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The Green's Function of the Sturm-Liouville Operator Acting on Graphs

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Abstract

Given the Green's function of a Sturm-Liouville operator defined on a graph. Form a new graph by identifying vertices. The Green's function of the Sturm-Liouville operator defined on the new graph is derived. A few basic examples are constructed.

1 Introduction

Describing the motion of a quantum mechanical particle on a one-dimensional network of thin metallic wires was first studied in the 1950s by Ruedenberg and Scherr [16]. They assumed organic molecules maintain a frame-like structure and that the electrons move within this frame. Recently, the topic has been the subject of many papers. They focus on construction of admissible Hamiltonian operators ([4], [9], [14]), formulation of the scattering problem ([1], [4], [13]), and analysis of a wavefunction at a junction ([3], [16], [17]) for finite graphs. Standard examples used are a lattice of wires ([2], [7]) and a star-like structure of a finite number (usually three) of wires ([9], [12], [13], [16]).

The motivation for this work was to determine properties of resonances on unbounded graphs. See [6] for more details.

2 Graphs and the Sturm-Liouville Operator

A graph is generally defined as a collection of points and lines connecting the points. When we say *curve*, we mean a differentiable isometric function α from a closed interval $I \subseteq \mathbb{R}$ into an Euclidean space where the distance between any two points in $\{\alpha(x) : x \in I\}$ is the arc-length measured along the curve.

A *graph*, $\Gamma = (\mathcal{V}(\Gamma), \mathcal{E}(\Gamma))$, is a pair consisting of *vertices*, denoted $\mathcal{V} \equiv \mathcal{V}(\Gamma)$, which is a nonempty collection of points, and *edges*, denoted $\mathcal{E} \equiv \mathcal{E}(\Gamma) = \{e_j : j \in J\}$ with J an indexed set, which is a collection of curves whose endpoints are in \mathcal{V} . The graph is weighted so that each element $e_j \in \mathcal{E}$ is assigned an extended positive real number ℓ_j representing the length of the edge. Let ∂e_j denote the set of at most two endpoints of the edge e_j . Given a vertex $\mathbf{v} \in \mathcal{V}$, $e_j \in \mathcal{E}$ is said to be *incident* on \mathbf{v} if $\mathbf{v} \in \partial e_j$. The set of all edges incident on \mathbf{v} will be denoted $\mathcal{I}_{\mathbf{v}} := \{e_j \in \mathcal{E} : \mathbf{v} \in \partial e_j\}$.

Each edge in \mathcal{E} is assumed to be isometric to a closed subset of the real line, it inherits an ordering of its elements the same as \mathbb{R} . This orientation will either be stated explicitly or drawn directly onto a representation of the graph. For a vertex $\mathbf{v} \in \mathcal{V}$, let $\mathcal{I}_{\mathbf{v}}^- \subseteq \mathcal{I}_{\mathbf{v}}$ be the set of all incident edges that are directed toward \mathbf{v} and $\mathcal{I}_{\mathbf{v}}^+ \subseteq \mathcal{I}_{\mathbf{v}}$ be the set of all edges that are directed away from \mathbf{v} . Given an oriented edge $e_j \in \mathcal{E}$ that is directed toward $\mathbf{v} \in \mathcal{V}$, call \mathbf{v} the *terminal* vertex of e_j . If e_j is directed away from $\mathbf{u} \in \mathcal{V}$, call \mathbf{u} the *initial* vertex of e_j . The *domain* of each e_j , $\mathcal{D}(e_j)$, is the set $\{\alpha^{-1}(x) : x \in e_j\}$ which is a closed interval on \mathbb{R} . The domain and orientation of each e_j can be changed if needed by a basic translation or reversal of orientation of α so long as the length of the interval remains ℓ_j .

If Γ is a graph and $\mathbf{v} \in \mathcal{V}$, then the *valence* (or *degree*) of \mathbf{v} , denoted $val(\mathbf{v})$, is the number of incident edges that meet at \mathbf{v} , counting loops twice. If $val(\mathbf{v}) = 1$, then \mathbf{v} is a *boundary vertex* of Γ . Any vertex \mathbf{v} with $val(\mathbf{v}) \geq 2$ is called an *internal vertex*.

The definition of a graph given above allows for loops, multiple edges connecting vertices, edges infinitely long with no endpoints, and isolated vertices. For brevity, we will assume that there are no isolated vertices, no edge isomorphic to the entire real line, and no loops (the one exception, however, will be Example 3.1). These can be accomplished by simply dropping or adding appropriate vertices to the graph. Additionally, we will use edges of finite length only and assume that all graphs have at most a countable number of vertices.

A Hilbert space on the graph Γ can now be defined as the direct sum of

Hilbert spaces on each edge. Hence, $\mathcal{H}^2(\Gamma) := \bigoplus_{j \in J} \mathcal{H}^2(e_j)$ where $\mathcal{H}^2(e_j)$ is the second order Sobolov space of complex square integrable functions on $\mathcal{D}(e_j)$. Elements of $\mathcal{H}^2(\Gamma)$ are families of functions written as $\psi := \{\psi_j : j \in J\}$ such that the domain of each ψ_j coincides with the domain of e_j . For each j , ψ_j' is absolutely continuous and ψ_j'' is square integrable. The inner product on $\mathcal{H}^2(\Gamma)$ is

$$\langle \varphi, \psi \rangle \equiv \int_{\Gamma} \varphi \psi := \sum_{j \in J} \int_{e_j} \overline{\varphi_j(x)} \psi_j(x) dx$$

for any $\varphi, \psi \in \mathcal{H}^2(\Gamma)$. Note, however, that the inner product is defined only if a countable set of terms is non-zero. For the case when J is uncountable, we must make the assumption that if $\psi \in \mathcal{H}(\Gamma)$, then there exists a countable subset $J' \subset J$ such that the support of ψ is $\cup_{j \in J'} e_j$. That is, ψ_j vanishes for every $j \in J \setminus J'$.

