how the vacuum energy behaves on quantum graphs and what connection there may be to quantum chaos.
CHAPTER II

DEFINITIONS AND NOTATION

In this chapter, we develop the physical system we are to deal with: the quantum graph. Once that is developed, vacuum energy is introduced formally. The definitions and notation presented here will be the groundwork for chapters IV and V while chapter III will include some of the basics and leave out some of the directed bond formalism.

A. Topology of Graphs

A graph $G(V, B)$ is a set of vertices $V$ and a set of bonds $B$ whose elements are characterized by two vertices which they are said to connect. Throughout, the sizes of the sets are $|V| = V$, $|B| = B$, and the vertices will be numbered $1, \ldots, V$ while the bonds will be numbered $1, \ldots, B$ arbitrarily. In this way the notation $\ell \in B$ will be mixed with $\ell \in \{1, \ldots, B\}$. An example of a graph is shown in figure 1.

If $i \neq j$, let $(i, j) \subset B$ be the set of bonds connecting vertices $i$ and $j$, and $(i, i) \subset B$ be the set of loops connecting $i$ to itself. In figure 1 we have two loops on vertex one, and three bonds connecting vertices one and two.

Usually, a vertex connectivity matrix, $C(V)$, is defined as a $V \times V$ matrix such

Fig. 1. A graph with 4 vertices and 11 bonds.
that

\[
C^{(V)}_{ij} = \begin{cases} 
|i,j| & \text{if } i \neq j \\
2|i,j| & \text{if } i = j.
\end{cases}
\]  

(2.1)

This describes the topology of the graph. Note, a loop contributes twice to its entry in the connectivity matrix; the reason for this becomes clear with the definition of valency of vertex \( i \),

\[
v_i = \sum_{j=1}^{V} C_{ij}.
\]  

(2.2)

Valency can be thought of as the number of bonds coming out of a vertex. A loop contributes two because it adds two ways to leave a vertex \( i \).

**Definition II.1.** A subgraph \( G'(V',B') \) consists of \( V' \subseteq V \) and \( B' \subseteq B \) such that all \( \ell \in B' \) connect vertices in \( V' \) only.

**Definition II.2.** A graph is connected if there do not exist two non-empty subsets of the vertices which partition \( V \) with the property that there is no bond connecting the subsets.

In all of our discussion, we will look at connected graphs. If a graph is disconnected, then we can use our analysis on each of the connected components separately.

Within this framework, we can define different types of graphs.

**Definition II.3.** A graph is simple if it contains no loops or multiple bonds. (i.e. \( |i,j| \in \{0,1\} \) and \( |i,i| = 0 \) for all \( i,j \in V \).)

In our quantum graphs, we will be able to change any graph into a simple graph without changing the spectrum or wave functions (see [22] for details). So we will use simple, connected graphs frequently in our discussion and without loss of generality from more arbitrary graphs.
Definition II.4. A simple graph is *complete* if every vertex is connected to every other vertex (i.e. each vertex has valency $v = V - 1$).

Definition II.5. A simple, connected graph is a *ring* if $V = B$ and each vertex has valency $v = 2$. A *nontrivial* ring has $V \geq 2$.

Definition II.6. A graph is *simply connected* if there does not exist a nontrivial ring as a subgraph.

Definition II.7. A graph is a *tree* if it is simple, connected, and simply connected.

Definition II.8. A graph is a *star graph* if it has one vertex with valency $V - 1$ and all other vertices are connected to it and have valency 1.

Examples of a complete graph, a ring and a star are shown in figure 2. Star graphs will be used at first in our discussion of vacuum energy due to their simplicity. This will give us the necessary insight to look at arbitrary graphs.

For any vertex $i$, 

$$S(i) := \bigcup_{j \in V} (i, j)$$

(2.3)

is the *star of vertex* $i$.

Henceforth, we will consider connected, simple graphs to simplify some particulars in the definitions.
Note that \((i,j)\) means the same thing as \((j,i)\). On occasion it is necessary to distinguish between directions along a bond, hence the following definition.

**Definition II.9.** Given a bond \(\ell \in (i,j)\) with \(i < j\) we associate two *directed bonds* with it, \(\ell^+ = (\ell,+)\) going from \(i\) to \(j\) and \(\ell^- = (\ell,-)\) going from \(j\) to \(i\). The *set of directed bonds going from \(i\) to \(j\)* is denoted by \([i,j]\).

Even though we can still define directed bonds on loops, the need for an \(i = j\) case is eliminated since we are only considering simple graphs.

The set of directed bonds, \(D\), is defined as \(D = \bigcup_{\ell \in B} \{\ell^+, \ell^-\}\). With this definition, it is clear that \(|D| = 2B\). Greek letters will be used to represent directed bonds while latin letters (particularly \(\ell\)) will be reserved for undirected bonds.

**Definition II.10.** Given a directed bond \(\alpha = (\ell,d)\) where \(d \in \{+, -\}\), we define the following

- The *reversal of \(\alpha\)*, denoted by \(\bar{\alpha}\), is given by \(\bar{\alpha} = (\ell, -d)\).
- We denote the undirected bond associated with \(\alpha\) as \(|\alpha| := \ell\).
- If \(\alpha \in [i,j]\), then define \(o(\alpha) = i\) as the *origin* of \(\alpha\) and \(t(\alpha) = j\) as the *terminus* of \(\alpha\).

Similar to the star of vertex \(i\), we can define the *outgoing star at vertex \(i\)*, \(S^+(i)\), and the *incoming star at vertex \(i\)*, \(S^-(i)\), as

\[
S^+(i) = \bigcup_{j \in V} [i,j], \quad \text{and} \quad S^-(i) = \bigcup_{j \in V} [j,i].
\]  

(2.4)

Much like the vertex connectivity matrix, we can define the directed bond connectivity matrix, \(C^{(D)}\), as a \(2B \times 2B\) matrix with

\[
C^{(D)}_{\alpha\beta} = \begin{cases} 
1 & \text{if for some } i \in V, \alpha \in S^-(i) \text{ and } \beta \in S^+(i) \\
0 & \text{otherwise.}
\end{cases}
\]  

(2.5)
In other words, \( C_{\beta \alpha}^{(D)} = 1 \) implies that \( \beta \) follows \( \alpha \) on the graph. This allows us to define a path on a graph easily.

**Definition II.11.** The ordered set of bonds \( p = (\alpha_1, \ldots, \alpha_n) \) is a path if for all \( i \in \{1, \ldots, n-1\} \), \( C_{\alpha_{i+1} \alpha_i}^{(D)} = 1 \).

- A path is **closed** if \( C_{\alpha_1 \alpha_n}^{(D)} = 1 \).
- A **periodic orbit** is a class of closed paths that only differ by a cyclic permutation, and is denoted as \( p = (\alpha_1, \ldots, \alpha_n) \). (See appendix A.1 for more explanation of this equivalence class.)

The periodic orbits will play a central role in our arguments since we will be able to express our vacuum energy as a sum over periodic orbits. If we take a periodic orbit over \( n \) bonds (which we denote as \( p \in \mathcal{P}_n \), \( p = (\alpha_1, \ldots, \alpha_n) \)), we can make another periodic orbit: \( p^2 = (\alpha_1, \ldots, \alpha_n, \alpha_1, \ldots, \alpha_n) \) over \( 2n \) bonds. Similarly, we can construct any \( p^r \) for \( r \in \mathbb{N} \). This leads us to the notion of a primitive periodic orbit.

**Definition II.12.** A periodic orbit \( p_0 \) is **primitive** if it cannot be represented as \( p_0 = p^r \) for any other periodic orbit \( p \) and any natural number \( r \).

With this definition, we can write any periodic orbit \( p \), as \( p = p_0^r \) where \( p_0 \) is a primitive periodic orbit. If \( p \) is primitive, \( r = 1 \) and \( p = p_0 \). This representation in terms of a primitive periodic orbit is unique, and \( r \) is called the **repetition number** of the orbit (sometimes written as \( r_p \) to emphasize the dependence on \( p \)).

**B. Metric Graphs**

In addition to the graph structure in section II.A, we add coordinates along each bond. Each \( \ell \in \mathcal{B} \) is given a length \( L_\ell \), and because length does not depend on direction, we can write \( L_{\ell^+} = L_{\ell^-} := L_\ell \). Now, to specify a point in the graph, we
We define a coordinate on a directed bond $\alpha \in [i, j]$ so that $x_\alpha$ is zero at $i$, is $L_\alpha$ at $j$, and increases linearly between $i$ and $j$. From this, it can be shown that $x_\alpha = L_\alpha - x_\alpha$ for all $\alpha \in \mathbf{D}$. Whenever we speak of coordinates along an undirected bond $\ell$, we tacitly assume we have picked the $\ell^+$ coordinates. Also, in general, we will not include the subscript on $x_\alpha$ since from context it should be clear which bond we are talking about.

Now we take the common definition of the set of square integrable functions on an interval and construct the analogue for the graph as

$$L^2(G) := L^2[0, L_1] \oplus \cdots \oplus L^2[0, L_B].$$

We have informally said we have numbered the bonds $1, \ldots, B$. We can adopt a similar numbering for directed bonds if $\ell^+$ is numbered the same as $\ell$ and $\ell^-$ is numbered as $\ell + B$. In this way, we have numbered our directed bonds $1, \ldots, 2B$. Now, $u \in L^2(G) \oplus L^2(G)$ is a vector of functions along the directed bonds if $u_\alpha(x) = u_\alpha(L_\alpha - x)$ for all $\alpha \in \mathbf{D}$. By specifying the directed bond $\alpha$ and coordinate along that bond $x$, we obtain the value of $u$ at that point on the graph, $u_\alpha(x)$. We impose $u_\alpha(x) = u_\alpha(L_\alpha - x)$ to maintain that $u$ gives only one value for every point on the graph. Here, we have eliminated the need for the subscript on the $x$ by having the directed bond information on our function.

To relate these terms easily, we define the function on $\alpha$:

$$i_{\bar{\alpha}}(x) := L_\alpha - x. \tag{2.6}$$

Since this is a function on $\alpha$, the corresponding function on $\bar{\alpha}$ is $i_{\bar{\alpha}}(x) = x$. Thus,
this function $i_{\alpha\alpha}$ can be described as taking a point with coordinate on $\alpha$ and giving the corresponding coordinate for it on $\bar{\alpha}$.

In the previous section, we defined paths on non-metric graphs. We can generalize this to metric graphs in the following definition.

**Definition II.13.** A **metric path** over $n > 1$ bonds from point $x$ on directed bond $\alpha_1$ to point $y$ on directed bond $\alpha_n$ is defined as $p_{x,y} = (x, \alpha_1, \ldots, \alpha_n, y)$ such that for all $i \in \{1, \ldots, n-1\}$, we have $C_{\alpha_{i+1}\alpha_i}^{(D)} = 1$.

- The **length** of $p_{x,y}$ is $L_{p_{x,y}} = y_{\alpha_n} - x_{\alpha_1} + L_{\alpha_1} + \cdots + L_{\alpha_n-1}$. ($x_{\alpha_1}$ and $y_{\alpha_n}$ are the coordinates of the points on $\alpha_1$ and $\alpha_n$ respectively)
- A metric path on only one bond (so $p_{x,y} = (x, \alpha, y)$) must have $y_{\alpha} > x_{\alpha}$ and the length is $L_{p_{x,y}} = y_{\alpha} - x_{\alpha}$.
- A metric path from $x$ to $y$ is **closed** if $x$ and $y$ are the same point (i.e. they lie on the same undirected bond and $i_{\alpha_1\alpha_1}(x) = i_{\alpha_1\alpha_n}(y)$), and we say that path begins and ends at $x$ (or equivalently, at $y$).
- A metric path is a **periodic path** if it is closed and $\alpha_n = \alpha_1$.
- A metric path is a **bounce path** if it is closed but not periodic. If a particle is imagined traveling along a bounce path, it returns to the point it originated from with the opposite momentum.

Pictures of how these paths look are given in figure 3. Notice that for a periodic path $L_{p_{x,x}} = L_{\alpha_1} + \cdots + L_{\alpha_n-1}$ while for a bounce path

$$L_{p_{x,x}} = 2L_{\alpha_1} - 2x_{\alpha_1} + L_{\alpha_2} + \cdots + L_{\alpha_n-1} = 2x_{\bar{\alpha_1}} + L_{\alpha_2} + \cdots L_{\alpha_n-1}.$$
Fig. 3. A metric path from \( x \) to \( y \) on a graph, a periodic path, and a bounce path, from left to right.

As before, we can obtain periodic orbits from our definition of periodic metric paths. As an example, if \( p = (\alpha_1, \alpha_2, \ldots, \alpha_n) \) is a closed (non-metric) path, it is equivalent to \( p' = (\alpha_i, \alpha_{i+1}, \ldots, \alpha_n, \alpha_1, \alpha_2, \ldots, \alpha_{i-1}) \) (i.e. \( p \in p \) and \( p' \in p \); see appendix A.1). Similarly, if

\[
p_{x,x} = (x, \alpha_1, \alpha_2, \ldots, \alpha_n, \alpha_1, x),
\]

it is equivalent to

\[
p_{y,y} = (y, \alpha_i, \alpha_{i+1}, \ldots, \alpha_n, \alpha_1, \alpha_2, \ldots, \alpha_{i-1}, \alpha_i, y)
\]

for any \( y \) on the bond \( \alpha_i \).

This equivalence relation gives us the same interpretation of periodic orbits as before and can be described as taking out the beginning and ending point information. For example, \( p_{x,x} \) has the information of all the bonds it travels on in addition to the fact that it begins and ends at point \( x \), but for a periodic orbit, the information of where it begins and ends is lost so that we know only the bonds it travels on.
C. Quantum Graphs

To make metric graphs into quantum graphs, we now define differential operators on them. In the literature one commonly finds the Schrödinger operator applied to the graph (see for example, [22]). This operator takes the form,

$$H_\alpha = \left( \frac{1}{i} \frac{d}{dx_\alpha} + A_\alpha \right)^2 + V_\alpha(x).$$  \hfill (2.7)

Here, $A_\alpha$ is related to a magnetic vector field, and it has the property that $A_\alpha = -A_\bar{\alpha}$, $\frac{d}{dx_\alpha}$ is the derivative along the bond $\alpha$ (it too has the property that $\frac{d}{dx_\alpha} = -\frac{d}{dx_{\bar{\alpha}}}$) and $V_\alpha(x)$ is a potential on the graph. In our manuscript, we set $A_\alpha = 0$ and $V_\alpha(x) \equiv 0$ for all $\alpha$, so $H_\alpha$ reduces to the Laplacian,

$$H_\alpha = -\frac{d^2}{dx^2}. \hfill (2.8)$$

The subscript on the $x$ is dropped since $\frac{d^2}{dx_\alpha} = \frac{d^2}{dx_{\bar{\alpha}}}$. With (2.8), the eigenvalue equation is

$$H_\alpha u_\alpha(x) = k^2 u_\alpha(x)$$ \hfill (2.9)

for all $\alpha \in D$. We will refer to $k^2$ as the energy and $k$ as the wave number.

This does not complete our quantum graph, for we still need to know what happens at the vertices to define our self-adjoint operator. The conditions at the vertices will be referred to as the boundary conditions. Commonly in the literature one finds the Neumann (also called Kirchhoff) boundary conditions for a single vertex $i$:

$$u_\alpha(0) = \phi_i, \quad \forall \alpha \in S^+(i),$$ \hfill (2.10)

$$\sum_{\alpha \in S^+(i)} u'_\alpha(0) = 0.$$ \hfill (2.11)
In passing, we mention (2.11) can be generalized to Robin conditions by changing it to:

\[ \sum_{\alpha \in S^+(i)} u_\alpha'(0) = \lambda \phi_i. \] (2.12)

The other common boundary condition is pure Dirichlet,

\[ u_\alpha(0) = 0, \quad \forall \alpha \in S^+(i). \] (2.13)

In general, the boundary conditions for a vertex \( i \) can be written in the form due to Kostrykin and Schrader [14],

\[ Au|_{S^+(i)}(0) + Bu'|_{S^+(i)}(0) = 0, \] (2.14)

where \( u|_{S^+(i)}(0) \) is the vector of functions on the directed bonds contained in \( S^+(i) \) evaluated at 0 (at vertex \( i \)), and \( u'|_{S^+(i)}(0) \) is the same for their derivatives. Since \( v_i = |S^+(i)| \) (the valency), \( A \) and \( B \) are \( v_i \) by \( v_i \) matrices. They have the properties that

- \( (A, B) \) is of maximal rank, and
- \( AB^\dagger \) is self-adjoint.