Many of the calculations later will depend on the functional value and first derivative of $\psi \in \mathcal{H}^2(\Gamma)$ near the vertices. Given any vertex $\mathbf{v} \in \mathcal{V}$ and any incident edge $e_j \in \mathcal{I}_{\mathbf{v}}$ on \mathbf{v} , let

$$\psi_j(\mathbf{v}) := \lim_{e_j \ni x \rightarrow \mathbf{v}} \psi_j(x)$$

and write the *oriented derivative* along e_j at \mathbf{v} as

$$D\psi_j(\mathbf{v}) := \begin{cases} \lim_{e_j \ni x \rightarrow \mathbf{v}} \psi_j'(x), & \text{if } e_j \in \mathcal{I}_{\mathbf{v}}^+; \\ - \lim_{e_j \ni x \rightarrow \mathbf{v}} \psi_j'(x), & \text{if } e_j \in \mathcal{I}_{\mathbf{v}}^-. \end{cases} \quad (2.1)$$

This definition agrees with [4] and [11].

We define the operator $\mathcal{L} \equiv \mathcal{L}(\Gamma, V)$ on $\mathcal{H}^2(\Gamma)$ as

$$\mathcal{L} \psi = \mathcal{L} \{\psi_j\} := \left\{ - \frac{d}{dx} \left(p_j \frac{d}{dx} \psi_j \right) + q_j \psi_j : j \in J \right\} \quad (2.2)$$

where $p := \{p_j : j \in J\}$ and $q := \{q_j : j \in J\}$ are families of real bounded measurable functions.

As defined, \mathcal{L} is a symmetric operator and not particularly interesting. It acts on a collection of lines that are non-interacting. This is remedied by studying the self-adjoint extensions of \mathcal{L} which correspond to assigning a specific set of boundary conditions to the vertices in the graph. Using the theory of von Neumann ([15],[18]), the self-adjoint extensions of two

semi-infinite edges coupled at a single point have been extensively studied (see [5] for a brief overview), but this is not the case for more general one-dimensional graphs. The very specific case of the operator \mathcal{L} with $p \equiv 1$ and $q \equiv 0$ acting on a connected graph consisting of n semi-infinite edges was determined to have n^2 self-adjoint extensions assuming that the functional elements are continuous at the single vertex [9]. An analysis of self-adjoint extensions for more complicated graphs has not been done due to the large number of parameters associated with the extensions.

\mathcal{L} is the general form of a Sturm-Liouville operator acting on a graph. We proceed to introduce boundary conditions to make the operator self-adjoint.

At the vertex $\mathbf{v} \in \mathcal{V}$, $\psi \in \mathcal{H}^2(\Gamma)$ will satisfy *Neumann boundary conditions (NBC)* if it is continuous at that vertex and the sum of the oriented derivatives over all incident edges vanishes. That is,

$$\psi_j(\mathbf{v}) = \psi_k(\mathbf{v}) \text{ for all } e_j, e_k \in \mathcal{I}_{\mathbf{v}}, \text{ and} \quad (2.3a)$$

$$\sum_{e_j \in \mathcal{I}_{\mathbf{v}}} D\psi_j(\mathbf{v}) = 0. \quad (2.3b)$$

Any function ψ is said to be *continuous* at the vertex $\mathbf{v} \in \mathcal{V}$ if it satisfies condition (2.3a). In this case, write $\psi(\mathbf{v})$ to represent the common functional value at \mathbf{v} . ψ is *continuous on Γ* if it is continuous on each edge and is continuous at every vertex in Γ .

Conversely, ψ satisfies *Dirichlet boundary conditions (DBC)* at \mathbf{v} if

$$D\psi_j(\mathbf{v}) = D\psi_k(\mathbf{v}) \text{ for all } e_j, e_k \in \mathcal{I}_{\mathbf{v}}, \text{ and} \quad (2.4a)$$

$$\sum_{e_j \in \mathcal{I}_{\mathbf{v}}} \psi_j(\mathbf{v}) = 0. \quad (2.4b)$$

The choice of names is self-evident when \mathbf{v} has only a single incident edge. If ψ satisfies (2.3) at \mathbf{v} , then $\psi'(\mathbf{v}) = 0$. If ψ satisfies (2.4) at \mathbf{v} , then $\psi(\mathbf{v}) = 0$. Let $D\psi(\mathbf{v})$ represent the sum of the oriented derivatives over all incident edges of \mathbf{v} in \mathcal{E} , *i.e.*,

$$D\psi(\mathbf{v}) := \sum_{e_j \in \mathcal{I}_{\mathbf{v}}} D\psi_j(\mathbf{v}) \quad (2.5)$$

which may or may not vanish, depending on the specific boundary condition of Γ assigned at \mathbf{v} .

Most papers in the bibliography about differential operators on graphs have internal vertices that satisfy *NBC* and boundary vertices satisfy either *DBC* and *NBC*, depending on the author's preference.

Presuming that every vertex in Γ satisfies (2.3) or (2.4) makes \mathcal{L} self-adjoint. Divide the set of vertices into two sets: \mathcal{V}_N and \mathcal{V}_D . Let $L = \mathcal{L}|_{\mathcal{D}(L)}$ be the operator with domain

$$\mathcal{D}(L) := \left\{ \psi \in \mathcal{H}^2(\Gamma) : \psi \text{ satisfies } NBC \text{ at every } \mathbf{v} \in \mathcal{V}_N \right. \\ \left. \text{and } \psi \text{ satisfies } DBC \text{ at every } \mathbf{v} \in \mathcal{V}_D \right\}. \quad (2.6)$$

It is straightforward to prove the following.

Proposition 2.1. *If $L = \mathcal{L}|_{\mathcal{D}(L)}$ is given by the formula (2.2) with domain (2.6), p is continuous and positive on Γ , and q is essentially bounded on Γ (that is, there exists $C > 0$ such that $\|q_j\|_{L^\infty(e_j)} < C$ for all $j \in J$), then L is self-adjoint.*

A more complicated differential operator was studied by Mehran [14] where the boundary conditions were dependent on the angles of incidence of the edges to the vertex. Exner *et al.* ([7] through [11]) assumes the slightly more general boundary condition at vertices that an element of in the domain of L satisfies (2.3) or (2.4) at each vertex except that the summation does not vanish but is proportional to the value of the continuous part at that vertex. All other references relating to differential operators of graphs ([1], [2], [3], [4], [12], [13], [16]) use *NBC* for internal vertices.

3 Determination of Green's Function on Arbitrary Graphs

Given the Sturm-Liouville operator L satisfying the conditions given in Proposition 2.1 on a graph Γ , the resolvent $R(\lambda) \equiv (L - \lambda)^{-1}$, where λ is in the resolvent set $\rho(L)$ of L , is an integral operator with kernel $g(\lambda; x, y)$,

$$[R(\lambda)\psi](x) = \int_{\Gamma} g(\lambda; x, y)\psi(y)dy$$

where $\psi \in \mathcal{H}^2(\Gamma)$. g is the *Green's function* of Γ . Unless explicitly needed, the dependence of g on λ will be suppressed.

Suppose we are given a countable collection of disjoint lines, each of finite length, whose endpoints satisfy *DBC* or *NBC*. The Green's function associated to the operator $L - \lambda$ is given in terms of the Green's functions of the individual lines provided that λ is in the resolvent set of L . More

generally, it is useful to relate the Green's function of a graph to a new one obtained by identifying some or all of its vertices. Let $\Gamma_o = (\mathcal{V}_o, \mathcal{E})$ be such a graph and g_o its Green's function. By identifying vertices in Γ_o , a new graph, $\Gamma = (\mathcal{V}, \mathcal{E})$, is formed. We now need to determine the new Green's function, g . Let L_o and L be the respective Strum-Liouville operators acting on Γ_o and Γ .

Formally, let $\mathcal{U}_o \subseteq \mathcal{V}_o$ be the set of vertices that have to be identified (they should all satisfy *NBC*). Define an equivalence relation, \sim , writing $\mathbf{u}_o \sim \mathbf{v}_o$ if $\mathbf{u}_o, \mathbf{v}_o \in \mathcal{U}_o$ have been identified. For $\mathbf{u}_o \in \mathcal{U}_o$, let $[\mathbf{u}_o] := \{\mathbf{v}_o \in \mathcal{U}_o : \mathbf{v}_o \sim \mathbf{u}_o\}$. This partitions \mathcal{U}_o into equivalence classes. Let \mathcal{U} be the set

$$\mathcal{U} := \mathcal{U}_o / \sim = \{[\mathbf{u}_o] : \mathbf{u}_o \in \mathcal{U}_o\}.$$

The set of vertices in Γ is now $\mathcal{V} := \mathcal{U} \cup (\mathcal{V}_o \setminus \mathcal{U}_o)$. An alternate way of representing elements of this equivalence class would be to write $\{\mathbf{v}_1, \dots, \mathbf{v}_n\} \rightarrow \mathbf{v}$ where the vertices $\mathbf{v}_1, \dots, \mathbf{v}_n$ have been identified to a single vertex and the new vertex is labelled \mathbf{v} . This notation will be useful for the examples given later.

Let $\tau : \mathcal{U}_o \rightarrow \mathcal{U}$ be the function defined as $\tau(\mathbf{u}_o) = [\mathbf{u}_o] =: \mathbf{u}$. For $\alpha_o \in \ell^2(\mathcal{U}_o)$, define a transformation $T : \ell^2(\mathcal{U}_o) \rightarrow \ell^2(\mathcal{U})$ as

$$(T\alpha_o)(\mathbf{u}) := \sum_{\{\mathbf{u}_o \in \mathcal{U}_o : \tau(\mathbf{u}_o) = \mathbf{u}\}} \alpha_o(\mathbf{u}_o). \quad (3.1)$$

T is a $|\mathcal{U}| \times |\mathcal{U}_o|$ matrix and each element is given by

$$T_{\mathbf{u} \mathbf{u}_o} = \begin{cases} 1, & \text{if } \tau(\mathbf{u}_o) = \mathbf{u}; \\ 0, & \text{otherwise.} \end{cases} \quad (3.2)$$

For $\alpha \in \ell^2(\mathcal{U})$, the adjoint of T is

$$(T^*\alpha)(\mathbf{u}_o) := \alpha(\tau(\mathbf{u}_o)). \quad (3.3)$$

If $\psi \in \mathcal{H}^2(\Gamma_o)$, then ψ will satisfy (2.3b) at the vertex $\mathbf{u} \in \mathcal{U}$ provided $(TD\psi)(\mathbf{u}) = 0$ where $D\psi \in \ell^2(\mathcal{U}_o)$ represents the sum of the oriented derivatives at each $\mathbf{u}_o \in \mathcal{U}_o$. A function $\varphi_o \in \mathcal{D}(L_o)$ automatically satisfies (2.3b) at $\mathbf{u} \in \mathcal{U}$ since $D\varphi_o(\mathbf{v}_o) = 0$ for all $\mathbf{v}_o \in [\mathbf{u}_o] = \mathbf{u}$. If the vector $\varphi_o(\mathcal{U}_o) \in \ell^2(\mathcal{U}_o)$ is in the range of T^* , then φ_o satisfies (2.3a) on Γ .