With these conditions, \( A + ikB \) is invertible for all \( k > 0 \) and one can construct a unitary scattering matrix for that vertex (see [14] and [15]) which we will call \( \sigma^{(i)}(k) \),

\[ \sigma^{(i)}(k) = -(A + ikB)^{-1}(A - ikB). \] (2.15)

This \( v_i \) by \( v_i \) matrix is indexed by undirected bonds in \( S(i) \). Thus, \( \sigma^{(i)}_{\ell \ell'}(k) \) describes transmission from bond \( \ell \) to \( \ell' \) through vertex \( i \). Since \( \sigma^{(i)}(k) \) is unitary, \( \sigma^{(i)}(k)(\sigma^{(i)}(k))^\dagger = I \) where \( (\sigma^{(i)}(k))^\dagger \) means the conjugate transpose of \( \sigma^{(i)}(k) \).

To sketch where this comes from, consider an incoming plane wave on bond \( \ell \) incident on vertex \( i \) (i.e. \( \ell \in S(i) \)). After reflections and transmissions we should
obtain the following (assuming an infinite star graph):

\[
\begin{align*}
    u_{\ell'}(x) &= \begin{cases} 
        e^{-ikx} + \sigma_{\ell\ell}(k)e^{ikx} & \text{if } \ell' = \ell \\
        \sigma_{\ell'\ell}(k)e^{ikx} & \text{otherwise},
    \end{cases}
    \forall \ell' \in S(i).
\end{align*}
\]

This equation defines the scattering matrix; we can find the values using our boundary conditions. Evaluating \( u_{\ell'} \) and its derivative at zero, we obtain that,

\[
\begin{align*}
    u_{\ell'}(0) &= \delta_{\ell\ell'} + \sigma_{\ell'\ell}(k) \\
    u'_{\ell'}(0) &= ik(-\delta_{\ell\ell'} + \sigma_{\ell'\ell}(k)).
\end{align*}
\]

From these equations one can read of two matrices, one for the values at the vertices and another for the derivatives at the vertices. Putting these into the general boundary conditions in (2.14),

\[
A(I + \sigma^{(i)}(k)) + ikB(-I + \sigma^{(i)}(k)) = 0.
\]

Naively solving this, we obtain (2.15). This is handled more rigorously in the above cited papers by Kostrykin and Schrader.

**Example.** To construct the boundary conditions given in (2.10) and (2.11) for a vertex \( i \) with valency \( v_i \) we use the following two \( v_i \) matrices:

\[
A = \begin{pmatrix} 
1 & -1 & 0 & \cdots & 0 \\
0 & 1 & -1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & -1 \\
0 & 0 & 0 & \cdots & 0
\end{pmatrix}, \quad
B = \begin{pmatrix} 
0 & 0 & 0 & \cdots & 0 \\
0 & 0 & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \cdots & 0 \\
1 & 1 & 1 & \cdots & 1
\end{pmatrix}
\]

These satisfy the properties: \((A, B)\) is of maximal rank and \(AB^\dagger\) is self-adjoint. Thus,
we can find $\sigma^{(i)}$ using (2.15), getting

$$
\sigma^{(i)} = \begin{pmatrix}
\frac{2}{v_i} - 1 & \frac{2}{v_i} & \cdots & \frac{2}{v_i} \\
\frac{2}{v_i} & \frac{2}{v_i} - 1 & \cdots & \frac{2}{v_i} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{2}{v_i} & \frac{2}{v_i} & \cdots & \frac{2}{v_i} - 1
\end{pmatrix}.
$$

(2.19)

With a $\sigma^{(i)}(k)$ for each vertex $i$, the scattering matrix for the whole graph can be given as a $2B$ by $2B$ matrix indexed by directed bonds,

$$S_{\beta\alpha}(k) = \begin{cases}
\sigma^{(t(\alpha))}_{|\beta||\alpha|}(k) & \text{if } C^{(D)}_{\beta\alpha} = 1 \\
0 & \text{otherwise}.
\end{cases}
$$

(2.20)

This matrix is also unitary since it is a direct product of unitary vertex scattering matrices.

For much of what we do we will consider the scattering matrix to be independent of the wave number, $k$. This vastly simplifies things, and is characteristic of both Neumann and Dirichlet data at vertices. If the Robin data in (2.12) is used, the scattering matrix becomes $k$-dependent and harder to work with in practice.

The following theorem, due to Kostrykin and Schrader [15], characterize $k$-independent scattering matrices.

**Theorem II.1.** If the scattering matrix for vertex $i$, $\sigma^{(i)}$, is $k$-independent, then $A(I + \sigma^{(i)}) = B(I - \sigma^{(i)}) = 0$, $(\sigma^{(i)})^2 = I$ and consequently, $\sigma^{(i)} = (\sigma^{(i)})^\dagger$.

**Proof.** This is given in the papers by Kostrykin and Schrader, but here we offer a little proof using (2.17) and the fact that $A + ikB$ is invertible.

We know that $\sigma^{(i)}$ must solve (2.17) for $k > 0$, but $\sigma^{(i)}$ is independent of $k$, so
the following two equations hold (for $k = 2$ and $k = 1$ respectively),

$$A(I + \sigma^{(i)}) + 2iB(-I + \sigma^{(i)}) = 0,$$

$$A(I + \sigma^{(i)}) + iB(-I + \sigma^{(i)}) = 0.$$  

Subtracting the second from the first, we obtain $B(I - \sigma^{(i)}) = 0$ and it follows that $A(I + \sigma^{(i)}) = 0$. Consequently,

$$A(I + \sigma^{(i)})(I - \sigma^{(i)}) = 0,$$

$$A(I - (\sigma^{(i)})^2) = 0.$$  

Similarly, $B(I - (\sigma^{(i)})^2) = 0$. From this, it is seen that $(A + ikB)(I - (\sigma^{(i)})^2) = 0$, and $A + ikB$ is invertible implies that $I - (\sigma^{(i)})^2 = 0$. Thus, $\sigma^{(i)}$ is its own inverse and since $\sigma^{(i)}$ is unitary, its inverse is $(\sigma^{(i)})^\dagger$. Thus, $\sigma^{(i)} = (\sigma^{(i)})^\dagger$. \hfill $\square$

This theorem will be important later when we address the method of images and cancellation of bounce orbits (see section III.C and chapter V).

Returning to (2.9), take a solution, $\psi \in L^2(G)$, to this equation, whose elements solve $H_\ell \psi_\ell = k^2 \psi_\ell$, $\forall \ell \in B$. We can extend $\psi$ to $L^2(G) \oplus L^2(G)$ naturally by $\psi_{\ell^+}(x) = \psi_\ell(L_\ell - x)$. Thus, in what is to follow we drop the ‘+’ from the $\ell^+$ with the understanding that we measure $\ell$ in $\ell^+$ coordinates.

The inner product $\langle \cdot | \cdot \rangle$ on $L^2(G)$ is given by,

$$\langle \psi | \phi \rangle := \sum_{\ell=1}^B \int_0^{L_\ell} \psi_\ell^*(x) \phi_\ell(x) dx, \quad \forall \psi, \phi \in L^2(G),$$  \hspace{1cm} (2.21)

just a sum over all $L^2[0, L_\ell]$ inner products, and here $\psi^*$ refers to complex conjugate of $\psi$. Orthogonal functions, $\psi$ and $\phi$, on $L^2(G)$ satisfy $\langle \psi | \phi \rangle = 0$.

Equation (2.9) can be written as $H_\ell \psi_\ell = k^2 \psi_\ell$ in coordinates or $\Delta \psi = k^2 \psi$ with $\psi \in L^2(G)$ and $\Delta = (H_1, \ldots, H_B)$. Let $\{\psi_n \in L^2(G)\}_{n=1}^\infty$ be normalized orthogonal
eigenfunctions with corresponding eigenvalues \( \{k_n\}_{n=1}^{\infty} \). The \( k_n \) degeneracy is removed by having a number of orthogonal eigenfunctions equal to the multiplicity of \( k_n \). The facts that we get a discrete spectrum and a complete set of eigenfunctions from our quantum graphs are well known (but nontrivial to prove).

If we write a function \( u \) as a linear combination of these eigenfunctions,

\[
    u = \sum_n a_n \psi_n, \quad \text{or in terms of bonds,} \quad u_\ell(x) = \sum_n a_n \psi_{n,\ell}(x).
\]

(2.22)

The \( a_n \) can be expressed in terms of inner products, notably \( a_n = \langle \psi_n | u \rangle \). Writing this out,

\[
    a_n = \sum_{\ell=1}^{B} \int_0^{L_\ell} \psi_n^*(x) u(x) dx.
\]

(2.23)

This will be needed in the next section when understanding how we can obtain vacuum energy.

D. Vacuum Energy in Quantum Graphs

With the necessary tools in place to study our graphs, we now discuss what we are to find in these graphs: vacuum energy.

With our units of \( \hbar = c = 1 \), we have \( k_n = \omega_n \), and introducing an exponential cutoff function (see chapter I) the vacuum energy is

\[
    E(t) = \frac{1}{2} \sum_n k_n e^{-k_n t}, \quad t > 0.
\]

(2.24)

For a system, the regular part of (2.24) contributes to the force while the divergent part does not contribute and can thus be discarded in our vacuum energy calculations (see [3] for more details). In all the problems we will study in detail, this divergent part amounts to the free space energy without boundaries imposed and we will call it
$E_{\text{weyl}}(t)$ due to its connection with the Weyl term in the spectral asymptotics. Thus, the energy we are interested in is

$$E_c = \lim_{t \to 0^+} \left[ \frac{1}{2} \sum_n k_n e^{-k_n t} - E_{\text{weyl}}(t) \right]. \quad (2.25)$$

For our graphs, $E_{\text{weyl}}(t) = \frac{L}{2t}$, where $L$ is the total length of the graph (i.e. $L = L_1 + L_2 + \cdots + L_B$). This is clearly divergent and its connection to the Weyl term will be clear later (see section III.B and chapter IV).

We will be largely concerned with the vacuum energy $E_c$ and to a lesser extent with the vacuum energy density (with $\xi = \frac{1}{4}$, see [33]).

The vacuum energy density at point $x$ on bond $\ell$ is $\rho_{\ell}(x,t)$ and is given by

$$\rho_{\ell}(x, t) = \frac{1}{2} \sum_n k_n e^{-k_n t} |\psi_{n;\ell}(x)|^2, \quad t > 0. \quad (2.26)$$

Here we have that $|\psi_{n;\ell}(x)|^2 = \psi_{n;\ell}^*(x) \psi_{n;\ell}(x)$. Notice that since each $\psi_n$ is assumed to be normalized,

$$\sum_{\ell} \int_0^{L_\ell} \rho_{\ell}(x, t) dx = \frac{1}{2} \sum_n k_n e^{-k_n t} \langle \psi_n | \psi_n \rangle = E(t). \quad (2.27)$$

We can construct $E(t)$ with the help of the cylinder kernel [27]. For this we add a $t$-dependence (such as a time) to our graphs, with $t > 0$ being the region of interest and consider the partial differential equation,

$$H_{\ell} \Psi_{\ell}(x, t) = \frac{\partial^2}{\partial t^2} \Psi_{\ell}(x, t), \quad (2.28)$$

with the same boundary conditions at the vertices as discussed in the previous section. This is a separable equation and we can write a solution to it as $\Psi_{\ell}(x, t) = \psi_{\ell}(x) \phi(t)$. This gives us the eigenvalue problem (2.9) and an equation for $\phi$,

$$H_{\ell} \psi_{\ell}(x) = k^2 \psi_{\ell}(x) \quad \text{and} \quad \frac{\partial^2}{\partial t^2} \phi(t) = k^2 \phi(t). \quad (2.29)$$
With \( t > 0 \) and the condition that \( \phi \to 0 \) as \( t \to \infty \), \( \phi_n(t) = e^{-k_n t} \) and the general solution is of the form,

\[
\Psi_\ell(x,t) = \sum_n a_n \psi_n;\ell(x)e^{-k_n t}
\]  \hspace{1cm} (2.30)

The cylinder kernel, \( T \), solves (2.28) with the initial condition,

\[
T_{\ell\ell'}(0; x, y) = \begin{cases} 
\delta(x - y), & \text{if } \ell = \ell' \\
0, & \text{otherwise.}
\end{cases}
\]  \hspace{1cm} (2.31)

Using (2.23) it can be shown that,

\[
T_{\ell\ell'}(t; x, y) = \sum_n \psi^*_n;\ell'(y)\psi_n;\ell(x)e^{-k_n t}.
\]  \hspace{1cm} (2.32)

Notice that \( \rho_\ell(x,t) = -\frac{1}{2}\frac{\partial}{\partial t} T_{\ell\ell}(t; x, x) \). Calculating the trace of \( T \),

\[
\text{Tr } T(t) = \sum_\ell \int_0^L T_{\ell\ell}(t; x, x) \, dx = \sum_n e^{-k_n t},
\]  \hspace{1cm} (2.33)

we can find \( E(t) \) by the relation,

\[
E(t) = -\frac{1}{2}\frac{\partial}{\partial t} \text{Tr } T(t).
\]  \hspace{1cm} (2.34)

Thus, if we can find \( T \) for a graph, \( E(t) \) (and therefore \( E_c \)) can be calculated from it. Moreover, \( \rho \) can also be found from \( T \) similarly.

Finally, to obtain a force, we must differentiate \( E_c \) with respect to a length which changes in our problem (for example, in the two parallel plate case, the distance between the plates).
CHAPTER III

QUANTUM STAR GRAPHS

To begin our discussion, we consider star graphs as defined by definition II.8 and seen in figure III. This chapter lacks the mathematical rigor apparent in chapters IV and V, and focuses on more physical and heuristic arguments to obtain all the results for star graphs in the context of vacuum energy. Many of the results in later chapters are summarized here as well as results found for just star graphs. A lot of this can also be found in the recent paper by S. A. Fulling, L. Kaplan, and J. H. Wilson [1]. Also, due to the nature of star graphs, directed bonds are not used in this discussion.

A. Setting up the Star Graph and Equal Bond Lengths

The first attempt at evaluating (2.25) will be to find the spectrum explicitly. We will find that this requires us to assume the bond lengths must be equal for our star graph (i.e. $L_1 = \cdots = L_B := L$).

We label our bonds 1, \ldots, $B$ and since there are $B + 1$ vertices. The $B$ end vertices are labeled by the bond they are attached to and the central vertex is labeled by 0. Notice that in this specific case, labeling by vertices and bonds is equivalent,

![Fig. 4. A star graph with unequal bond lengths.](image-url)
so bond $\ell$ has end vertex $\ell$. This particular labeling for star graphs will be used in later sections.

The eigenvalue equation is (dropping directed bonds),

$$\frac{d^2}{dx^2} \psi_\ell(x) = k^2 \psi_\ell(x). \quad (3.1)$$

We take each $\ell^+$ to go from the central vertex out, so the coordinates of $\ell$ start at 0 at the central vertex and attain $L_\ell$ at each end vertex. The conditions at the vertices will be completely Neumann as in (2.10) and (2.11), and we will write them in the form,

$$\sum_\ell \psi_\ell'(0) = 0 \quad (3.2)$$

$$\psi_1(0) = \cdots = \psi_B(0) = C \quad (3.3)$$

$$\psi_\ell'(L_\ell) = 0 \quad \forall \ell \in B. \quad (3.4)$$

Solutions of (3.1) with (3.4) imposed have the form

$$\psi_\ell(x) = A_\ell \cos(k(L_\ell - x)). \quad (3.5)$$

Thus, imposing (3.2) and (3.3) should give us our spectrum, $\{k_n\}$. There are two cases to consider for this:

1. $\psi_1(0) = \cdots = \psi_B(0) \neq 0$. In this case, $C = A_\ell \cos(kL_\ell) \neq 0$, $\forall \ell \in B$, and so $\psi_\ell(x) = C \frac{\cos(k(L_\ell - x))}{\cos(kL_\ell)}$. Differentiating $\psi_\ell$ with this data and using (3.2) we obtain,

$$\sum_{\ell=1}^B \tan(kL_\ell) = 0. \quad (3.6)$$

Solving this for $k$, the part of the spectrum for this case is found (which we call $\{k_n^{(1)}\}$). In the special case where each $L_\ell$ is incommensurate (i.e. $\sum_\ell m_\ell L_\ell = 0$ with $m_\ell \in \mathbb{Z}$, has no solution except when $m_\ell = 0 \ \forall \ell \in B$, see [22]) this
expression gives all the eigenvalues, but finding a closed form for them is not feasible although a case 2 is not necessary anymore. To get a closed form, we assume that $L_1 = \cdots = L_B := L$, and we get,

$$\sin(k_n^{(1)}L) = 0 \implies k_n^{(1)} = \frac{n\pi}{L}, \quad n \in \mathbb{N}. \quad (3.7)$$

We introduce the notation $k_n^{(1)}$ to differentiate these eigenvalues from those in case 2 below. Each of these eigenvalues does not have a degeneracy associated with it.

2. $\psi_1(0) = \cdots = \psi_B(0) = 0$. In this case, eigenvalues come from,

$$A_\ell \cos(k_\ell L_\ell) = 0,$$

but since we have equal bond lengths and disregard the trivial solution, our values satisfy,

$$\cos(k_n^{(2)}L) = 0 \implies k_n^{(2)} = \left(n + \frac{1}{2}\right)\frac{\pi}{L}, \quad n \in \mathbb{N}. \quad (3.8)$$

To get degeneracy for these eigenvalues we have to return to (3.2) to obtain,

$$\sum_{\ell=1}^{B} A_\ell = 0,$$

which will give $B - 1$ distinct solutions. Thus, each $k_n^{(2)}$ has a degeneracy of $B - 1$.

Now, we can find $\text{Tr} \ T(t)$ from (2.33) by breaking up our spectrum into $k_n^{(1)}$ and
Fig. 5. A model of a $B = 4$ bond star graph with pistons. The (Neumann) pistons model the end vertices of the star graph and feel an outward force from the vacuum energy.

\[ k_n^{(2)} , \]

\[
\text{Tr } T(t) = \sum_{n=0}^{\infty} e^{-\frac{n\pi t}{L}} + (B - 1) \sum_{n=0}^{\infty} e^{-\left(n+\frac{1}{2}\right) \frac{\pi t}{L}}
\]

\[
= \frac{BL}{\pi} \frac{1}{t} + \frac{1}{2} - \frac{(B - 3)\pi}{24L} t + O(t^2). \quad (3.9)
\]

Now, using (2.34) and (2.25) with the knowledge that $E_{\text{weyl}}(t) = \frac{BL}{2\pi t}$, we obtain the vacuum energy directly,

\[
E_c = \frac{(B - 3)\pi}{48L}. \quad (3.10)
\]

To obtain the overall force on the graph, we differentiate with respect to the length, $L$. In this equal bond case, we obtain a repulsive force for $B > 3$. This force can be imagined by considering Neumann pistons in the place of end vertices as seen in figure 5. The Casimir force pushes or pulls on these pistons based on the number of bonds, as we found; this example is in [1]. The significance of the repulsive pistons is also discussed in [1] as well as numerical evaluations of the force for unequal bond lengths. It is found that even with unequal bonds, the force is repulsive for a high number of bonds.
B. Trace Formula on a Star Graph

For a star graph, the vertex scattering matrix for the central vertex, $\sigma^{(0)}$, is of main interest. All other end vertices have $\sigma^{(i)} = (\pm 1)$ (+1 for a Neumann vertex and $-1$ for a Dirichlet vertex), so by (2.20) we can obtain $S$ in block matrix form as a $2B$ by $2B$ matrix,

$$S = \begin{pmatrix} 0 & \sigma^{(0)} \\ (\pm 1)_B & 0 \end{pmatrix}, \quad (3.11)$$

where $(\pm 1)_B$ is a $B$ by $B$ square matrix with an assortment of $+1$ and $-1$ along its diagonal depending on if an end vertex is Neumann or Dirichlet respectively. For all Neumann conditions $(\pm 1)_B = I$.

We use the form of the trace formula found in [22] (for $H_{\ell} = -\frac{d^2}{dx^2}$),

$$d(k) := \sum_n \delta(k - k_n) = \frac{\mathcal{L}}{\pi} + \text{Re} \frac{1}{\pi} \sum_p A_p \frac{L_p}{r_p} e^{ikL_p}. \quad (3.12)$$

In this expression, the spectrum $\{k_n\}$ has been related to the periodic orbits $p$. The value $\mathcal{L} = L_1 + \cdots + L_B$ is the total length of the graph and the value $r_p$ is the repetition of the periodic orbit as explained in section II.B. For a given periodic orbit $p = (\alpha_1, \ldots, \alpha_n)$ going over $n$ bonds, $A_p = S_{\alpha_1\alpha_n}S_{\alpha_n\alpha_{n-1}} \cdots S_{\alpha_2\alpha_1}$ is the amplitude of the orbit and $L_p = L_{\alpha_1} + \cdots + L_{\alpha_n}$ is the length of the orbit. Also, note the first term is the Weyl term and is sometimes written as $d_{\text{weyl}}(k) = \frac{\mathcal{L}}{\pi}$.

To obtain vacuum energy we just apply the function $f(k) = \frac{1}{2}ke^{-kt}$, to get that,

$$E(t) = \frac{1}{2} \int_0^\infty ke^{-kt}d(k) \, dk. \quad (3.13)$$

Substituting this in and evaluating it (skipping all of the problems which arise),
we obtain

$$E(t) = \frac{L}{2\pi t^2} - \text{Re} \frac{1}{2\pi} \sum_p \frac{A_p}{L_p r_p} + O(t).$$

(3.14)

It can be seen from this that the divergent first term is just $E_{\text{weyl}}(t)$ which we said was the divergent part and is to be discarded to find $E_c$. So, using (2.25) the vacuum energy is found,

$$E_c = -\frac{1}{2\pi} \text{Re} \sum_p \frac{A_p}{L_p r_p}. \quad (3.15)$$

At no point have we assumed we were dealing with star graphs, so this expression is true for general graphs as will be shown carefully in chapters IV and V. Also, the ‘Re’ is not needed in the above expression, as explained in appendix A.2. This expression can be reformulated in terms of primitive periodic orbits, $p_0$, as defined in definition II.12,

$$E_c = -\frac{1}{2\pi} \text{Re} \sum_{p_0} \sum_{r=1}^{\infty} \frac{(A_{p_0})^r}{L_{p_0} r^2}. \quad (3.16)$$

Both (3.15) and (3.16) are equivalent.

Now, considering a quantum star graph, all periodic orbits can be written as $p = (\ell_1^+, \ell_1^-, \ell_2^+, \ell_2^-, \ldots, \ell_n^+, \ell_n^-)$, so instead of a sum over $p$ we can sum over $\bar{p} = (\ell_1, \ell_2, \ldots, \ell_n)$. This construction in terms of this $\bar{p}$ is unique to star graphs due to the form all $p$ on the star graph take. It can be seen that $L_p = 2L_{\bar{p}}$ and $r_p = r_{\bar{p}}$. To simplify $A_p$, we assume Neumann conditions at the end vertices as we did in the previous section. This makes the amplitude unaltered when it hits an end vertex, so we are in effect only looking at the central vertex. The amplitude becomes simply

$$A_p = A_{\bar{p}} = S_{\ell_1^+ \ell_1^-} S_{\ell_2^+ \ell_2^-} \cdots S_{\ell_n^+ \ell_n^-} = \sigma_{\ell_1 \ell_n}^{(0)} \sigma_{\ell_n \ell_{n-1}}^{(0)} \cdots \sigma_{\ell_2 \ell_1}^{(0)}.$$

Note that elements of $\sigma^{(0)}$ are indexed by undirected bonds unlike the $S$ matrix. Making these substitutions to change $p$ to $\bar{p}$ we can rewrite (3.15) for star graphs.
as,

\[ E_c = -\frac{1}{4\pi} \text{Re} \sum_{\bar{p}} \frac{A_{\bar{p}}}{L_{\bar{p}} r_{\bar{p}}} \]  \hspace{1cm} (3.17)

We can break up the sum over \( \bar{p} \) into two sums: the first as a sum over the number of undirected bonds traversed, \( n \), and the second as a sum over \( \bar{p} \) that traverse \( n \) bonds (we write this as \( \bar{p} \in \bar{P}_n \)). If we also assume that all bonds are equal, then for all \( \bar{p} \in \bar{P}_n \), \( L_{\bar{p}} = nL \), and

\[ E_c = -\frac{1}{4\pi L} \text{Re} \sum_{n=1}^{\infty} \sum_{\bar{p} \in \bar{P}_n} \frac{1}{n} \sum \frac{A_{\bar{p}}}{r_{\bar{p}}} \]  \hspace{1cm} (3.18)

Now, we use the following two facts to put the energy in terms of matrix eigenvalues.

- \( \sum_{\bar{p} \in \bar{P}_n} \frac{A_{\bar{p}}}{r_{\bar{p}}} = \frac{\text{Tr}(\sigma^{(0)})}{n} \). The proof of this mirrors that of lemma IV.1 (with \( s = 0 \)).

- If \( \{\lambda_j\}_{j=1}^B \) are the eigenvalues of \( \sigma^{(0)} \), then \( \text{Tr}(\sigma^{(0)}) = \sum_{j=1}^B (\lambda_j)^n \)

With these, \( E_c \) for star graphs with equal bond lengths can be put in terms of the central vertex scattering matrix eigenvalues (with Neumann conditions at the end vertices),

\[ E_c = -\frac{1}{4\pi L} \text{Re} \sum_{j=1}^B \sum_{n=1}^{\infty} \frac{(\lambda_j)^n}{n^2} \]  \hspace{1cm} (3.19)

Now, to check this against what we have already found for equal bond lengths, we need the scattering matrix for a Neumann vertex found in (2.19). In the star graph, \( v_0 = B \), and finding the eigenvalues for this matrix, we get \( \lambda_1 = 1 \) and \( \lambda_2 = \lambda_3 = \cdots = \lambda_B = -1 \). With these, \( E_c \) can be evaluated exactly and it is just (3.10). Thus, these methods agree for equal bonds. This same approach can be taken for the \( S \) matrix discussed at the beginning of this section, but the calculations are a bit more difficult and a connection to the method of images described in the next section would not be clear. Because the first method of images given for star graphs
in the next section focuses on the central vertex, we will find (3.17).

C. Method of Images on a Star Graph

The method of images takes a free space solution to a partial differential equation and finds a corresponding solution to a problem constrained with boundary conditions. We will apply this method to the free space cylinder kernel,

\[ T_0(t; |x - y|) = \frac{t/\pi}{t^2 + (x - y)^2}. \tag{3.20} \]

This comes from solving \(-\frac{\partial^2}{\partial t^2} T_0(t; x) = \frac{\partial^2}{\partial x^2} T_0(t; x)\) on the whole \(x\)-axis and \(t > 0\) with the initial condition \(T_0(0; x) = \delta(x)\). With (3.20), we can construct the cylinder kernel for our graph by the method of images below and thus, we obtain the vacuum energy and its density.

To do the method of images, we can take a free space solution to the one-dimensional problem (something which can separate into \(-\frac{d^2}{dx^2} u(x) = k^2 u(x)\) as the \(x\) part) and propagate it through all metric paths (see definition II.13) beginning at a point \(y\) on bond \(\ell\) and ending at a point \(x\) on bond \(\ell'\). Starting at point \(y\) amounts to shifting the coordinates of the function at this point, so in effect we can define \(\bar{u}(x) := u(x - y)\) and we now have \(\bar{u}\) starting at point 0. In this way, we will only consider the method of images on functions \(u(x)\) with our transformations going over a metric path \(p_{0,x}\). In the end, applying \(u(x - y)\) to this method (instead of \(u(x)\)) gives the most general solution. As we can see by (3.20), our cylinder kernel has the form \(T_0(t; |x - y|)\), so we will apply our method below to its \(x\) variable.

When speaking of metric paths, we discuss paths that go from \(y\) on \(\ell\) to \(x\) on \(\ell'\), but due to the above argument, when we write down an expression we will set \(y = 0\). Everytime a metric path passes through a vertex the solution is transformed, much
like reflection in the case of two plates. The details of this transformation will be left for chapter V (where it is called the $K$-transformation), but we just note here that $N_\ell$ is the transformation associated with vertex $\ell$ while $K_{\ell'\ell}$ describes the effect of going from bond $\ell$ to $\ell'$ through the central vertex. These transformations are determined by the boundary conditions at the vertices which they describe.

**Example.** For a completely Neumann graph, it turns out that

$$ [N_\ell u](x) = u(2L_\ell - x), \quad \text{and} \quad (3.21) $$

$$ [K_{\ell'\ell} u](x) = \left( \frac{2}{B} - \delta_{\ell'\ell} \right) u(-x). \quad (3.22) $$

The coefficient in (3.22) bears similarity to (2.19). This resemblance is no coincidence as is described below in (3.24).

Indeed, if $u$ solves a partial differential equation which separates into $-\frac{d^2}{dx^2} \psi(x) = k^2 \psi(x)$ as its $x$ part, then so do the above two transformed functions. If we consider $u_\ell(x) = u(x) + [N_\ell u](x)$, then $u'_\ell(x) = u'(x) - u'(2L_\ell - x)$ and thus, $u'_\ell(L_\ell) = 0$, so $N_\ell$ makes $u$ satisfy the Neumann condition at the end vertex.

On the other hand, if we consider $u_{\ell'}(x) = u(x)\delta_{\ell'\ell} + [K_{\ell'\ell} u](x)$, then we have,

$$ u_1(0) = u_2(0) = \cdots = u_B(0) = \frac{2}{B} u(0) \quad \text{and} \quad (3.23) $$

$$ \sum_{\ell' = 1}^{B} u'_{\ell'}(0) = u'(0) - \left[ \frac{B}{2} - 1 \right] u'(0) = 0, $$

so the $K_{\ell'\ell}$ transformation makes the solution satisfy the Neumann (i.e. Kirchhoff) condition at the central vertex. Note that we had the original solution originate on bond $\ell$ here.

For our star graphs, we can separate all metric paths from a point $y(=0)$ on $\ell$ to $x$ on $\ell'$ into four types listed below and shown in figure 6.
Fig. 6. The four types of metric paths from \( y \) to \( x \) on a star graph.

1. Beginning at \( y \) on \( \ell \) going \textit{towards} the central vertex and ending at \( x \) on \( \ell' \) going \textit{away} from the central vertex.

2. Beginning at \( y \) on \( \ell \) going \textit{away} from the central vertex and ending at \( x \) on \( \ell' \) going \textit{away} from the central vertex.

3. Beginning at \( y \) on \( \ell \) going \textit{towards} the central vertex and ending at \( x \) on \( \ell' \) going \textit{towards} the central vertex.

4. Beginning at \( y \) on \( \ell \) going \textit{away} from the central vertex and ending at \( x \) on \( \ell' \) going \textit{towards} the central vertex.

We will construct a metric path of type 1 and from that get 2, 3 and 4.

A metric path of type 1 can be written as

\[
P_{y,x} = (y, \ell^-, \ell_1^+, \ell_1^-, \ldots, \ell_n^+, \ell_n^-, \ell'_{\ell}, x)
\]

and we propagate \( u \) along this path so that

\[
u(x) \xrightarrow{P_{y,x}} [\Phi_{\ell', \ell_n, \ldots, \ell_1, \ell}](x) := [K_{\ell \ell_n} N_{\ell_n} K_{\ell_n \ell_{n-1}} \cdots N_{\ell_2} K_{\ell_2 \ell_1} N_{\ell_1} K_{\ell_1 \ell} u](x).
\]

Here \( K_{\ell_1 \ell} \) describes \( u \) propagating from \( \ell \) to \( \ell_1 \) through the central vertex, \( N_{\ell_1} \) describes the reflection off of the end vertex, \( \ell_1 \), and so on. Note that in the special case when \( n = 0 \) we set \( \Phi_{\ell', \ell} = K_{\ell \ell} \). Also, \( y \) is not included in the expression due to setting it to zero as justified above.
Using this, the four types can be represented in the following manner,

1. \( u(x) \mapsto [\Phi_{\ell', \ell_n, \ldots, \ell_1, \ell} u](x) \)

2. \( u(x) \mapsto [\Phi_{\ell', \ell_n, \ldots, \ell_1, \ell N} u](x) \)

3. \( u(x) \mapsto [N_{\ell} \Phi_{\ell', \ell_n, \ldots, \ell_1, \ell} u](x) \)

4. \( u(x) \mapsto [N_{\ell} \Phi_{\ell', \ell_n, \ldots, \ell_1, \ell N} u](x) \)

Adding up all possibilities of metric paths (\( y = 0 \) to \( x \)) just amounts to a sum over all \( n \) and all possibilities of \( \ell_1, \ldots, \ell_B \). This gives us a solution to the problem on bond \( \ell' \). If \( \ell' = \ell \) we must add the free space solution by itself and \( N_{\ell} u \) which we have neglected in this development (though it is of type 4). The solution then takes the form:

\[
u_{\ell \ell'}(x) = \delta_{\ell \ell'} (u(x) + [N_{\ell} u](x)) + \sum_{n=0}^{\infty} \sum_{p_n} [\Phi_{\ell', \ell_n, \ldots, \ell_1, \ell} u](x) + [N_{\ell} \Phi_{\ell', \ell_n, \ldots, \ell_1, \ell} u](x) + [N_{\ell} \Phi_{\ell', \ell_n, \ldots, \ell_1, \ell N} u](x) + [N_{\ell} \Phi_{\ell', \ell_n, \ldots, \ell_1, \ell N} u](x) \quad (3.23)
\]

This construction is completely general (in the context of star graphs) and even \( k \)-dependent scattering matrices can be used though relating these to the given transformations is difficult. For our purposes, we will assume that our transformation at the end vertices is the Neumann transformation given in (3.21) while at the central vertex we have a \( k \)-independent \( \sigma^{(0)} \) and thus,

\[
[K_{\ell' \ell} u](x) = \sigma^{(0)}_{\ell' \ell} u(-x).
\quad (3.24)
\]

Using these two transformations, the solution can be re-written with \( A_{p_n} = \sigma^{(0)}_{\ell_n \ell_{n-1}} \cdots \sigma^{(0)}_{\ell_2 \ell_1} \)
and \( L_{p_n} = L_{\ell_1} + \cdots + L_{\ell_n} \) as,

\[
\begin{align*}
   u_{\ell\ell'}(x) &= \delta_{\ell\ell'}(u(x) + u(2L_{\ell} - x)) + \\
   &\sum_{n=0}^{\infty} \sum_{p_n} A'_{\ell\ell'} \left[ -2L_{p_n} - x \right] + A_{\ell'p_n,\ell} u(2(L_{\ell} + L_{p_n}) + x) + \\
   &A_{\ell'p_n,\ell} u(-2(L_{p_n} + L_{\ell'}) + x) + A_{\ell'p_n,\ell} u(2(L_{\ell} + L_{p_n} + L_{\ell'}) - x). \quad (3.25)
\end{align*}
\]

It is interesting to note that the argument of \( u \) in each case is the length of the metric path described (with \( y = 0 \)).