To construct the Green's function for Γ , solve the differential equation

$$(L - \lambda)\varphi = f \quad (3.4)$$

where $\lambda \in \mathbb{C} \setminus [0, \infty)$, f is any function on \mathcal{E} , and $\varphi \in \mathcal{D}(L)$ is the unique solution satisfying the assigned boundary conditions for Γ (thus, $\varphi = R(\lambda)f$). Consider the corresponding differential equation in Γ_o ,

$$(L_o - \lambda)\varphi_o = f, \quad (3.5)$$

where $\varphi_o \in \mathcal{D}(L_o)$ and is given by

$$\varphi_o(x) = \int_{\Gamma_o} g_o(x, y) f(y) dy. \quad (3.6)$$

We shall assume standard properties of Green's function for g_o , which are obvious when Γ_o is a disjoint collection of lines, and then verify these properties for the new Green's function g which we construct.

Assume that φ is a perturbation of φ_o , so

$$\varphi = \varphi_o + \psi \quad (3.7)$$

where $\psi \in \mathcal{H}^2(\Gamma)$. Applying $(\mathcal{L} - \lambda)$ to both sides of (3.7) and using (3.4) and (3.5), then

$$(\mathcal{L} - \lambda)\psi = 0. \quad (3.8)$$

Borrowing notation from physics literature, let $\langle \cdot |$ and $|\cdot\rangle$ respectively denote row and column vectors. In addition, for any function $h : A \rightarrow \mathbb{C}$, where $A = \{a_1, \dots, a_n, \dots\}$ is a countable set, let

$$|h(a)\rangle_{a \in A} \equiv |h(A)\rangle := \begin{pmatrix} h(a_1) \\ \vdots \\ h(a_n) \\ \vdots \end{pmatrix}$$

with similar notation for the row vector $\langle h(a)|_{a \in A} \equiv \langle h(A)|$.

For fixed y , $g_o(x, y)$ satisfies the homogeneous equation provided $x \neq y$, so we take

$$\psi(x) = \langle g_o(x, \mathcal{U}_o) | \alpha(\mathcal{U}_o) \rangle \quad (3.9)$$

where $|\alpha(\mathcal{U}_o)\rangle$ is a scaling vector that is to be determined.

For every $\mathbf{u}_o, \mathbf{v}_o \in \mathcal{U}_o$,

$$Dg_o(\mathbf{u}_o, \mathbf{v}_o) = \begin{cases} 0, & \text{if } \mathbf{u}_o \neq \mathbf{v}_o; \\ -\frac{1}{p(\mathbf{u}_o)}, & \text{if } \mathbf{u}_o = \mathbf{v}_o. \end{cases} \quad (3.10)$$

Differentiation at vertices is given by (2.5) and will always be assumed to be with respect to the variable x . The above equation is well known and easily verifiable for the case of isolated edges.

Differentiating both sides of (3.9) with respect to x and evaluating when $x = \mathbf{u}_o \in \mathcal{U}_o$ and using (3.10), we have

$$D\psi(\mathbf{u}_o) = \langle Dg_o(\mathbf{u}_o, \mathcal{U}_o) | \alpha(\mathcal{U}_o) \rangle = -\frac{\alpha(\mathbf{u}_o)}{p(\mathbf{u}_o)},$$

implying that $|\alpha(\mathcal{U}_o)\rangle = -|p(\mathbf{u}_o)D\psi(\mathbf{u}_o)\rangle_{\mathbf{u}_o \in \mathcal{U}_o}$. Writing (3.9) as a vector where we let x take on every vertex in \mathcal{U}_o , then

$$|\psi(\mathcal{U}_o)\rangle = -g_o(\mathcal{U}_o, \mathcal{U}_o) |p(\mathbf{u}_o)D\psi(\mathbf{u}_o)\rangle_{\mathbf{u}_o \in \mathcal{U}_o}. \quad (3.11)$$

$g_o(\mathcal{U}_o, \mathcal{U}_o)$ is a $|\mathcal{U}_o| \times |\mathcal{U}_o|$ matrix that is non-singular since a non-trivial null space would imply that λ is an eigenvalue satisfying DBC on \mathcal{U}_o . Define its inverse as

$$\Lambda \equiv \Lambda(\lambda) := g_o(\mathcal{U}_o, \mathcal{U}_o)^{-1}. \quad (3.12)$$

Now (3.11) can be written as

$$|p(\mathbf{u}_o)D\psi(\mathbf{u}_o)\rangle_{\mathbf{u}_o \in \mathcal{U}_o} = -\Lambda |\psi(\mathcal{U}_o)\rangle. \quad (3.13)$$

Substituting into (3.9) gives

$$\psi(x) = -\langle g_o(x, \mathcal{U}_o) | p(\mathbf{u}_o)D\psi(\mathbf{u}_o) \rangle_{\mathbf{u}_o \in \mathcal{U}_o} = \langle g_o(x, \mathcal{U}_o) | \Lambda |\psi(\mathcal{U}_o)\rangle. \quad (3.14)$$

Since φ and φ_o both satisfy (2.3a) for any vertex $\mathbf{u}_o \in \mathcal{U}_o$, then so must ψ . Referring to (3.7), one boundary condition of ψ is

$$|\psi(\mathcal{U}_o)\rangle = T^* |\varphi(\mathcal{U})\rangle - |\varphi_o(\mathcal{U}_o)\rangle. \quad (3.15)$$

Since φ and φ_o both satisfy (2.3b) for any vertex $\mathbf{u} \in \mathcal{U}$, then so must ψ . Thus, $T\Lambda |\psi(\mathcal{U}_o)\rangle = 0$. Applying $T\Lambda$ to both sides of (3.15) and solving for $|\varphi(\mathcal{U})\rangle$ gives

$$|\varphi(\mathcal{U})\rangle = (T\Lambda T^*)^{-1} T\Lambda |\varphi_o(\mathcal{U}_o)\rangle, \quad (3.16)$$

provided that $T\Lambda T^*$ is invertible. $T\Lambda T^*$ is invertible provided λ is not in the spectrum of L_o , that is, $\lambda \notin \sigma(L_o)$.