The formula (3.25) can now be applied to the free space cylinder kernel in (3.20) to get a cylinder kernel for our quantum star graph which satisfies the initial condition given in (2.31) and the boundary conditions at the vertices. As mentioned before, these transformations act on the \( x \) variable in (3.20), and we obtain,

\[
T_{\ell\ell'}(t; x, y) = \delta_{\ell\ell'}(T_0(t; |x - y|) + T_0(t; |2L_{\ell} - x - y|)) + \\
\sum_{n=0}^{\infty} \sum_{p_n} [A_{\ell'p_n,\ell} T_0(t; |x - 2L_{p_n} - y|) + \\
+ A_{\ell'p_n,\ell} T_0(t; 2(L_{\ell} + L_{p_n}) + x - y)] + \\
+ A_{\ell'p_n,\ell} T_0(t; |2L_{p_n} + L_{\ell'} + x - y|) + \\
+ A_{\ell'p_n,\ell} T_0(t; 2(L_{\ell} + L_{p_n} + L_{\ell'}) - x - y)]. \quad (3.26)
\]
Now set $\ell = \ell'$ and $x = y$,

$$T_{\ell \ell}(t; x, x) = T_0(t; 0) + T_0(t; |2L_\ell - 2x|) +$$

$$\sum_{n=0}^{\infty} \sum_{p_n} [A_{\ell p_n} T_0(t; |2L_{p_n} + 2x|) + A_{\ell p_n} T_0(t; |2(L_\ell + L_{p_n})|) +$$

$$A_{\ell p_n} T_0(t; |2(L_{p_n} + \ell)|) +$$

$$A_{\ell p_n} T_0(t; |2(2L_\ell + L_{p_n}) - 2x|)]. \quad (3.27)$$

This accounts for all closed metric paths beginning and ending at $x$ and it should be noted that the first and last terms in the sum are due to bounce paths (for the definition of bounce paths, see definition II.13) while the middle two are periodic paths (and $T_0(t; |2L_\ell - 2x|)$ is also due to a bounce path).

We see from the previous vacuum energy expression (3.15) that only periodic paths will end up contributing, and it will be shown formally in chapter V that bounce paths all sum to a constant in the trace, called $C_{BP}$ here. This “cancellation” of bounce paths hinges on theorem II.1. The constant $C_{BP}$ is related to an index theory for graphs and is discussed in [34]. Here, on the other hand, we will just discard the bounce paths.

Using (2.33) for the trace of $T$,

$$\text{Tr } T(t) = T_0(t; 0)\mathcal{L} + C_{BP} + \sum_{n=0}^{\infty} \sum_{\ell=1}^{B} \sum_{p_n} A_{\ell p_n} T_0(t; |2(L_\ell + L_{p_n})|)2L_\ell, \quad (3.28)$$

where $C_{BP}$ is the constant described above. Let $\ell = \ell_0$ and change variables in the sum so that $\ell_0 \rightarrow \ell_1$ (i.e. $n \rightarrow n + 1$) to obtain,

$$\text{Tr } T(t) = T_0(t; 0)\mathcal{L} + C_{BP} + \sum_{n=1}^{\infty} \sum_{p_n} 2A_{p_n} T_0(t; 2L_{p_n})L_{\ell_1}. \quad (3.29)$$

Note, $A_{p_n \ell_1} = \sigma_{\ell_1 \ell_n}^{(0)} \sigma_{\ell_n \ell_{n-1}}^{(0)} \cdots \sigma_{\ell_2 \ell_1}^{(0)} = A_{\bar{\ell}}$ with $A_{\bar{\ell}}$ defined in the previous section.
and \( \bar{p} \in \bar{P}_n \). In a similar manner, we get \( L_{\mathbf{p}_n} = L_{\bar{\mathbf{p}}} \). These values are independent of cyclic permutations, so we can break up the sum over \( \mathbf{p}_n \) into the equivalence class of cyclic permutations of \( \mathbf{p}_n \) and the cyclic permutations themselves (see appendix A.1 for explanation of this equivalence class). These equivalence classes are the periodic orbits given by \( \bar{p} \). The sum of cyclic permutations is then,

\[
\sum_{n=1}^{\infty} \sum_{\bar{p} \in \bar{P}_n} \sum_{\mathbf{p}_n} 2A_{\bar{p}} T_0(t; 2L_{\bar{p}}) L_{\ell_1} = \sum_{n=1}^{\infty} \sum_{\bar{p} \in \bar{P}_n} 2A_{\bar{p}} T_0(t; 2L_{\bar{p}}) \frac{L_{\bar{p}}}{r_{\bar{p}}} \tag{3.30}
\]

The appearance of \( r_{\bar{p}} \) is due to the fact that if \( \sigma \) is the permutation transformation, then after \( n_{\bar{p}} := n/r_{\bar{p}} \) permutations \( \sigma^{n_{\bar{p}}}(\mathbf{p}_n) = \mathbf{p}_n \). Therefore, \( \sum_{\mathbf{p}_n} L_{\ell_1} = L_{\bar{p}_0} \) where \( \bar{p}_0 \) is the primitive periodic orbit such that \( \bar{p}_0^{r_{\bar{p}}} = \bar{p} \). Furthermore, \( L_{r_{\bar{p}_0}} = L_{\bar{p}}/r_{\bar{p}} \). Thus, our expression can be rewritten in terms of \( \bar{p} \),

\[
\text{Tr } T(t) = T_0(t; 0) \mathcal{L} + C_{BP} + \sum_{n=1}^{\infty} \sum_{\bar{p} \in \bar{P}_n} 2A_{\bar{p}} \frac{L_{\bar{p}}}{r_{\bar{p}}} T_0(t; 2L_{\bar{p}}). \tag{3.31}
\]

In the end, the \( T_0(t; 0) \mathcal{L} \) term becomes the \( E_{\text{weyl}}(t) \) term where \( \mathcal{L} \) is still the total length of the graph.

Differentiating to find \( E(t) \) and thus \( E_c \), the constant for bounce paths falls out and we get the same expression as before,

\[
E_c = -\frac{1}{4\pi} \sum_{n=1}^{\infty} \sum_{\bar{p} \in \bar{P}_n} \frac{A_{\bar{p}}}{L_{\bar{p}} r_{\bar{p}}} = -\frac{1}{4\pi} \sum_{\bar{p}} \frac{A_{\bar{p}}}{L_{\bar{p}} r_{\bar{p}}}. \tag{3.32}
\]

This may look different from (3.18), but in fact they are equal (see appendix A.2). The real part is only kept in the trace formula approach to emphasize that the energy is real-valued.

The vacuum energy density can be found from (3.27) with

\[
\rho_{\ell}(x, t) = -\frac{1}{2} \frac{\partial}{\partial t} T_{\ell \ell}(t; x, x),
\]
but no particular insight can be immediately seen from writing this out. Analyzing this object would be of interest, and it remains an open problem at the moment. All that can be said at the moment is if bounce paths are not taken into account in the vacuum energy density, then the vacuum energy density is a constant throughout the graph.

D. Analyzing the Vacuum Energy Expression

The equation in (3.15) is what we are to analyze. A full explanation of the numerical analysis associated with this is found in [1]. In all of our analysis, we have assumed Neumann boundary conditions at the end vertices, and that gave us (3.6) as the secular equation which gives us the spectrum, \( \{k_n\} \). If instead we put Dirichlet conditions on some vertices, our secular equation becomes

\[
\sum_{\ell=1}^{B} \tan(k L_\ell + \theta_\ell) = 0,
\]

(3.33)

where \( \theta_\ell = 0 \) if vertex \( \ell \) is Neumann and \( \theta_\ell = \pi \) if vertex \( \ell \) is Dirichlet.

What is to follow is due to independent work by our collaborator Lev Kaplan. The expression for vacuum energy in terms of the spectrum given in (2.25) can be numerically evaluated to any degree of accuracy as described in [1]. In this way, we can analyze our periodic orbit expression while comparing it to the actual energy. As in eq. (24) in [1], we can take the contribution to the vacuum energy due to the shortest primitive periodic orbits with a central Neumann vertex,

\[
E_{c}^{\text{shortest}} = -\frac{1}{4\pi} \sum_{\ell=1}^{B} \sum_{r=1}^{\infty} \frac{1}{r^2} \left( \frac{2}{B} - 1 \right) r \frac{\cos(r \theta_\ell)}{L_\ell}.
\]

(3.34)

Using this along with numerical comparisons with the actual energies, we find that not only do we get repulsive casimir forces for unequal bond lengths, but \( E_{c}^{\text{shortest}} \)}
gives a relatively simple way to guess the sign of the force (and hence its repulsive or attractive nature) for a large numbers of bonds (again, see [1] for more details).

We can further add on longer periodic orbits numerically and test how the expression we have found converges. This is done in the same paper as above by cutting off the sum at a maximum periodic orbit length, $L_{\text{max}}$. The error in the case of Neumann pistons in a star graph goes as $L_{\text{max}}^{-1}$. In the case of mixed Neumann and Dirichlet parts, the orbits of different length contribute with different sign since due to $\theta_{\ell}$ above; the error in this case falls off as $L_{\text{max}}^{-3/2}$. Thus, the expression for vacuum energy seems to converge. In the next chapter, we will find that in general, the vacuum energy expression does converge. It is in fact conditionally convergent, but any reasonable grouping of terms should give a sensible result.

The insight given by studying quantum star graphs leads naturally to more general graphs where we will find the same vacuum energy expression.
CHAPTER IV

THE TRACE FORMULA APPROACH

In the previous chapter, we found the vacuum energy through two main methods, but we left out the main details of the mathematical derivation of each. We first show that the vacuum energy found in (3.15) is convergent, though conditionally. Using the ideas here, we go back to the trace formula and formally derive (3.15). With this, it will be shown that the vacuum energy is continuous in the lengths of the bonds. The results in this chapter will be in a paper by G. Berkolaiko, J. Harrison, and J. H. Wilson [35].

A. Convergence of Vacuum Energy Expression

As stated in section III.B, (3.15) is true for any graph with a $k$-independent scattering matrix, not only for star graphs. This is because the trace formula is derived in [19] for general graphs with $k$-independent scattering matrices. Here we drop the ‘Re’ because of the argument given in appendix A.2.

The grouping we will consider is,

$$E_c = -\frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{p \in P_n} \frac{A_p}{L_p r_p}. \quad (4.1)$$

The sum over $p \in P_n$ is a finite sum, and we represent it as

$$\left| \sum_{p \in P_n} \frac{A_p}{L_p r_p} \right| = \left| \sum_{p \in P_n} \int_0^{\infty} \frac{A_p}{r_p} e^{-s L_p} ds \right|. \quad (4.2)$$

The equality can be established by simple evaluation of the integral given. To find an upper bound for these terms, we establish a lemma.
Lemma IV.1.

\[ \sum_{p \in \mathcal{P}_n} \frac{A_p}{r_p} e^{-sL_p} = \frac{1}{n} \text{Tr} \left( e^{-sL} \right)^n \]

with \( e^{-sL} \) defined below in (4.5).

Proof. To begin, recall that if \( p \in \mathcal{P}_n \), then \( p = (\alpha_1, \ldots, \alpha_n) \). Furthermore, \( \frac{n}{r_p} := n_p \) is the number of \( p \in p \) where \( p \) are merely vectors of directed bonds. For further explanation of this see appendix A.1. Therefore the following equality holds,

\[ n \sum_{p \in \mathcal{P}_n} \frac{A_p}{r_p} e^{-sL_p} = \sum_{p \in \mathcal{P}_n} \sum_{p \in p} A_p e^{-sL_p}. \tag{4.3} \]

Given this, we have \( p = (\alpha_1, \ldots, \alpha_n) \),

\[ A_p = S_{\alpha_1 \alpha_n} S_{\alpha_2 \alpha_{n-1}} \cdots S_{\alpha_2 \alpha_1}, \]

and \( L_p = L_{\alpha_1} + \cdots + L_{\alpha_n} \). Applying this,

\[ \sum_{p \in \mathcal{P}_n} \sum_{p \in p} A_p e^{-sL_p} = \sum_{p \in \mathcal{P}_n} e^{-sL_{\alpha_n}} S_{\alpha_1 \alpha_n} e^{-sL_{\alpha_n-1}} S_{\alpha_2 \alpha_{n-1}} \cdots e^{-sL_1} S_{\alpha_2 \alpha_1}, \tag{4.4} \]

where we have introduced \( \mathcal{P}_n \) as the set of vectors of \( n \) directed bonds. Now define the following matrix,

\[ e^{-sL} = \begin{pmatrix}
  e^{-sL_1} & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\
  0 & e^{-sL_2} & \cdots & 0 & 0 & 0 & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & e^{-sL_B} & 0 & 0 & \cdots & 0 \\
  0 & 0 & \cdots & 0 & e^{-sL_1} & 0 & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & 0 & 0 & e^{-sL_2} & \cdots & 0 \\
  \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
  0 & 0 & \cdots & 0 & 0 & 0 & \cdots & e^{-sL_B}
\end{pmatrix}. \tag{4.5} \]
With the matrix multiplication $e^{-sL}S$, we can write (4.4) as,

$$
\sum_{\alpha_1} \sum_{\alpha_2} \cdots \sum_{\alpha_n} (e^{-sL}S)_{\alpha_1\alpha_n}(e^{-sL}S)_{\alpha_n\alpha_{n-1}} \cdots (e^{-sL}S)_{\alpha_2\alpha_1} = \text{Tr} \left( e^{-sL}S \right)^n. \quad (4.6)
$$

With this lemma, we can prove convergence of (4.1).

Theorem IV.1. If $L_{\text{min}} = \min_j \{L_j\}$, then

$$
\left| \sum_{p \in \mathcal{P}_n} \frac{A_p}{L_p r_p} \right| \leq \frac{2B}{n^2 L_{\text{min}}}.
$$

Thus, (4.1) with the given grouping, converges.

Proof. Beginning with (4.2), we can interchange the sum and the integral since the sum is finite and using lemma IV.1,

$$
\left| \sum_{p \in \mathcal{P}_n} \frac{A_p}{L_p r_p} \right| = \left| \int_0^\infty \frac{1}{n} \text{Tr} \left( e^{-sL}S \right)^n ds \right|. \quad (4.7)
$$

Now consider $L_{\text{min}} = \min_\alpha \{L_\alpha\}$, so that $L_\alpha = L_{\text{min}} + L'_\alpha$ with $L'_\alpha \geq 0$ for all $\alpha$. Using this with (4.5), $e^{-sL} = e^{-sL_{\text{min}}} e^{-sL'}$ and the trace becomes,

$$
\text{Tr} \left( e^{-sL}S \right)^n = e^{-snL_{\text{min}}} \text{Tr} \left( e^{-sL'}S \right)^n. \quad (4.8)
$$

To obtain an upper bound to the trace, let $Q(s) = e^{-sL'}S$. Take the eigenvalues $\{\lambda_\alpha\}_{\alpha=1}^{2B}$ and left eigenvectors eigenvectors $\{v_\alpha\}_{\alpha=1}^{2B}$ normalized to one, then

$$
\langle Q^\dagger(s)v_\alpha, Q^\dagger(s)v_\alpha \rangle = |\lambda_\alpha|^2. \quad (4.9)
$$

The left-hand side of (4.9) can be written as $\langle v_\alpha, Q(s)Q^\dagger(s)v_\alpha \rangle$. Looking at $Q(s)Q^\dagger(s)$ then,

$$
Q(s)Q^\dagger(s) = e^{-sL'}SS^\dagger e^{-sL'} = e^{-2sL'}.
$$
The last equality is established since $S$ is unitary (i.e. $SS^\dagger = I$).