Rewriting (3.14) using (3.15) and (3.16) gives

$$\psi(x) = \langle g_o(x, \mathcal{U}_o) | \Lambda [T^*(T\Lambda T^*)^{-1} T\Lambda - 1] | \varphi_o(\mathcal{U}_o) \rangle.$$

From (3.6) we have $|\varphi_o(\mathcal{U}_o)\rangle = \int_{\Gamma_o} |g_o(\mathcal{U}_o, y)\rangle f(y) dy$, so (3.7) becomes

$$\begin{aligned} \varphi(x) &= \int_{\Gamma_o} g_o(x, y) f(y) dy \\ &\quad + \int_{\Gamma_o} \langle g_o(x, \mathcal{U}_o) | \Lambda [T^* (T \Lambda T^*)^{-1} T \Lambda - 1] | g_o(\mathcal{U}_o, y) \rangle f(y) dy \end{aligned}$$

and we arrive at the following theorem.

Theorem 3.1 (The Main Theorem). *Given the Strum-Liouville operator $L_o - \lambda$, where $\lambda \in \mathbb{C} \setminus [0, \infty)$, defined on a graph $\Gamma_o = (\mathcal{V}_o, \mathcal{E})$ with Green's function $g_o \equiv g_o(\lambda)$, form a new graph $\Gamma = (\mathcal{V}, \mathcal{E})$ by identifying subsets of vertices in $\mathcal{U}_o \subseteq \mathcal{V}_o$ of Γ_o (every vertex in \mathcal{U}_o must satisfy NBC). Let T be given by (3.1) and Λ be given by (3.12). The Green's function $g \equiv g(\lambda)$ of the Strum-Liouville operator $L - \lambda$ defined on Γ exists provided p is continuous on Γ and is*

$$g(x, y) = g_o(x, y) + \langle g_o(x, \mathcal{U}_o) | \Lambda [T^* (T \Lambda T^*)^{-1} T \Lambda - 1] | g_o(\mathcal{U}_o, y) \rangle. \quad (3.17)$$

A specialized case of this theorem was calculated in [1] using the M.G. Krein resolvent formula.

Remark 1. By (3.17), g is defined on $\Gamma_o \times \Gamma_o$, not $\Gamma \times \Gamma$. When evaluating g at a vertex $\mathbf{v} \in \Gamma$, it is necessary to choose a vertex $\mathbf{v}_o \in \Gamma_o$ such that $\tau(\mathbf{v}_o) = \mathbf{v}$ and replace \mathbf{v} in g with \mathbf{v}_o . This is shown to be well-defined by Property 5 below. The partial derivative of g evaluated at a vertex $\mathbf{v} \in \Gamma$ is still a summation over all incident edges given by (2.5) and (2.1).

As given, this theorem only applies to an initial graph consisting of a disjoint collection of lines. It can, nevertheless, be applied to arbitrary graphs as well. It need only be demonstrated that (3.10) holds for the new graph Γ . This is a special case of Property 6 below.

Proposition 3.2 (Properties of the Green's Function on a Graph). *Given a graph Γ as in Theorem 3.1 with Strum-Liouville operator $L - \lambda$ of Γ , the Green's function $g(\lambda)$ for $\lambda \in \mathbb{C} \setminus [0, \infty)$ has the following properties:*

1. $g(\bar{\lambda}; x, y) = \overline{g(\lambda; y, x)}$ for all $x, y \in \Gamma$.
2. Let $x, y \in \Gamma \setminus \mathcal{V}$. $g(\lambda; x, y)$ is continuous. For y fixed, $\frac{\partial}{\partial x} g(\lambda; x, y)$ and $\frac{\partial^2}{\partial x^2} g(\lambda; x, y)$ are continuous functions with respect to x provided $x \neq y$.

3. $\frac{\partial}{\partial x}g(\lambda; x, y)$ has a jump discontinuity at $y \in \Gamma \setminus \mathcal{V}$:

$$\left. \frac{\partial}{\partial x}g(\lambda; x, y) \right|_{x=y^-}^{x=y^+} = -\frac{1}{p(y)}.$$

4. For $x \in \Gamma \setminus \mathcal{V}$, g satisfies the homogeneous equation

$$(L - \lambda)[g(\lambda; \cdot, y)](x) = 0$$

provided $x \neq y$.

5. For y fixed, $g(\lambda; \mathbf{u}, y)$ satisfies (2.3a) for all $\mathbf{u} \in \mathcal{U}$.

6. For $\mathbf{u} \in \mathcal{U}$,

$$Dg(\lambda; \mathbf{u}, y) = \begin{cases} 0, & \text{if } y \neq \mathbf{u}; \\ -\frac{1}{p(y)}, & \text{if } y = \mathbf{u}. \end{cases}$$

(This simultaneously demonstrates (2.3b) and (3.10) hold for the Green's function on Γ).

7. $g(\lambda; x, y)$ is analytic in λ and extends to the resolvent set of L .

Proof. Properties 1 through 4 are all inherited from the properties of g_o by virtue of (3.17).

To establish Property 5, use (3.17) evaluated at all values of x for those vertices that have been identified. Writing the collection of functions as a vector, we have

$$\begin{aligned} |g(\mathcal{U}_o, y)\rangle &= |g_o(\mathcal{U}_o, y)\rangle + g_o(\mathcal{U}_o, \mathcal{U}_o)\Lambda[T^*(T\Lambda T^*)^{-1}T\Lambda - 1]|g_o(\mathcal{U}_o, y)\rangle \\ &= T^*(T\Lambda T^*)^{-1}T\Lambda|g_o(\mathcal{U}_o, y)\rangle \end{aligned} \quad (3.18)$$

which implies that $|g(\mathcal{U}_o, y)\rangle$ is in the range of T^* (refer to the paragraph following (3.3)). Thus, g is continuous at each $\mathbf{u} \in \mathcal{U}$.

Property 6 will be established in two parts by showing (i) if $y \notin \mathcal{U}_o$, then $T\Lambda|g(\mathcal{U}_o, y)\rangle = 0$ and (ii) $Dg(\mathcal{U}, \mathcal{U})$ is a diagonal matrix with entries $-\frac{1}{p(\mathbf{u}_1)}, \dots, -\frac{1}{p(\mathbf{u}_m)}$ where $\{\mathbf{u}_1, \dots, \mathbf{u}_m\} = \mathcal{U}$.

To prove (i), apply $T\Lambda$ to both sides of (3.18). Then

$$T\Lambda|g(\mathcal{U}_o, y)\rangle = T\Lambda T^*(T\Lambda T^*)^{-1}T\Lambda|g_o(\mathcal{U}_o, y)\rangle = T\Lambda|g_o(\mathcal{U}_o, y)\rangle. \quad (3.19)$$

Since g_o satisfies the boundary condition (2.3a) by assumption, then for $y \notin \mathcal{U}_o$ we have

$$|Dg_o(\mathcal{U}_o, y)\rangle = 0. \quad (3.20)$$

Let $y \notin \mathcal{U}_o$ be fixed. Starting with $T|p(\mathbf{u}_o)D\psi(\mathbf{u}_o)\rangle_{\mathbf{u}_o \in \mathcal{U}_o}$, apply (3.13) with $g(x, y)$ substituted for $\psi(x)$, apply (3.19), and apply (3.13) again with $g_o(x, y)$ substituted for $\psi(x)$. Thus,

$$\begin{aligned} T|p(\mathbf{u}_o)Dg(\mathbf{u}_o, y)\rangle_{\mathbf{u}_o \in \mathcal{U}_o} &= -T\Lambda|g(\mathcal{U}_o, y)\rangle = -T\Lambda|g_o(\mathcal{U}_o, y)\rangle \\ &= T|p(\mathbf{u}_o)Dg_o(\mathbf{u}_o, y)\rangle_{\mathbf{u}_o \in \mathcal{U}_o}. \end{aligned}$$

Since $Dg(\mathbf{u}_o, y) = 0$ for all $\mathbf{u}_o \in \mathcal{U}_o$ where $y \notin \mathcal{U}_o$, then

$$T|p(\mathbf{u}_o)Dg(\mathbf{u}_o, y)\rangle_{\mathbf{u}_o \in \mathcal{U}_o} = 0.$$

From the initial definition of T (3.1), the \mathbf{u} -th component of

$$T|p(\mathbf{u}_o)Dg(\mathbf{u}_o, y)\rangle_{\mathbf{u}_o \in \mathcal{U}_o}$$

is

$$\sum_{\{\mathbf{u}_o \in \mathcal{U}_o : \mathbf{u}_o \mapsto \mathbf{u}\}} p(\mathbf{u}_o)Dg(\mathbf{u}_o, y) = p(\mathbf{u})Dg(\mathbf{u}, y) = 0.$$

This implies that $Dg(\mathbf{u}, y) = 0$ since p is continuous and non-zero at all vertices given in the equation above.

To prove (ii), calculate $|Dg(\mathcal{U}, \mathbf{v})\rangle$ for all $\mathbf{v} \in \mathcal{U}$. From Remark 1, choose $\mathbf{v}_o \in \mathcal{U}_o$ such that $\mathbf{v}_o \mapsto \mathbf{v}$. Now calculate $|Dg(\mathcal{U}, \mathbf{v}_o)\rangle$. In a similar manner to the calculations in (i), start with $|p(\mathbf{u})Dg(\mathbf{u}, \mathbf{v}_o)\rangle_{\mathbf{u} \in \mathcal{U}}$, apply the identity $|Dg(\mathcal{U}, y)\rangle = T|Dg(\mathcal{U}_o, y)\rangle$, apply (3.13) with $g(x, y)$ substituted for $\psi(x)$, apply (3.19), and apply (3.13) again with $g_o(x, y)$ substituted for $\psi(x)$. Thus,

$$\begin{aligned} T|p(\mathbf{u})Dg(\mathbf{u}, \mathbf{v}_o)\rangle_{\mathbf{u} \in \mathcal{U}} &= T|p(\mathbf{u}_o)Dg(\mathbf{u}_o, \mathbf{v}_o)\rangle_{\mathbf{u}_o \in \mathcal{U}_o} = -T\Lambda|g(\mathcal{U}_o, \mathbf{v}_o)\rangle \\ &= -T\Lambda|g_o(\mathcal{U}_o, \mathbf{v}_o)\rangle = T|p(\mathbf{u}_o)Dg_o(\mathbf{u}_o, \mathbf{v}_o)\rangle_{\mathbf{u}_o \in \mathcal{U}_o}. \end{aligned} \tag{3.21}$$

From (3.10), $|p(\mathbf{u}_o)Dg_o(\mathbf{u}_o, \mathbf{v}_o)\rangle_{\mathbf{u}_o \in \mathcal{U}_o}$ is a $|\mathcal{U}_o|$ -dimensional column vector with 0 everywhere except the \mathbf{v}_o -th place, which is -1 . Applying T to that vector transforms it to a $|\mathcal{U}|$ -dimensional column vector with 0 everywhere except the \mathbf{v} -th place, which is -1 . (ii) now follows.

To establish Property 7, note that the operator $R(-1)$ has integral kernel $g(-1; x, y)$ which is square integrable on $\Gamma \times \Gamma$ and therefore compact. This implies $R(-1)$ has discrete spectrum and so does $L = R(-1)^{-1} - 1$. Therefore, $R(\lambda)$ is a Hilbert-Schmidt operator given by the kernel

$$\sum_{j \in J} \frac{u_j(x)u_j(y)}{\lambda_j - \lambda}$$

where $\{u_j\}$ are the eigenfunctions of L with corresponding eigenvalues $\{\lambda_j\}$. Each u_j may be chosen to be real, since L has real coefficients. Thus, $g(\lambda; x, y)$ is analytic for $\lambda \in \mathbb{C} \setminus [0, \infty)$ and extends to $\rho(L)$.