Thus, using the above and $\min_{\alpha} L'_\alpha = 0$,

$$\langle Q(s)v_\alpha, Q(s)v_\alpha \rangle = \langle v_\alpha, e^{-2sL}v_\alpha \rangle \leq \max_{\|v\|=1} \langle v, e^{-2sL}v \rangle = e^{-2s\min_{\alpha} L'_\alpha} = 1.$$  

From (4.9) and the above we obtain $|\lambda_\alpha| \leq 1$, and therefore,

$$|\text{Tr} (e^{-sL}S)^n| = |\text{Tr} (Q(s))^n| \leq \sum_{\alpha=1}^{2B} |\lambda_\alpha|^n \leq 2B. \quad (4.10)$$  

With this we can obtain from (4.7),

$$\left| \frac{1}{n} \int_0^{\infty} \text{Tr} (e^{-snL}S)^n \, ds \right| \leq \frac{1}{n} \int_0^{\infty} e^{-snL_{\text{min}}} |\text{Tr} (e^{-sL}S)^n| \, ds \leq \frac{2B}{n^2L_{\text{min}}}.$$  

\[\square\]

B. Proof of the Vacuum Energy Expression

With the ideas of the previous section, we return to the trace formula and derive the expression for the vacuum energy, $E_c$. The trace formula we will use here, in contrast to (3.12) will be convergent.

**Theorem IV.2.** Given the definition of $E_c$ in (2.25), we find for general quantum graphs with $k$-independent scattering matrices that,

$$E_c = -\frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{p \in P_n} A_p \frac{L_p}{L_p r_p}.$$  

**Proof.** The convergent trace formula as given in [22] is

$$d(k) := \sum_n \delta_\epsilon(k - k_n) = \frac{L}{\pi} + \frac{1}{\pi} \sum_{n=1}^{\infty} \sum_{p \in P_n} A_p \frac{L_p}{r_p} \cos(kL_p)e^{-\epsilon L_p}, \quad \epsilon > 0, \quad (4.11)$$  

where $\delta_\epsilon(k) = \frac{\epsilon/\pi}{e^{\epsilon/\pi} + 1}$ (so that $\delta_\epsilon(k) \to \delta(k)$ as $\epsilon \to 0$). This may look different from
(3.12), but in fact, they are equivalent and appendix A.2 discusses this.

It can be shown that,

\[
\lim_{\epsilon \to 0^+} \frac{1}{2} \int_0^\infty k e^{-kt} d(k) \, dk = \frac{1}{2} \sum_n k_n e^{-k_n t} = E(t). \tag{4.12}
\]

Therefore, equating both sides,

\[
E(t) = \frac{L}{2\pi} \int_0^\infty k e^{-kt} \, dk + \lim_{\epsilon \to 0^+} \frac{1}{2\pi} \sum_{n=1}^\infty \sum_{p \in \mathcal{P}_n} A_p \frac{L_p}{r_p} \int_0^\infty k \cos(kL_p)e^{-kt} \, dk \, e^{-\epsilon L_p} \tag{4.13}
\]

Considering the integral inside the sum by itself and applying the Laplace transform for it and the inverse Laplace transform,

\[
L_p \int_0^\infty k \cos(kL_p)e^{-kt} \, dk = -\frac{\partial}{\partial t} \left[ L_p \int_0^\infty \cos(kL_p)e^{-kt} \, dk \right]
= -\frac{\partial}{\partial t} \left[ \frac{L_p t}{L_p^2 + t^2} \right]
= -\frac{\partial}{\partial t} \left[ t \int_0^\infty \cos(st)e^{-sL_p} \, ds \right]
= - t \int_0^\infty \cos(st)e^{-sL_p} \, ds + t \int_0^\infty s \sin(st)e^{-sL_p} \, ds. \tag{4.14}
\]

We now take the same grouping as in (4.1), so that the element of interest is,

\[
\left| \sum_{p \in \mathcal{P}_n} \frac{A_p}{r_p} \left[ - t \int_0^\infty \cos(st)e^{-sL_p} \, ds + t \int_0^\infty s \sin(st)e^{-sL_p} \, ds \right] e^{-\epsilon L_p} \right|
\leq \left| \int_0^\infty \sum_{p \in \mathcal{P}_n} \frac{A_p}{r_p} \cos(st)e^{-sL_p-\epsilon L_p} \, ds \right| + \left| t \int_0^\infty \sum_{p \in \mathcal{P}_n} \frac{A_p}{r_p} s \sin(st)e^{-sL_p-\epsilon L_p} \, ds \right|. \tag{4.15}
\]

In the last expression, we used the triangle inequality since the sum is finite. Looking
at the first term then,

$$\left| \int_0^\infty \sum_{p \in \mathcal{P}_n} \frac{A_p}{r_p} \cos(st) e^{-(s+\epsilon)L_p} \ ds \right| \leq \int_0^\infty \left| \sum_{p \in \mathcal{P}_n} \frac{A_p}{r_p} e^{-(s+\epsilon)L_p} \right| \left| \cos(st) \right| \ ds$$

$$\leq \int_0^\infty \left| \sum_{p \in \mathcal{P}_n} \frac{A_p}{r_p} e^{-(s+\epsilon)L_p} \right| \ ds.$$  \hfill (4.16)

Now we can apply lemma IV.1 so that,

$$\int_0^\infty \left| \sum_{p \in \mathcal{P}_n} \frac{A_p}{r_p} e^{-(s+\epsilon)L_p} \right| \ ds = \int_0^\infty \left| \frac{1}{n} \Tr (e^{-(s+\epsilon)L} S)^n \right| \ ds,$$  \hfill (4.17)

and following the proof of theorem IV.1 exactly, we obtain,

$$\left| \int_0^\infty \sum_{p \in \mathcal{P}_n} \frac{A_p}{r_p} \cos(st) e^{-(s+\epsilon)L_p} \ ds \right| \leq \frac{2B}{n^2 L_{\text{min}}}.$$  \hfill (4.18)

Since we send $t \to 0^+$, we can say $t < 1$ and applying the same argument to the second term with $\sin(st)$, we get a similar inequality. In fact,

$$\left| \int_0^\infty \sum_{p \in \mathcal{P}_n} \frac{A_p}{r_p} s \sin(st) e^{-(s+\epsilon)L_p} \ ds \right| \leq \frac{2B}{n^3 L_{\text{min}}^2}.$$  \hfill (4.19)

After evaluating the integral inside the sum in (4.13) we obtain,

$$\left| - \sum_{p \in \mathcal{P}_n} A_p \frac{L_p}{r_p} \frac{\partial}{\partial t} \left[ \frac{t}{L_p^2 + t^2} \right] e^{-\epsilon L_p} \right| \leq \frac{2B}{n^2 L_{\text{min}}} + \frac{2B}{n^3 L_{\text{min}}^2}.$$  \hfill (4.20)

Thus, the sum converges absolutely by comparison to a $\sum_{n=1}^\infty n^{-2}$ series, and the convergence does not depend on $\epsilon$ or $t$, so it converges uniformly in both of these variables and we can bring the limit $\epsilon \to 0^+$ inside the sum, so

$$E(t) = \frac{\mathcal{L}}{2\pi t^2} - \frac{1}{2\pi} \sum_{n=1}^\infty \sum_{p \in \mathcal{P}_n} A_p \frac{L_p}{r_p} \frac{\partial}{\partial t} \left[ \frac{t}{L_p^2 + t^2} \right].$$  \hfill (4.21)
Returning to our definition of $E_c$ in (2.25) we get,

$$E_c = \lim_{t \to 0^+} -\frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{p \in P_n} A_p \frac{L_p}{r_p} \frac{\partial}{\partial t} \left[ \frac{t}{L_p^2 + t^2} \right] .$$  \hfill (4.22)

As stated previously, the term inside the sum is uniformly convergent in $t$, so we can bring the limit inside the sum, and obtain,

$$E_c = -\frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{p \in P_n} A_p \frac{L_p}{r_p} .$$  \hfill (4.23)

This argument proves our equation for vacuum energy in quantum graphs and its convergence. With this, we can do some formal analysis on our expression.

C. Analysis of the Vacuum Energy

Consider the case when all bonds of the graph are equal, so that if $p \in P_n$, then $L_p = nL$.

**Corollary IV.1.** If all bonds on a quantum are all equal to $L$, then the vacuum energy can be written as,

$$E_c = -\frac{1}{2\pi L} \sum_{\alpha=1}^{2B} \sum_{n=1}^{\infty} \frac{(\lambda_\alpha)^n}{n^2} ,$$

where $\{\lambda_\alpha\}_{\alpha=1}^{2B}$ are the eigenvalues of the $S$ matrix.

**Proof.** First, if $p \in P_n$, then $L_p = nL$, and we can use the expression for vacuum energy in theorem IV.2 to show,

$$E_c = -\frac{1}{2\pi L} \sum_{n=1}^{\infty} \frac{1}{n} \sum_{p \in P_n} \frac{A_p}{r_p} .$$  \hfill (4.24)
Using lemma IV.1 with $s = 0$ we then get,
\[ E_c = -\frac{1}{2\pi L} \sum_{n=1}^{\infty} \frac{1}{n^2} \text{Tr} (S^n). \] (4.25)

If $\{\lambda, \alpha = 1, 2, \ldots, 2B\}$ are the eigenvalues of $S$, then the corollary follows directly. \(\square\)

We can also show that our expression is continuous in the lengths of the bonds. For $0 < \epsilon \leq L_{\text{min}}$, theorem 4.1.1 can be modified to state,
\[ \left| \sum_{p \in P_n} \frac{A_p}{L_p r_p} \right| \leq \frac{2B}{n^2 \epsilon}. \] (4.26)

This tells us that $E_c$ converges uniformly in $L = (L_1, \ldots, L_B)$ for the domain, $[\epsilon, \infty)^B$, and is thus continuous in $L$ on those intervals. This does not imply that it converges uniformly on $(0, \infty)^B$ though. Now, we define the new notation $N_p = (N_p^{(1)}, \ldots, N_p^{(B)})$ so that, $L_p = N_p \cdot L$. Each $N_p^{(\ell)}$ is how many times the periodic orbit, $p$, went over bond $\ell$. This is used to state the following:

**Theorem IV.3.** The expression derived in theorem IV.2,
\[ E_c(L) = -\frac{1}{2\pi} \sum_{n=1}^{\infty} \sum_{p \in P_n} \frac{A_p}{(N_p \cdot L)r_p} \]
is infinitely differentiable with respect each $L_\ell$ and each derivative can be computed by differentiating term by term. Each derivative is itself uniformly convergent on $[\epsilon, \infty)$ with $\epsilon > 0$ for each bond length and each derivative is continuous in the lengths of the bonds.

**Proof.** To appear in the upcoming paper [35]. \(\square\)

Physical arguments aside, the first derivative with respect to bond $L_\ell$ gives the force tending to extend or contract a bond $\ell$, and this shows that the force is continuous in the bond lengths and can be differentiated term by term.
D. Remarks

In this chapter, we have shown that the vacuum energy expression we found converges, rigorously derived the vacuum energy expression, and argued that it is continuous in the lengths of the bonds (as well as infinitely differentiable). These give a solid foundation for the expression of vacuum energy using the trace formula. Though we have gained many insights into the vacuum energy in quantum graphs, this approach offers no direct way to find the vacuum energy density. This motivates the alternate approach presented in section III.C and chapter V of the method of images which, in effect, re-derives the trace formula.
CHAPTER V

THE METHOD OF IMAGES ON QUANTUM GRAPHS

Here we refine, abstract and give rigorous treatment to the method of images as described in section III.C. This will in effect, re-derive the trace formula, but more directly than that, this method can be applied to the cylinder kernel to obtain the vacuum energy and its density. This chapter will focus on this method and give as two of its results: the vacuum energy expression and its density. We also discuss briefly the connection this has with the actual trace formula and how the bounce paths give us an index theory for graphs as is discussed in the paper by S. A. Fulling, P. Kuchment, and J. H. Wilson [34].

A. The $K$ transformation and a General Solution on a Quantum Graph

We begin our discussion with what is called the $K$ transformation. We first develop the transformation for infinite star graphs and call it $\kappa^{(i)}$ (constructed for vertex $i$). Upon going to general finite graphs, we will construct the $K$ transformation in a similar manner to how we constructed the $S$ matrix in section II.C.

Consider the infinite star graph with coordinates starting with 0 at vertex $i$ and increasing away from the vertex on each bond (see figure 7). There are boundary conditions at the central vertex and a partial differential equation on the bonds which is separable in the graph coordinate (for example, (2.28) separates in the coordinate as seen in (2.29)). If $u$ solves this same partial differential equation on the whole real line, we call it a free space solution. In our arguments we will only discuss the graph coordinate $x$, suppressing the other coordinate from the partial differential equation.

An example is given in section III.C where the free space solution, $T_0$, given in (3.20) solves $-\frac{\partial^2}{\partial x^2}T_0(t; x) = \frac{\partial^2}{\partial t^2}T_0(t; x)$. In graph coordinates this equation was just
(2.28) which separated into (2.29). We will return to $T_0$ when we discuss the trace of the cylinder kernel for arbitrary graphs and hence, the vacuum energy.

With $u$ as our free space solution, the $\kappa^{(i)}$ transformation is defined to be the non-trivial transformation such that,

$$u_{\ell'}(x) = \begin{cases} u(x) + \kappa_{i \ell}^{(i)} u(x), & \text{if } \ell = \ell', \\ \kappa_{i \ell}^{(i)} u(x), & \text{otherwise}, \end{cases}$$

solves the partial differential equation on the graph and satisfies the boundary conditions at the vertex $i$ for all choices of $\ell$. Using $\kappa^{(i)}$, and we can obtain $K_{\beta \alpha}$ for an arbitrary finite graph by,

$$[K_{\beta \alpha} u](x) = \begin{cases} \kappa_{\beta | \alpha | \alpha}^{(t(\alpha))} \{ u \circ i_{\alpha \bar{\alpha}} \}, & \text{if } C_{\beta \alpha}^{(D)} = 1 \\ 0, & \text{otherwise}. \end{cases}$$

The introduction of $i_{\alpha \bar{\alpha}}$ (2.6) here is due to $u$ being on bond $\alpha$ whereas in the above construction of $\kappa^{(i)}$ it was technically on bond $\bar{\alpha}$, so $\kappa_{\beta | \alpha | \alpha}^{(t(\alpha))}$ works on functions with $\bar{\alpha}$ coordinates while $u$ is in $\alpha$ coordinates.

Now, we will construct the general solution under the method of images in much the same way as is done in section III.C. This part is merely motivation and not proof (the proof is given in appendix B). At the beginning of section III.C, we discussed why $p_{y,x}$ can be reduced to $p_{0,x}$ by defining a separate $\bar{u}(x) := u(x - y)$. The same

![Fig. 7. An infinite star graph with 5 bonds.](image-url)
Fig. 8. The four types of metric paths from \( y \) to \( x \) on a general graph.

argument holds for general graphs. Therefore, to get a solution that begins at \( y(=0) \) on directed bond \( \alpha \) and is measured at \( x \) on directed bond \( \beta \), we propagate \( u \) through all metric paths between them; a metric path which accomplishes this is one of four types:

1. The metric path starts at \( y \) going in the \( \alpha \) direction and ends at \( x \) going in the \( \beta \) direction.

2. The metric path starts at \( y \) going in the \( \bar{\alpha} \) direction and ends at \( x \) going in the \( \beta \) direction.

3. The metric path starts at \( y \) going in the \( \bar{\alpha} \) direction and ends at \( x \) going in the \( \bar{\beta} \) direction.

4. The metric path starts at \( y \) going in the \( \alpha \) direction and ends at \( x \) going in the \( \bar{\beta} \) direction.

In the case of a closed path, 1 and 3 would be periodic paths whereas 2 and 4 would be bounce paths. Pictures of these 4 types are included in figure 8.

To continue this construction, we assume that for each metric path we have the \( K \) transformation acting on \( u \) everytime it goes between two directed bonds, so if
\[ p_{0,x} = (0, \alpha, \alpha_1, \alpha_2, \ldots, \alpha_{n-1}, \beta, x), \]

\[ u \xrightarrow{p_{0,x}} \Phi_{\beta\alpha_n-1\cdots\alpha_1\alpha} u := K_{\beta\alpha_n-1} K_{\alpha_n-1\alpha_{n-2}} \cdots K_{\alpha_2\alpha_1} K_{\alpha_1\alpha} u. \]

This will sometimes be written as \( \Phi_{\beta p_{n-1}\alpha} \) where \( p_{n-1} = (\alpha_1, \ldots, \alpha_{n-1}) \) and if \( n = 1 \), \( \Phi_{\beta\alpha} = K_{\beta\alpha} \). As before, we can write the above 4 types as:

1. \( u \xmapsto{} \Phi_{\beta p_{n-1}\alpha} u \)

2. \( u \xmapsto{} \Phi_{\beta p_{n-1}\bar{\alpha}} u \)

3. \( u \xmapsto{} \Phi_{\bar{\beta} p_{n-1}\bar{\alpha}} u \)

4. \( u \xmapsto{} \Phi_{\bar{\beta} p_{n-1}\alpha} u \)

Now to obtain a general solution, we sum over the number of bonds an orbit goes over (\( n = 1 \) to \( \infty \)) and all the orbits of this size (we write as \( p_{n-1} \in \mathbb{P}_{n-1} \)). This construction yields the general formula given in the theorem below.

**Theorem V.1.** If \( u \) is a free space solution to the partial differential equation applied to our graph, then a formal solution to the same partial differential equation applied to every bond of a quantum graph with boundary conditions at the vertices takes the form (suppressing any other coordinate),

\[ u_{\beta\alpha}(x) = \sum_{n=1}^{\infty} \sum_{p_{n-1} \in \mathbb{P}_{n-1}} \left[ [\Phi_{\beta p_{n-1}\alpha} u](x) + [\Phi_{\beta p_{n-1}\beta} \{u \circ i_{\alpha}\beta\}](x) \right. \]

\[ + \left. \{\Phi_{\bar{\beta} p_{n-1}\bar{\alpha}} \{u \circ i_{\alpha}\bar{\alpha}\} \circ i_{\bar{\beta}\beta}(x) + [\Phi_{\bar{\beta} p_{n-1}\beta} \circ i_{\bar{\beta}\beta}(x)] \right) \]

\[ = \begin{cases} u(x) & \text{if } \beta = \alpha \\ u \circ i_{\alpha\alpha}(x) & \text{if } \beta = \bar{\alpha} \\ 0 & \text{otherwise,} \end{cases} \]
for all $\beta$ and $x$ measured on directed bond $\beta$; $u_{\beta \alpha}$ is also a function on directed bonds $\beta$ (i.e. $u_{\beta \alpha} = u_{\beta \alpha} \circ i_{\beta \beta}$).

**Proof.** See appendix B.

The mapping $i_{\beta \beta}$ appears in this theorem because $[K_{\bar{\beta} \alpha} u]$ outputs a function in $\bar{\beta}$ coordinates, so applying $i_{\beta \beta}$ puts us back in $\beta$ coordinates. Similarly, $i_{\alpha \bar{\alpha}}$ appears since $u$ is initially on bond $\alpha$, so for $K_{\alpha \bar{\alpha}}$ to act on it, we must first apply $i_{\alpha \bar{\alpha}}$ to it.

In the next section, we will find an appropriate $K$ transformation to analyze a partial differential equation which can be separated into our well known eigenvalue problem, $H_\alpha u_\alpha = k^2 u_\alpha$.

**B. Relating $K$ Transformations to the $S$ matrix**

The above construction implies that all we need to find is a $\kappa^{(i)}$ transformation for every vertex $i$. Naturally, there is a connection to the vertex scattering matrix, $\sigma^{(i)}$ when these matrices are $k$-independent. The following theorem gives this connection.

**Theorem V.2.** Consider (1) a quantum graph with $H := H_1 = \cdots = H_B = -\partial^2 / \partial x^2$ and boundary conditions which give a $k$-independent scattering matrix, $S$, (2) a separable equation $H u(t, x) = \bar{H}_t u(t, x)$ where $\bar{H}_t$ is some linear differential operator on $u$ acting on its $t$ coordinate (e.g. $\bar{H}_t = \partial^2 / \partial t^2$ for the cylinder equation), and (3) a free space solution of the partial differential equation, $u$. Then the $K$-transformation (5.2) is

$$[K_{\bar{\beta} \alpha} u](t, x) = S_{\bar{\beta} \alpha} u(t, L_\alpha + x)$$

**Proof.** To establish this, we consider an infinite quantum star graph on a vertex $i$ with boundary conditions as defined in (2.14) and we will suppress the $t$ coordinate
in $u$. These become for our infinite star graph,

$$A\bar{u}(0) + B\bar{u}'(0) = 0 \quad (5.3)$$

with the conditions on $A$ and $B$ discussed in section II.C. In this case, $\bar{u} = (u_1, \ldots, u_B)$ is the vector of functions on each infinite bond and $\bar{u}(0)$ amounts to evaluating all of these at 0 (the vertex $i$).

The first claim is $[\kappa^{(i)}_{\ell\ell'}u](x) = \sigma^{(i)}_{\ell\ell'}u(-x)$. Since $u$ is a free space solution, (5.1) implies that we need to check if

$$u_{\ell'}(x) = \delta^\ell_{\ell'}u(x) + \sigma^{(i)}_{\ell\ell'}u(-x), \quad (5.4)$$

is a solution to the infinite star graph for all $\ell$. For one, since each term is a solution to the above partial differential equation, this too is a solution to it on each bond by superposition. Thus, we just need to check if this satisfies the boundary conditions.

If (5.4) is a solution for all $\ell$ then the boundary conditions must be satisfied for the matrix $\bar{u} = Iu(x) + \sigma^{(i)}u(-x)$. To see if this fits the boundary conditions, define the matrix $C$ as,

$$C := A\bar{u}(0) + B\bar{u}'(0) = A(I + \sigma^{(i)})u(0) + B(I - \sigma^{(i)})u'(0). \quad (5.5)$$

By theorem II.1, $A(I + \sigma^{(i)}) = B(I - \sigma^{(i)}) = 0$ for $k$-independent $\sigma^{(i)}$. Thus, $C = 0$ and therefore, the boundary conditions are satisfied, so $[\kappa^{(i)}_{\ell\ell'}u](x) = \sigma^{(i)}_{\ell\ell'}u(-x)$ is a legitimate transformation.

The $K$-transformation is then,

$$[K_{\beta\alpha}u](t) = [\kappa^{(t(\alpha))}_{|\beta|\alpha}(u \circ i_{\alpha\alpha})](x) = \sigma^{(t(\alpha))}_{|\beta|\alpha}u(L_{\alpha} + x), \quad \text{if } C^{(D)}_{\beta\alpha} = 1.$$

The $\sigma^{(t(\alpha))}_{|\beta|\alpha}$ term is the same as for the $S$ matrix in (2.20), so $[K_{\beta\alpha}u](x) = S_{\beta\alpha}u(L_{\alpha} + x)$ if $C^{(D)}_{\beta\alpha} = 1$, and both the $K$ transformation and $S$ give 0 when $C^{(D)}_{\beta\alpha} = 0$. Thus,
\[ [K_{\beta\alpha}u](x) = S_{\beta\alpha}u(L_{\alpha} + x) \text{ for all } \beta \text{ and } \alpha. \]

After establishing our \( K \)-transformation, we can rewrite the formal solution in theorem VI.1 (suppressing the \( t \)-coordinate),

\[
u_{\beta\alpha}(x) = \sum_{n=1}^{\infty} \sum_{p_{n-1} \in \mathbb{P}_{n-1}} \left[ A_{\beta p_{n-1} \alpha} u(L_{\alpha} + L_{p_{n-1}} + x) + A_{\beta p_{n-1} \bar{\alpha}} u(-L_{p_{n-1}} - x) \right.
\]
\[
\left. + A_{\beta p_{n-1} \alpha} u(-L_{p_{n-1}} - L_{\beta} + x) + A_{\beta p_{n-1} \alpha} u(L_{\alpha} + L_{p_{n-1}} + L_{\beta} - x) \right]
\]
\[
\begin{cases} 
  u(x) & \text{if } \beta = \alpha \\
  u(L_{\alpha} - x) & \text{if } \beta = \bar{\alpha} \\
  0 & \text{otherwise}.
\end{cases}
\] (5.6)

In the expression, we introduce,

\[ A_{\beta p_{n-1} \alpha} = S_{\beta \alpha n-1} S_{\alpha n-1 \alpha n-2} \cdots S_{\alpha 2 \alpha 1} S_{\alpha 1 \alpha} \]

and \( L_{p_{n-1}} = L_{\alpha_1} + \cdots + L_{\alpha_{n-1}}. \)

Issues of convergence aside, we will apply this expression to a general kernel to obtain the trace of it. Different \( \bar{H}_t \) can be used for different kernels. For instance, to obtain the cylinder kernel we use \( \bar{H}_t = \partial^2 / \partial t^2 \). This will lead to the vacuum energy and its density.

The general kernel we discuss has the form \( G_0(t; |x - y|) \) in free space, and the method above is applied to the \( x \)-coordinate. The solution will be the equivalent kernel for the graph. The initial conditions that a kernel on the graph satisfies are,

\[
G_{\beta\alpha}(0; x, y) = \begin{cases} 
  \delta(x - y), & \text{if } \beta = \alpha \\
  \delta(L_{\alpha} - x - y), & \text{if } \beta = \bar{\alpha} \\
  0, & \text{otherwise}.
\end{cases}
\] (5.7)
In the expression for \( G_{\beta \alpha}(t; x, y) \), \( x \) is measured along bond \( \beta \) and \( y \) is measured along bond \( \alpha \). Originating \( G_0(t; |x - y|) \) on bond \( \alpha \) and applying the method of images in (5.6) to the \( x \)-coordinate gives a solution which satisfies the above initial conditions.

As the first step in obtaining the trace of \( G \), we set \( \beta = \alpha = \ell^+ \) and \( y = x \) after applying (5.6),

\[
G_{\ell \ell}(t; x, x) = G_0(t; 0) + \sum_{n=1}^{\infty} \sum_{p_{n-1} \in P_{n-1}} \left[ A_{\ell^+ p_{n-1} \ell^+} G_0(t; L \ell + L_{p_{n-1}}) \right.
\]

\[
+ A_{\ell^+ p_{n-1} \ell^-} G_0(t; L_{p_{n-1}} + 2x) + A_{\ell^- p_{n-1} \ell^+} G_0(t; L_{p_{n-1}} + L \ell) \]

\[
+ A_{\ell^- p_{n-1} \ell^-} G_0(t; 2L \ell + L_{p_{n-1}} - 2x) \].
\]

(5.8)

The first and third terms in the above sum are due to the periodic paths while the second and fourth are due to bounce paths.

C. The Trace of a Kernel on a Quantum Graph

Before discussing and proving the main theorem of this section, we separate out the parts of the trace,

\[
\text{Tr } G(t) = G_{\text{weyl}}(t) + G_{\text{BP}}(t) + G_{\text{PO}}(t).
\]

(5.9)

The three parts of the trace are due to the Weyl term, the bounce paths (BP), and the periodic orbits (PO) respectively. Writing these out,

\[
G_{\text{weyl}}(t) = \sum_{\ell=1}^{B} \int_{0}^{L \ell} G(t; 0) \, dx = \mathcal{L} G(t; 0),
\]

(5.10)

\[
G_{\text{BP}}(t) = \sum_{\ell=1}^{B} \int_{0}^{L \ell} \sum_{n=1}^{\infty} \sum_{p_{n-1} \in P_{n-1}} \left[ A_{\ell^+ p_{n-1} \ell^-} G_0(t; L_{p_{n-1}} + 2x) \right.
\]

\[
+ A_{\ell^- p_{n-1} \ell^-} G_0(t; 2L \ell + L_{p_{n-1}} - 2x) \] \]

(5.11)
and

\[
G_{\text{PO}}(t) = \sum_{\ell=1}^{B} \int_{0}^{L_{\ell}} \sum_{n=1}^{\infty} \sum_{p_{n-1} \in I_{n-1}} \left[ A_{\ell^{+}p_{n-1}^{+}} \rho_{0}(t; L_{\ell} + L_{p_{n-1}}) \right. \\
+ \left. A_{\ell^{-}p_{n-1}^{+}} \rho_{0}(t; L_{p_{n-1}} + L_{\ell}) \right] dx.
\] (5.12)

Clearly, we have

\[
G_{\text{Weyl}}(t) + G_{\text{BP}}(t) + G_{\text{PO}}(t) = \sum_{\ell=1}^{B} \int_{0}^{L_{\ell}} G_{\ell\ell}(t; x, x) \, dx.
\]

To establish the next theorem, we will need one crucial lemma in order to obtain that the bounce paths reduce down to a nice closed form.

**Lemma V.1.** If the scattering matrix \( S \) of a graph is \( k \)-independent, then

\[
\sum_{\alpha_{n}=1}^{2B} A_{\alpha_{n}^{+}\alpha_{n-1}^{+}\cdots\alpha_{1}^{+}\alpha_{n}} = \delta_{\alpha_{1}^{+}\alpha_{n-1}^{+}} A_{\alpha_{n-1}^{+}\cdots\alpha_{1}^{+}}.
\]

**Proof.** We know \( A_{\alpha_{n}^{+}\alpha_{n-1}^{+}\cdots\alpha_{1}^{+}\alpha_{n}} = S_{\alpha_{n}^{+}\alpha_{n-1}^{+}} S_{\alpha_{n-1}^{+}\alpha_{n-2}^{+}} \cdots S_{\alpha_{2}^{+}\alpha_{1}^{+}} S_{\alpha_{1}^{+}\alpha_{n}} \) by definition. Thus, we can write our sum as,

\[
\sum_{\alpha_{n}=1}^{2B} A_{\alpha_{n}^{+}\alpha_{n-1}^{+}\cdots\alpha_{1}^{+}\alpha_{n}} = A_{\alpha_{n-1}^{+}\cdots\alpha_{1}^{+}} \sum_{\alpha_{n}=1}^{2B} S_{\alpha_{1}^{+}\alpha_{n}} S_{\alpha_{n-1}^{+}\alpha_{n}}.
\]

For both elements in the sum on the right-hand side to be nonzero, we must have \( t(\alpha_{n-1}) = o(\alpha_{1}) =: i \) and \( \alpha_{n} \in S^{+}(i) \). Thus, using \( |\alpha_{n}| = |\alpha_{n}| \) and the equivalence of \( S^{+}(i) \) to \( S(i) \),

\[
\sum_{\alpha_{n}=1}^{2B} S_{\alpha_{1}^{+}\alpha_{n}} S_{\alpha_{n-1}^{+}\alpha_{n}} = \sum_{\alpha_{n} \in S^{+}(i)} \sigma_{|\alpha_{n}|^{(i)} \alpha_{n}^{(i)} |\alpha_{n-1}^{(i)} |\alpha_{n}|^{(i)}} = \sum_{\ell \in S^{(i)}} \sigma_{|\alpha_{1}^{(i)} \ell^{(i)} |\alpha_{n-1}^{(i)}}.\]
It has already been established in theorem II.1 that \((\sigma^{(i)})^2 = I\), so

\[
\sum_{\ell \in S(i)} \sigma_\ell^{(i)} \sigma^{(i)}_\ell |_{\alpha_1} |_{\alpha_{n-1}} = \delta_{\alpha_1 \alpha_{n-1}}.
\]

\hspace{1cm} \blacksquare

**Theorem V.3.** Assume the conditions of theorem V.2 and that \(G_0(t; |x - y|)\) is the free space kernel of \(HG_0 = \tilde{H} G_0\). Assume further that (5.8) converges uniformly for \(x \in [0, L_\ell]\), then the trace of the corresponding kernel, \(G\), for a graph is

\[
\text{Tr } G(t) = \mathcal{L}G_0(t; 0) + \frac{1}{2} \left[ \sum_{\alpha=1}^{2B} S_{\alpha\alpha} \right] \int_0^\infty G_0(t; x) \, dx + \sum_p A_p \frac{L_p}{r_p} G_0(t; L_p).
\]

The sum over \(p\) is a sum over all periodic orbits and \(A_p, L_p,\) and \(r_p\) are respectively the amplitude, length and repetition number of the periodic orbit \(p\).

**Proof.** The condition that (5.8) converge uniformly for \(x \in [0, L_\ell]\) allows us to manipulate the sums and integrals. Such a condition may be able to be relaxed in favor of conditions on \(G_0\).

First, this will be broken up into two parts. We have already established that \(G_{\text{weyl}}(t) = \mathcal{L}G(t; 0)\), we just need to work with the periodic orbit part and the bounce path part.