□

Observe that $\sigma(L) \subseteq \sigma(L_o) \cup \{\lambda \in \mathbb{R} : T\Lambda T^* \text{ is not invertible}\}$.

4 Examples

The first example is a very basic application of Theorem 3.1 which can be used in its general form to create loops and cycles in the new graph and will be applied to join a collection of disjoint graphs.

Proposition 4.1 (Arbitrary Join at a Single Vertex). *Given the Sturm-Liouville operator $L_o - \lambda$, where $\lambda \in \rho(L_o)$, defined on the graph Γ_o with Green's function g_o , choose distinct NBC vertices $\mathbf{v}_1, \dots, \mathbf{v}_n$ in Γ_o and form a new graph Γ determined by the mapping $\{\mathbf{v}_1, \dots, \mathbf{v}_n\} \rightarrow \mathbf{v}$. The Green's function g of the Sturm-Liouville operator $L - \lambda$ defined on Γ exists provided $\lambda \in \rho(L)$ and p is continuous on Γ and is*

$$g(x, y) = g_o(x, y) + \frac{\left(\sum_{i,j} \Lambda_{ij} g_o(x, \mathbf{v}_i)\right) \left(\sum_{i,j} \Lambda_{ij} g_o(\mathbf{v}_j, y)\right)}{\sum_{i,j} \Lambda_{ij}} - \sum_{i,j} \Lambda_{ij} g_o(x, \mathbf{v}_i) g_o(\mathbf{v}_j, y).$$

(The variables in the summations range from 1 to n .)

Proof. Define functions $\gamma_i(x) := g_o(x, \mathbf{v}_i)$ and $\gamma_j(y) := g_o(\mathbf{v}_j, y)$ where $i, j \in \{1, \dots, n\}$, then

$$\langle g_o(x, \mathcal{U}_o) | \Lambda | g_o(\mathcal{U}_o, y) \rangle = \sum_{i,j} \Lambda_{ij} \gamma_i(x) \gamma_j(y).$$

The mapping $\{\mathbf{v}_1, \dots, \mathbf{v}_n\} \rightarrow \mathbf{v}$ implies that T is an $n \times 1$ matrix with 1's for all entries. And so

$$(T\Lambda T^*)^{-1} = \frac{1}{\sum_{i,j} \Lambda_{ij}} I_1,$$

where I_1 is the 1-dimensional identity matrix. If \mathbf{w} an $n \times 1$ matrix with components (w_1, \dots, w_n) , then

$$\Lambda T^* (T \Lambda T^*)^{-1} T \Lambda \mathbf{w} = \frac{\sum_{i,j} \Lambda_{ij} w_j}{\sum_{i,j} \Lambda_{ij}} \begin{pmatrix} \sum_j \Lambda_{1j} \\ \vdots \\ \sum_j \Lambda_{nj} \end{pmatrix},$$

implying that

$$\langle g_o(x, \mathcal{U}_o) | \Lambda T^* (T \Lambda T^*)^{-1} T \Lambda | g_o(\mathcal{U}_o, y) \rangle = \frac{\left(\sum_{i,j} \Lambda_{ij} \gamma_i(x) \right) \left(\sum_{i,j} \Lambda_{ij} \gamma_j(y) \right)}{\sum_{i,j} \Lambda_{ij}}.$$

The result of the proposition follows from (3.17). □

For simplicity in Examples 4.2 and 4.4, let $k^2 = \lambda$, with the root taken in the lower-half plane for $\lambda \in \mathbb{C} \setminus [0, \infty)$.

Given a single finite line segment with domain $[0, \ell]$, the Green's function of the free Hamiltonian (*i.e.* $p \equiv 1, q \equiv 0$) satisfying *NBC* at both vertices is

$$g(x, y) = -\frac{1}{2k} \left[\frac{2 \cos kx \cos ky}{\tan k\ell} + \sin k(x+y) + \sin k|x-y| \right]. \quad (4.1)$$

Note that $g(0, 0) = g(\ell, \ell) = -k^{-1} \cot k\ell$ and $g(0, \ell) = g(\ell, 0) = -k^{-1} \csc k\ell$. Eigenvalues occur when g is not defined, namely when $k\ell$ is an integer multiple of π .

Example 4.2. *Green's function of the free Hamiltonian operator on a single loop.* Given a finite line segment of length ℓ , construct a loop. Let the initial and terminal vertices be \mathbf{u}_o and \mathbf{v}_o respectively. Form a new graph determined by the mapping $\{\mathbf{u}_o, \mathbf{v}_o\} \rightarrow \mathbf{v}$. Since

$$\Lambda = k \begin{pmatrix} \cot k\ell & -\csc k\ell \\ -\csc k\ell & \cot k\ell \end{pmatrix},$$

then $\sum_{i,j} \Lambda_{ij} = 2k(\cot k\ell - \csc k\ell)$. Additionally, $\gamma_1(x) = g_o(x, 0) = -k^{-1} \left(\frac{\cos kx}{\tan k\ell} + \sin kx \right)$ and $\gamma_2(x) = g_o(x, \ell) = -k^{-1} \frac{\cos kx}{\sin k\ell}$. Now

$$\sum_{i,j} \Lambda_{ij} \gamma_i(x) \gamma_j(y) = -k^{-1} \left(\frac{\cos k(x+y)}{\tan k\ell} + \sin k(x+y) \right),$$

and so

$$\frac{(\sum_{i,j} \Lambda_{ij} \gamma_i(x))(\sum_{i,j} \Lambda_{ij} \gamma_j(y))}{\sum_{i,j} \Lambda_{ij}} = -\frac{1}{2k} \left[\frac{\cos k(x-y)}{\sin k\ell} + \frac{\cos k(x+y)}{\tan k\ell} + \sin k(x+y) \right].$$

Thus, by Proposition 4.1,

$$g(x, y) = -\frac{1}{2k} \left[(\cot k\ell + \csc k\ell) \cos k(x-y) + \sin k|x-y| \right].$$

Eigenvalues occur when $k\ell$ is an integer multiple of 2π .