**Periodic Orbit Part**

From (5.12) above, there is no \(x\) dependence, so we can integrate through by \(x\) and simplify,

\[
G_{\text{PO}}(t) = \sum_{n=1}^\infty \sum_{p_{n-1} \in P_{n-1}} \sum_{\ell_1=1}^B [A_{\ell_1} + A_{\ell_1}] G(t; L_{p_{n-1}} + L_\ell) L_\ell.
\]

The two amplitudes given here decouple if instead of \(\ell\) we sum over the directed bond
Using this and combining $\alpha_n$ into $p_{n-1}$ to get $p_n$, the sum becomes,

$$G_{PO}(t) = \sum_{n=1}^{\infty} \sum_{p_n \in \mathbb{P}} A_{p_n \alpha_n} G(t; L_{p_n}) L_{\alpha_n}.$$

Now we break up the sum over $p_n$ into a sum over periodic orbits, $p$, and a sum of vectors in these orbits. Note from appendix A.1 that if $p_n \in p$, $A_{p_n \alpha_n} = A_p$ and $L_{p_n} = L_p$, and thus,

$$G_{PO}(t) = \sum_{n=1}^{\infty} \sum_{p_n \in \mathbb{P}} \sum_{p \in p} A_p G(t; L_p) L_{\alpha_n}.$$

In the last sum, $\sum_{p \in p} L_{\alpha_n} = L_{p_0}$ where $p_0$ is the primitive periodic orbit such that $p = p_{r_p}$. This length can be represented as $L_{p_0} = L_p/r_p$, so the sum simplifies down,

$$G_{PO}(t) = \sum_{n=1}^{\infty} \sum_{p \in \mathbb{P}} A_p \frac{L_p}{r_p} G(t; L_p). \quad (5.13)$$

**Bounce Path Part**

Similar to the first lines of the periodic orbit part above, we can collect terms and decouple the amplitudes, so changing our $\ell$ to $\alpha_n$ as before,

$$G_{BP}(t) = \frac{1}{2} \sum_{n=1}^{\infty} \sum_{p_{n-1} \in \mathbb{P}} \sum_{\alpha_n = 1}^{2B} A_{\alpha_n p_{n-1} \alpha_n} \int_{L_{p_{n-1}}}^{L_{p_{n-1}}+2L_{\alpha_n}} G(t; x) \, dx.$$
We now simplify this expression by considering the cutoff function,

\[ H(y - x) = \begin{cases} 
1, & x \leq y \\
0, & x > y.
\end{cases} \]

Instead of \( G(t; x) \) in the integral, consider \( \hat{G}(t; x) = G(t; x)H(y - x) \). Then we know that there exists \( m \in \mathbb{N} \) such that \((m - 1)L_{\min} \leq y \) and \( mL_{\min} > y \), then for \( n \geq m \) and all \( \mathbf{p}_n \in \mathbb{P}_n \) and \( \alpha_{n+1} \), we have \( L_{\mathbf{p}_n} > y \) and that implies,

\[
\int_{L_{\mathbf{p}_n}}^{L_{\mathbf{p}_n} + 2L_{\alpha_{n+1}}} \hat{G}(t; x) \, dx = 0.
\]

This cuts off our sum in \( n \) at the value \( n = m \) and we now utilize the two cases:

- If \( y < L_{\mathbf{p}_{m-1}} \), then \( \int_{L_{\mathbf{p}_{m-1}}}^{L_{\mathbf{p}_{m-1}} + 2L_{\alpha_m}} \hat{G}(t; x) \, dx = 0 = \int_y^{L_{\mathbf{p}_{m-1}}} \hat{G}(t; x) \, dx. \)

- If \( y \geq L_{\mathbf{p}_{m-1}} \), then \( (m - 1)L_{\min} \leq L_{\mathbf{p}_{m-1}} \) and so using \( mL_{\min} > y \) we obtain \( y < L_{\mathbf{p}_{m-1}} + L_{\min} < L_{\mathbf{p}_{m-1}} + 2L_{\alpha_m} \), and we can then equate the two integrals:

\[
\int_{L_{\mathbf{p}_{m-1}}}^{L_{\mathbf{p}_{m-1}} + 2L_{\alpha_m}} \hat{G}(t; x) \, dx = \int_y^{L_{\mathbf{p}_{m-1}}} \hat{G}(t; x) \, dx.
\]

Both of these cases show that,

\[
\int_{L_{\mathbf{p}_{m-1}}}^{L_{\mathbf{p}_{m-1}} + 2L_{\alpha_m}} \hat{G}(t; x) \, dx = \int_y^{L_{\mathbf{p}_{m-1}}} \hat{G}(t; x) \, dx.
\]

Therefore, we have the bounce path part with the given cutoff,

\[
\hat{G}_{\text{BP}}(t) = \frac{1}{2} \sum_{n=1}^{m} \sum_{\mathbf{p}_{n-1} \in \mathbb{P}_{n-1}} \sum_{\alpha_n=1}^{2B} A_{\alpha_n \mathbf{p}_{n-1} \alpha_n} \int_{L_{\mathbf{p}_{n-1}}}^{L_{\mathbf{p}_{n-1}} + 2L_{\alpha_n}} \hat{G}(t; x) \, dx
\]

\[
= \frac{1}{2} \sum_{n=1}^{m-1} \sum_{\mathbf{p}_{n-1} \in \mathbb{P}_{n-1}} \sum_{\alpha_n=1}^{2B} A_{\alpha_n \mathbf{p}_{n-1} \alpha_n} \int_{L_{\mathbf{p}_{n-1}}}^{L_{\mathbf{p}_{n-1}} + 2L_{\alpha_n}} \hat{G}(t; x) \, dx
\]

\[
+ \frac{1}{2} \sum_{\mathbf{p}_{m-1} \in \mathbb{P}_{m-1}} \sum_{\alpha_m=1}^{2B} A_{\alpha_m \mathbf{p}_{m-1} \alpha_m} \int_y^{L_{\mathbf{p}_{m-1}}} \hat{G}(t; x) \, dx. \tag{5.14}
\]
Utilizing lemma V.1 and concentrating on the second set of sums in (5.14),

\[
\sum_{p_{m-1} \in \mathbb{F}_{m-1}} \sum_{\alpha_{m-1} = 1}^{2B} A_{\alpha_{m-1}} p_{m-1} \int_{L_{p_{m-1}}}^{y} \hat{G}(t; x) \, dx
\]

\[
= \sum_{p_{m-3} \in \mathbb{F}_{m-3}} \sum_{\alpha_{m-2} = 1}^{2B} A_{\alpha_{m-2}} p_{m-3} \int_{L_{p_{m-3}}}^{y} \hat{G}(t; x) \, dx. \quad (5.15)
\]

This was the \(m\)th term in the series. For the \((m - 1)\) term, the bullets above can be modified to show that \(y < L_{p_{m-2}} + 2L_{\alpha_{m-1}}\) and this gives the result,

\[
\int_{L_{p_{m-2}}}^{L_{p_{m-2}} + 2L_{\alpha_{m-1}}} \hat{G}(t; x) \, dx = \int_{L_{p_{m-2}}}^{y} \hat{G}(t; x) \, dx.
\]

Similar to (5.15), we can separate out the \((m - 1)\) term and write it as,

\[
\sum_{p_{m-2} \in \mathbb{F}_{m-2}} \sum_{\alpha_{m-1} = 1}^{2B} A_{\alpha_{m-1}} p_{m-2} \int_{L_{p_{m-2}}}^{y} \hat{G}(t; x) \, dx
\]

\[
= \sum_{p_{m-4} \in \mathbb{F}_{m-4}} \sum_{\alpha_{m-3} = 1}^{2B} A_{\alpha_{m-3}} p_{m-4} \int_{L_{p_{m-3}}}^{y} \hat{G}(t; x) \, dx. \quad (5.16)
\]

The next step in this argument is also the inductive step. If we separate out the \((m - 2)\) term and add it to the simplified \(m\) term in (5.15) note that we get two integrals added together: \(\int_{L_{p_{m-2}}}^{L_{p_{m-3}} + 2L_{\alpha_{m-2}}} \hat{G}(t; x) \, dx + \int_{L_{p_{m-3}}}^{y} \hat{G}(t; x) \, dx = \int_{L_{p_{m-3}}}^{y} \hat{G}(t; x) \, dx\). Then lemma V.1 can be applied again. This is done for both the \(m\) term and \((m - 1)\) term separately all the way down to the first and second terms, which gives,

\[
\hat{G}_{BP}(t) = \frac{1}{2} \sum_{\alpha_{1}}^{2B} A_{\alpha_{1}} \int_{0}^{y} \hat{G}(t; x) \, dx + \frac{1}{2} \sum_{\alpha_{1} = 1}^{2B} \delta_{\alpha_{1}} \int_{L_{\alpha_{1}}}^{y} \hat{G}(t; x) \, dx.
\]

Clearly, \(\delta_{\alpha_{1}} = 0\) and in the first term, we can take \(y \to \infty\) to get back \(G_{BP}(t)\):

\[
G_{BP}(t) = \frac{1}{2} \left[ \sum_{\alpha_{1}}^{2B} S_{\alpha_{1}} \right] \int_{0}^{\infty} G(t; x) \, dx \quad (5.17)
\]

With (5.13) and (5.17) we have \(\text{Tr} \ G(t)\). □
As discussed above, the condition of uniform convergence on (5.8) may be able to be relaxed to conditions on $G_0$. This should even go back to conditions on $u$ which make (5.6) converge. In the discussion to follow, it is taken for granted that (5.8) converges uniformly on $x$.

D. Applications of the Kernel Trace including Vacuum Energy

A number of things can be found through the expression in theorem V.3. To begin, recall from (2.19) that in the case of Neumann conditions $\forall i \in \mathbf{V}$ and $\ell, \ell' \in S(i)$,

\[\sigma^{(i)}_{\ell\ell'} = \frac{2}{v_i} - \delta_{\ell\ell'}\text{ where } v_i = |S(i)|\text{ is the valency of } i.\]

Looking at the bounce path contribution then,

\[
\sum_{\alpha=1}^{2B} S_{\alpha\alpha} = \sum_{i=1}^{V} \sum_{\ell \in S(i)} \sigma^{(i)}_{\ell\ell} = \sum_{i=1}^{V} \left( \frac{2}{v_i} - 1 \right) v_i = 2(V - B). \tag{5.18}
\]

The term $V - B$ is the Euler characteristic of our graph, and this constant term is related to an index theory on graphs as is discussed in [34]. Indeed, there is such an index theorem for any quantum graph with $k$-independent boundary conditions, although the index is not equal to the Euler characteristic in general.

This bounce term is a ‘trace’ in the sense that it is a sum of traces as observed in (5.18). This motivates the definition,

\[
\mathbf{Tr} S := \sum_{\alpha=1}^{2B} S_{\alpha\alpha} = \sum_{i=1}^{V} \mathbf{Tr} \sigma^{(i)} \tag{5.19}
\]

For the bounce path contribution to add up to a constant the integral, $\int_0^\infty G_0(t; x) \, dx$, must be independent of the extra variable $t$. For example, this is true for the free
space cylinder kernel $T_0$ and the free space heat kernel $K_0$,

$$T_0(t; |x - y|) = \frac{t/\pi}{t^2 + (x - y)^2}, \quad (5.20)$$

$$K_0(t; |x - y|) = \frac{1}{\sqrt{4\pi t}} e^{-\frac{(x-y)^2}{4t}}. \quad (5.21)$$

In the case of $T_0$, $\tilde{H}_t = \frac{\partial^2}{\partial t^2}$, and in the case of $K_0$, $\tilde{H}_t = -\frac{\partial}{\partial t}$. We can also apply this method to the resolvent kernel given by,

$$G_0(k^2; |x - y|) = \frac{i}{2k} e^{ik|x-y|} \quad (5.22)$$

Since this is an integral kernel, to get it in terms of $k$ we need to consider $d(k^2) = 2k \, dk$. Thus, $G_0(k; |x - y|) = ie^{ik|x-y|}$. Applying this by itself will give something divergent (it will be a sum of delta functions). To get around this, we apply $\tilde{G}_0(k; |x - y|) = ie^{ik|x-y| - \epsilon|x-y|}$ for some small $\epsilon > 0$. Now from,

$$\frac{1}{\pi} \text{Im Tr } \tilde{G}(k) = \sum_n \delta_\epsilon(k - k_n), \quad (5.23)$$

with $\delta_\epsilon(k) = \frac{\epsilon}{\epsilon^2 + k^2}$ so that as $\epsilon \to 0$, $\delta_\epsilon(k) \to \delta(k)$. The $\{k_n\}$ is the spectrum given by the eigenvalue problem we have considered throughout. Using this, we obtain by theorem V.3,

$$\sum_n \delta_\epsilon(k - k_n) = \frac{L}{\pi} + \frac{1}{2} \text{Tr } S \delta_\epsilon(k) + \frac{1}{\pi} \sum_p A_p \frac{L_p}{r_p} \cos(kL_p) e^{-\epsilon L_p}. \quad (5.24)$$

This is the convergent trace formula, and if we let $\epsilon \to 0$ we get the trace formula (4.11).

Returning to the vacuum energy, we apply $T_0$ to theorem V.3,

$$\text{Tr } T(t) = \frac{L}{\pi t} + \frac{1}{4} \text{Tr } S + \sum_p A_p \frac{L_p}{r_p} \frac{t/\pi}{t^2 + L_p^2}. \quad (5.25)$$

Indeed, the bounce paths now cancel when differentiating and using (2.34) to get $E(t)$
and then applying (2.25) to get

\[ E_c = -\frac{1}{2\pi} \sum_p \frac{A_p}{L_p r_p}, \]  

(5.26)

our familiar \( E_c \) for quantum graphs. We can also go back in our derivation to (5.8) and apply \( T_0 \) to obtain \( T_{\ell\ell}(t; x, x) \), and hence \( \rho_\ell(t, x) = -\frac{1}{2\pi} \frac{\partial}{\partial t} T_{\ell\ell}(t; x, x) \).
CHAPTER VI

CONCLUSIONS

We have found by the trace formula and the method of images the vacuum energy expression for general quantum graphs with $k$-independent scattering matrices using an ultra-violet cutoff,

$$E_c = -\frac{1}{2\pi} \sum_p \frac{A_p}{L_p r_p}.$$ 

Both methods given were first done in chapter III in the context of quantum star graphs without the same amount of rigor as was covered for general graphs in chapters IV and V. Several results though were special to quantum star graphs. In modeling this system with tiny pistons as the end vertices, we find (with Neumann conditions) that the vacuum energy causes a repulsive force for a larger number of bonds (when $B > 3$ for the equal bond case). In addition, through numerical calculations [1] one finds that this expression converges if the periodic orbit lengths are cut off at some $L_{\text{max}}$.

Through rigorous application of the trace formula, we formally found the vacuum energy expression for general graphs (with $k$-independent scattering matrices) in chapter IV. This proof also showed that the expression is uniformly convergent in the lengths of the bonds for each $L_\ell \in [\epsilon, \infty)$ and thus continuous in those bond lengths on the same intervals. This hints that the vacuum energy does not vary wildly for small perturbations in the bond lengths. As expected though, as one of the bonds $\ell_0$ shrinks so $L_{\ell_0} \to 0$, then the expression does diverge. This can be seen by just considering the orbit on $\ell_0$, $p = (\ell_0^+, \ell_0^-)$, then $L_p^{-1} \to \infty$. The same thing happens in the very short distance limit in standard Casimir-effect calculations disregarding the atomic makeup of the plates.
Furthermore, the vacuum energy has continuous first derivatives in the lengths of the bonds (and by theorem IV.3, all derivatives are also continuous). The Casimir force is found by differentiating the vacuum energy with respect to a changing length, and thus, this expression is also continuous in bond lengths. All of this will appear in the upcoming paper [35].

Putting in equal bonds into the equation for the vacuum energy, corollary IV.1 relates the vacuum energy to the eigenvalues, \( \{\lambda_\alpha\} \), of the scattering matrix \( S \),

\[
E_c = -\frac{1}{2\pi L} \sum_{\alpha=1}^{2B} \sum_{n=1}^{\infty} \frac{(\lambda_\alpha)^n}{n^2}.
\]

By inspection it is clear that this is convergent since \( |\lambda_\alpha| = 1 \) because \( S \) is unitary.

We also applied the method of images to our quantum graph in chapter V. This method takes a free space solution to a problem and outputs a solution which applies on the entire quantum graph. In principle the method of images can be applied to scattering matrices that are \( k \)-dependent. The biggest problem here is handling the resulting \( K \) transformation becomes difficult. It is possible that by using an asymptotic approach information about the vacuum energy with these other transformations could be obtained, but this has yet to be looked into. With the knowledge of how the cylinder kernel is related to the vacuum energy, the cylinder kernel for a graph can be obtained by this method and analyzed for the vacuum energy. This method reproduces the result of the trace formula. An advantage to this approach over the trace formula comes from the fact that one can obtain the vacuum energy density to analyze. It is not clear that the expression for the density reduces down to such a nice formula like \( E_c \), but seeing how it behaves, even just numerically, would be of interest. Another advantage of this method of images is that it is applicable other systems than graphs (such as billiards, manifolds, etc.).
Now that there is an expression for the vacuum energy in quantum graphs, it should be possible to see what connection it has to the spectral statistics of the system. With the connection that quantum graphs have to other systems, this could shed light on how other systems’ vacuum energy behaves.
REFERENCES


APPENDIX A

COMBINATORICS

1. Periodic Orbits as Equivalence Classes

The information in this part of the appendix is not new but is placed here for completeness and to help understanding of the finer points of the periodic orbits as equivalence classes.

Consider the vector of directed $p = (\alpha_1, \ldots, \alpha_n)$. If each $C^{(D)}_{\alpha_{i+1} \alpha_i} = 1$, then $p$ is a path, and if $C^{(D)}_{\alpha_1 \alpha_n} = 1$, then it is periodic. We need not assume this vector is a periodic path since we have $A_p := S_{\alpha_1 \alpha_n} S_{\alpha_n \alpha_{n-1}} \cdots S_{\alpha_2 \alpha_1}$ and this is zero if $p$ is not a periodic path.

Now take $\sigma$ to be the permutation transformation on a vector of directed bonds, so that

$$
\sigma((\alpha_1, \alpha_2, \ldots, \alpha_n)) = (\alpha_2, \ldots, \alpha_n, \alpha_1)
$$

(A.1)

Now, there exists a minimum $n_p \in \mathbb{N}$ such that $\sigma^{n_p}(p) = p$. With this, we have the equivalence class defined by $\sigma$ on $p$, so

$$
p = \{p, \sigma(p), \sigma^2(p), \ldots, \sigma^{n_p-1}(p)\}.
$$

(A.2)

We have $n_p | n$ and $r_p$ is defined by $r_p n_p = n$. This is the repetition number of the path much like we have discussed in definition II.12 when we defined primitive periodic orbits.

Observe that $A_p = A_{\sigma(p)} = \cdots = A_{\sigma^{n_p-1}(p)} =: A_p$ and similarly, we can equate $L_p = L_p$ since lengths of all paths in $p$ are the same. Also, $r_p = r_p$ is still the repetition number of the periodic orbit as is described at the end of section II.A.
2. Equivalence of Trace Formulae

The trace formula in (4.11) is equivalent to (3.12) given here with the $\epsilon$ term,

$$d(k) := \sum_n \delta_\epsilon(k - k_n) = \frac{\mathcal{L}}{\pi} + \text{Re} \frac{1}{\pi} \sum_p A_p \frac{L_p}{r_p} e^{ikL_p - \epsilon L_p}.$$  \hfill (A.3)

This trace formula is derived for $k$-independent scattering matrices, and when the boundary conditions are of the type given by (2.14) we have $\sigma^{(i)} = (\sigma^{(i)})^\dagger$ for all $i \in V$ as shown in theorem II.1. Now consider $p = (\alpha_1, \alpha_2, \ldots, \alpha_n)$ and define the time reversal of $p$ as $p^* = (\bar{\alpha}_n, \ldots, \bar{\alpha}_2, \bar{\alpha}_1)$. Clearly, $L_{p^*} = L_p$ and $r_{p^*} = r_p$. Furthermore,

$$A_{p^*} = S_{\bar{\alpha}_n \alpha_1} S_{\bar{\alpha}_1 \bar{\alpha}_2} \cdots S_{\bar{\alpha}_{n-1} \bar{\alpha}_n} = \sigma^{(t(\bar{\alpha}_1))}|_{\bar{\alpha}_n || \alpha_1} \sigma^{(t(\bar{\alpha}_2))}|_{\bar{\alpha}_1 || \alpha_2} \cdots \sigma^{(t(\bar{\alpha}_n))}|_{\bar{\alpha}_{n-1} || \bar{\alpha}_n}.$$  

Now in the above $t(\bar{\alpha}_1) = o(\bar{\alpha}_n) = t(\alpha_n)$ and similarly $t(\bar{\alpha}_j) = o(\bar{\alpha}_{j-1}) = t(\alpha_{j-1})$ for $1 < j \leq n$. Using this, the fact that $\sigma^{(i)} = (\sigma^{(i)})^\dagger$, and $|\bar{\alpha}| = |\alpha|$,

$$A_{p^*} = \left(\sigma^{(t(\alpha_1))}|_{\alpha_1 || \alpha_n}\right)^* \left(\sigma^{(t(\alpha_2))}|_{\alpha_2 || \alpha_1}\right)^* \cdots \left(\sigma^{(t(\alpha_{n-1}))}|_{\alpha_{n-1} || \alpha_{n-1}}\right)^* = (S_{\alpha_1 \alpha_n} S_{\alpha_n \alpha_{n-1}} \cdots S_{\alpha_2 \alpha_1})^* = (A_p)^*.$$  

Now define,

$$\mathcal{S} := \sum_p A_p \frac{L_p}{r_p} e^{ikL_p - \epsilon L_p}. \hfill (A.4)$$

This can be rewritten so that,

$$\mathcal{S} = \sum_p A_{p^*} \frac{L_{p^*}}{r_{p^*}} e^{ikL_{p^*} - \epsilon L_{p^*}} = \sum_p (A_p)^* \frac{L_p}{r_p} e^{ikL_p - \epsilon L_p}.$$  

Adding these two together, we obtain a new expression for $\mathcal{S}$,

$$\mathcal{S} = \sum_p \text{Re}\{A_p\} \frac{L_p}{r_p} e^{ikL_p - \epsilon L_p}.$$
Then,

$$\text{Re } S = \sum_p \text{Re}\{A_p\} \frac{L_p}{r_p} \cos(kL_p)e^{-\epsilon L_p}$$

$$= \frac{1}{2} \sum_p A_p \frac{L_p}{r_p} \cos(kL_p)e^{-\epsilon L_p} + \frac{1}{2} \sum_p (A_p)^* \frac{L_p}{r_p} \cos(kL_p)e^{-\epsilon L_p}$$

$$= \frac{1}{2} \sum_p A_p \frac{L_p}{r_p} \cos(kL_p)e^{-\epsilon L_p} + \frac{1}{2} \sum_p (A_p)^* \frac{L_p^*}{r_p^*} \cos(kL_p^*)e^{-\epsilon L_p^*}$$

$$= \sum_p A_p \frac{L_p}{r_p} \cos(kL_p)e^{-\epsilon L_p}.$$

This shows the equivalence of (4.11) to (3.12), and through a similar argument it can be shown that \( \sum_p \frac{A_p}{L_p r_p} \) is real, so (3.17) and (3.32) are also the same and the real part can be dropped from (3.15).
APPENDIX B

PROOF OF THE GENERAL METHOD OF IMAGES FORMULA

In this appendix, we prove theorem VI.1. Before proving it, we prove a lemma which will aid in our proof.

Lemma VI.1. Consider (1) a free space solution, \( u \), to a partial differential equation and (2) a finite quantum graph with the same partial differential equation applied to each bond. Then for \( \gamma \in S^{-}(i) \),

\[
g_{\epsilon}(x) = \delta_{\epsilon \gamma} u \circ i_{\gamma \gamma}(x) + [K_{\epsilon \gamma} u](x),
\]

satisfies the partial differential equation for all \( \epsilon \in S^{+}(i) \) and the boundary conditions at vertex \( i \).

Proof. Let \( \ell := |\gamma| \) and \( \ell' := |\epsilon| \) and using the definition of the \( K \)-transform in (5.2) at a single vertex (\( i \) in this case), \([K_{\epsilon \gamma} u] = [\kappa_{\ell' \ell}(u \circ i_{\gamma \gamma})]\). Also, \( \delta_{\epsilon \gamma} = \delta_{\ell \ell'} \) and define \( \bar{u} := u \circ i_{\gamma \gamma} \). This \( \bar{u} \) is also a free space solution and we have,

\[
g_{\epsilon} = \delta_{\ell \ell'} \bar{u} + [\kappa_{\ell' \ell}(\bar{u})].
\]

By definition of the \( \kappa^{(i)} \) transformation, this satisfies the boundary conditions at the vertex \( i \) when you consider all \( \epsilon \in S^{+}(i) \).

\(\square\)

Theorem VI.1. If \( u \) is a free space solution to the partial differential equation applied to our graph, then a formal solution to the same partial differential equation applied to every bond of a quantum graph with boundary conditions at the vertices takes the
form (suppressing any other coordinate),

\[ u_{\beta\alpha}(x) = \sum_{n=1}^{\infty} \sum_{p_{n-1} \in P_{n-1}} \left[ \Phi_{\beta p_{n-1}} \ u(x) + [\Phi_{\beta p_{n-1}} \ {u \circ i_{\alpha\alpha}}] \right](x) \]

\[ + [\Phi_{\beta p_{n-1}} \ {u \circ i_{\alpha\alpha}}] \circ i_{\beta\beta}(x) + [\Phi_{\beta p_{n-1}} \ {u \circ i_{\alpha\alpha}}] \circ i_{\beta\beta}(x) \]

\[ + \begin{cases} 
    u(x) & \text{if } \beta = \alpha \\
    u \circ i_{\alpha\alpha}(x) & \text{if } \beta = \bar{\alpha} \\
    0 & \text{otherwise},
\end{cases} \]

for all \( \beta \) and \( x \) measured on directed bond \( \beta \); \( u_{\beta\alpha} \) is also a function on directed bonds \( \beta \) (i.e. \( u_{\beta\alpha} = u_{\beta\alpha} \circ i_{\beta\beta} \)).

**Proof.** To begin with, we first establish that this function is a function on directed bonds.

Consider,

\[ u_{\beta\alpha}(x) = \sum_{n=1}^{\infty} \sum_{p_{n-1} \in P_{n-1}} \left[ \Phi_{\beta p_{n-1}} \ u(x) + [\Phi_{\beta p_{n-1}} \ {u \circ i_{\alpha\alpha}}] \right](x) \]

\[ + [\Phi_{\beta p_{n-1}} \ {u \circ i_{\alpha\alpha}}] \circ i_{\beta\beta}(x) + [\Phi_{\beta p_{n-1}} \ {u \circ i_{\alpha\alpha}}] \circ i_{\beta\beta}(x) \]

\[ + \begin{cases} 
    u(x) & \text{if } \bar{\beta} = \alpha \\
    u \circ i_{\alpha\alpha}(x) & \text{if } \bar{\beta} = \bar{\alpha} \\
    0 & \text{otherwise},
\end{cases} \]

To compute \( u_{\beta\alpha} \circ i_{\beta\beta} \), notice that \( i_{\beta\bar{\beta}} \circ i_{\beta\beta}(x) = x \) and that \( \bar{\beta} = \alpha \) is equivalent to
\[ \beta = \bar{\alpha} \text{ while } \bar{\beta} = \bar{\alpha} \text{ is equivalent to } \beta = \alpha, \text{ so} \]
\[ u_{\beta\alpha} \circ i_{\bar{\beta}\beta}(x) = \sum_{n=1}^{\infty} \sum_{p_{n-1} \in P_{n-1}} \left[ [\Phi_{\beta p_{n-1} \alpha} u] \circ i_{\bar{\beta}\beta}(x) + [\Phi_{\beta p_{n-1} \alpha} \{ u \circ i_{\alpha\bar{\alpha}} \}] \circ i_{\bar{\beta}\beta}(x) \right. \]
\[ + \left. [\Phi_{\beta p_{n-1} \alpha} \{ u \circ i_{\alpha\bar{\alpha}} \}](x) + [\Phi_{\beta p_{n-1} \alpha} u](x) \right] \]
\[ \begin{cases} u \circ i_{\alpha\bar{\alpha}}(x) & \text{if } \beta = \bar{\alpha} \\ u(x) & \text{if } \beta = \alpha \\ 0 & \text{otherwise.} \end{cases} \]

From this, it is easily checked that \( u_{\beta\alpha} \circ i_{\bar{\beta}\beta}(x) = u_{\beta\alpha} \), so it is a function on directed bonds.

We now break up the sum into many parts (suppressing the \( x \)),
\[ u^{(n)}_{\beta\alpha} = \sum_{p_n \in P_n} \left[ [\Phi_{\beta p_n \alpha} u] + [\Phi_{\beta p_n \alpha} \{ u \circ i_{\alpha\bar{\alpha}} \}] \right] \]
\[ + \sum_{p_{n-1} \in P_{n-1}} \left[ [\Phi_{\beta p_{n-1} \alpha} u] + [\Phi_{\beta p_{n-1} \alpha} \{ u \circ i_{\alpha\bar{\alpha}} \}] \right] \circ i_{\bar{\beta}\beta}, \quad n > 0 \quad (B.1) \]
\[ u^{(0)}_{\beta\alpha} = [K_{\beta\alpha} u] + [K_{\beta\alpha} \{ u \circ i_{\alpha\bar{\alpha}} \}] + \begin{cases} u(x), & \text{if } \beta = \alpha \\ u \circ i_{\alpha\bar{\alpha}}(x), & \text{if } \beta = \bar{\alpha} \\ 0, & \text{otherwise.} \end{cases} \quad (B.2) \]

Clearly, we have \( u_{\beta\alpha} = \sum_{n=0}^{\infty} u^{(n)}_{\beta\alpha} \). These functions by themselves are not functions on directed bonds. Individually though, we claim that each \( u^{(n)}_{\beta\alpha} \) satisfies the boundary conditions at any given vertex and thus, by superposition \( u_{\beta\alpha} \) satisfies the boundary condition at all vertices.

To begin, we look at the \( n = 0 \) case. We shall look at the generic vertex \( i \), so we only have to look at \( \beta \in S^+(i) \). There are three cases to consider for this,
• $\alpha \in S^-(i)$. In this case, $K_{\beta\alpha} = 0$ and we can apply lemma VI.1 with $u$, $\gamma = \alpha$, and $\epsilon = \beta$ to obtain,

$$u_{\beta\alpha}^{(0)} = \delta_{\alpha\beta} u \circ i_{\alpha\alpha}(x) + [K_{\beta\alpha} u] + [K_{\beta\alpha} \{u \circ i_{\alpha\alpha}\}] .$$

By lemma, for all possibilities of $\beta \in S^+(i)$ this satisfies the boundary conditions at vertex $i$, and is a solution to the partial differential equation.

• $\alpha \in S^+(i)$. In this case, $K_{\beta\alpha} = 0$ and we can again apply lemma VI.1 but now with $u \circ i_{\alpha\alpha}$, $\gamma = \alpha$, and $\epsilon = \beta$ to obtain,

$$u_{\beta\alpha}^{(0)} = \delta_{\alpha\beta} u(x) + [K_{\beta\alpha} \{u \circ i_{\alpha\alpha}\}] + [K_{\beta\alpha} u] .$$

Again, for all possibilities of $\beta \in S^+(i)$ this satisfies the boundary conditions at vertex $i$ and the partial differential equation on the graph.

• $|\alpha| \not\in S(i)$. In this somewhat trivial case, $K_{\beta\alpha} = 0$ and $K_{\beta\bar{\alpha}} = 0$, so

$$u_{\beta\alpha}^{(0)} = [K_{\beta\alpha} \{u \circ i_{\alpha\alpha}\}] + [K_{\beta\alpha} u]$$

satisfies the boundary conditions at $i$ (though trivially).

Having established (B.2), we now handle the $n > 0$ cases.

Again, we look at the same vertex $i$ and consider $\beta \in S^+(i)$ and $\alpha_n \in S^-(i)$.

Consider the function,

$$g_{\alpha_n} = \sum_{p_{n-1} \in \mathcal{P}_{n-1}} \left[ [\Phi_{\alpha_n p_{n-1} \alpha} u] + [\Phi_{\alpha_n p_{n-1} \bar{\alpha}} \{u \circ i_{\alpha\alpha}\}] \right] .$$

Despite the indexing on this formula, $g_{\alpha_n}$ is defined on the whole real line and is a free space solution to the partial differential equation, so we can apply it with $\gamma = \alpha_n$.
and $\epsilon = \beta$ to our lemma VI.1,

$$g_{\beta \alpha} = \delta_{\beta \alpha} g_{\alpha} \circ i_{\alpha \alpha} + [K_{\beta \alpha} g_{\alpha}]. \quad (B.3)$$

Thus, $g_{\beta \alpha}$ satisfies the boundary conditions at vertex $i$ and the partial differential equations. By superposition, so does the following function,

$$\sum_{\alpha_n \in S^{-}(i)} g_{\beta \alpha} = g_{\beta} \circ i_{\beta} + \sum_{\alpha_n=1}^{2B} [K_{\beta \alpha} g_{\alpha}], \quad (B.4)$$

where we have used the fact that $K_{\beta \alpha} = 0$ when $\alpha_n \notin S^{-}(i)$.

Evaluating each term,

$$g_{\beta} \circ i_{\beta} = \sum_{P_{n-1} \in P_{n-1}} \left[ [\Phi_{\beta P_{n-1} \alpha} u] + [\Phi_{\beta P_{n-1} \alpha} \{u \circ i_{\alpha \alpha}\}] \right] \circ i_{\beta}, \quad \text{and} \quad (B.5)$$

$$\sum_{\alpha_n=1}^{2B} [K_{\beta \alpha} g_{\alpha}] = \sum_{P_n \in P_n} \left[ [\Phi_{\beta P_n \alpha} u] + [\Phi_{\beta P_n \alpha} \{u \circ i_{\alpha \alpha}\}] \right]. \quad (B.6)$$

From this it can be seen that,

$$u^{(n)}_{\beta \alpha} = g_{\beta} \circ i_{\beta} + \sum_{\alpha_n=1}^{2B} [K_{\beta \alpha} g_{\alpha}].$$

Thus, each $u^{(n)}_{\beta \alpha}$ satisfies the boundary conditions at vertex $i$ and satisfies the partial differential equation. Thus, by superposition of solutions, so does $u_{\beta \alpha}$. Furthermore, it is a function on directed bonds, so it is a legitimate formal solution to the entire partial differential on the graph. (Formal in the sense that it might diverge).
VITA

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- Sigma Xi, 2007
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- James G. Potter Scholarship 2006, $500
- Honors Incentive Award 2005, 2006, $2,000
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CONFERENCES


• Quantum Graphs, their Spectra and Applications, Newton Institute, Cambridge, 2007. (Invited talk)

PAPERS IN PREPARATION