□

Given the Sturm-Liouville operator $L_o - \lambda$ defined on a graph Γ_o consisting of n pairwise disjoint graphs $\Gamma_1, \dots, \Gamma_n$ with respective Green's functions g_1, \dots, g_n . Overall, the Green's function g_o on Γ_o is given by $g_o(x, y) = \delta_{st} g_j(x, y)$ where $x \in \Gamma_s, y \in \Gamma_t$ for $s, t \in \{1, \dots, n\}$ and δ_{st} is the Kronecker-delta function (*i.e.* $\delta_{st} = 1$ if $s = t$ and $\delta_{st} = 0$ otherwise).

Corollary 4.3 (Linking Disjoint Graphs at a Single Vertex). *Using the notation from the preceding paragraph, for each $j = 1, \dots, n$, choose a vertex $\mathbf{v}_j \in \Gamma_j$ that satisfies NBC and form a new graph Γ determined by the mapping $\{\mathbf{v}_1, \dots, \mathbf{v}_n\} \rightarrow \mathbf{v}$. The Green's function g of the Sturm-Liouville operator $L - \lambda$ defined on Γ exists provided p is continuous on Γ . If $x \in \Gamma_s$ and $y \in \Gamma_t$ for $s, t \in \{1, \dots, n\}$, then the Green's function is*

$$g(x, y) = \delta_{st} g_s(x, y) + \left(\frac{\omega_s \omega_t}{\sum_j \omega_j} - \delta_{st} \omega_s \right) g_s(x, \mathbf{v}_s) g_t(\mathbf{v}_t, y), \quad (4.2)$$

where $\omega_j := g_j(\mathbf{v}_j, \mathbf{v}_j)^{-1}$.

Proof. Λ is a diagonal matrix with entries $\omega_1, \dots, \omega_n$ implying that $\sum_{i,j} \Lambda_{ij} = \sum_i \omega_i$. Since $x \in \Gamma_s, y \in \Gamma_t$, and $g_o(x, y) = \delta_{st} g_s(x, y)$, then

$$\begin{aligned} \sum_{s,t} \Lambda_{st} g_o(x, \mathbf{v}_s) &= \omega_s g_p(x, \mathbf{v}_s), \\ \sum_{s,t} \Lambda_{st} g_o(\mathbf{v}_t, y) &= \omega_t g_t(\mathbf{v}_t, y), \text{ and} \\ \sum_{s,t} \Lambda_{st} g_o(x, \mathbf{v}_s) g_o(\mathbf{v}_t, y) &= \delta_{st} \omega_s g_s(x, \mathbf{v}_s) g_t(\mathbf{v}_t, y). \end{aligned}$$

Apply Proposition 4.1 and the result immediately follows.

□

Example 4.4. *The Green's Function of the free Hamiltonian operator for a Bounded Finite Star.* Let Γ_\circ consist of n disjoint graphs $\Gamma_1, \dots, \Gamma_n$, each a single finite edge with domain $[0, \ell_j]$ where $j \in \{1, \dots, n\}$ with all vertices satisfying *NBC*. For each $j = 1, \dots, n$, label \mathbf{v}_j as the terminal vertex of the edge in Γ_j . Let Γ be the star obtained by the mapping $\{\mathbf{v}_1, \dots, \mathbf{v}_n\} \rightarrow \mathbf{v}$ (see Figure 1 for a diagram of Γ). By (4.1), $\omega_j = -k \tan k\ell_j$ for each $j = 1, \dots, n$. And so $g_s(x, \mathbf{v}_s) = g_s(x, \ell_s) = -\frac{\cos kx}{k \sin k\ell_s}$ and $g_t(\mathbf{v}_t, y) = g_t(\ell_t, y) = -\frac{\cos ky}{k \sin k\ell_t}$. By Corollary 4.3, we have if $x \in \Gamma_s, y \in \Gamma_t$ for $s, t \in \{1, \dots, n\}$, then the Green's function of the free Hamiltonian on Γ is

$$g(x, y) = -\frac{1}{k} \left[\left(\frac{\sec k\ell_s \sec k\ell_t}{\sum_j \tan k\ell_j} - \delta_{st} \tan k\ell_s \right) \cos kx \cos ky \right. \\ \left. + \frac{\delta_{st}}{2} \left(\sin k(x + y) + \sin k|x - y| \right) \right].$$

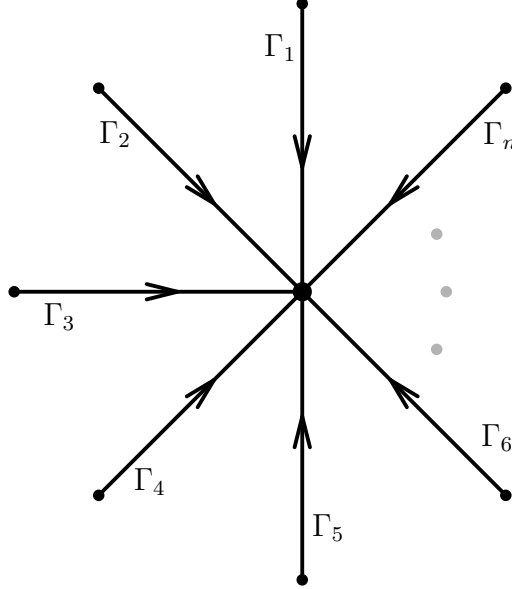


Figure 1: A Bounded Star.

□

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