Boundary value problems for Schrödinger operators on a path

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Abstract:

In this work, we concentrate on determining explicit expressions, via suitable orthogonal polynomials on the line, for the Green function associated with any regular boundary value problem on a weighted path, whose weights are determined by the coefficients of the three terms recurrence relation defining the polynomials. Our study is similar to what is known for boundary value problems associated with ordinary differential equations.

1 Introduction

In this work we analyze linear boundary value problems on a finite weighted path associated with Schrödinger operators with non constant potential. In spite of its relevance the Green function on a path have been obtained only for some boundary conditions, mainly for Dirichlet conditions or more generally for the so–called *Sturm–Liouville boundary conditions*, see [1, 2, 3, 6, 9]. Recently, some of the authors have obtained the Green function on a path for general boundary value problems related to Schrödinger operator with constant conductances and potential, [4].

We aim here at determining explicit expressions, via suitable orthogonal polynomials on the line, for the Green function associated with any regular boundary value problem on a weighted path, whose weights are determined by the coefficients of the three terms recurrence relation defining the polynomials. Our study is similar to what is known for boundary value problems associated with ordinary differential equations, [7, Chapters 7,11,12].

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The boundary value problems here considered are of two types that correspond to the cases in which the boundary has either two or one vertices. In each case, it is essential to describe the solutions of the Schröndinger equation on the interior nodes of the path. We show that it is possible to obtain explicitly such solutions in terms of the chosen orthogonal polynomials. As an immediate consequence of this property, we can easily characterize those boundary value problems that are regular and then we obtain their corresponding Green function.

2 Schrödinger operators on a path

Let P_{n+2} be a path with $n+2$ vertices, with vertex set $V = \{0, \dots, n+1\}$ and let $\mathcal{C}(V)$ be the vector space of real functions. Given $c \in \mathcal{C}(V)$ such that $c(k) > 0$ for any $k = 0, \dots, n$, we define the conductance on P_{n+2} as $c : V \times V \to [0, +\infty)$ such that $c(k, k+1) = c(k+1, k) = c(k)$ and $c(k, m) = 0$ otherwise.

The Schrödinger operator with potential $q \in \mathcal{C}(V)$ is the self–adjoint operator $\mathcal{L}_q : \mathcal{C}(V) \to \mathcal{C}(V)$ defined by

$$\begin{aligned}
\mathcal{L}_q(u)(0) &= c(0)[u(0) - u(1)] + q(0)u(0), \\
\mathcal{L}_q(u)(k) &= c(k)[u(k) - u(k+1)] + c(k-1)[u(k) - u(k-1)] + q(k)u(k), \\
\mathcal{L}_q(u)(n+1) &= c(n)[u(n+1) - u(n)] + q(n+1)u(n+1).
\end{aligned}$$

Observe that for any $1 \le k \le n$, this operator can be re–written as

$$\mathcal{L}_q(u)(k) = -c(k+1)u(k+1) + [c(k) + c(k-1) + q(k)]u(k) - c(k-1)u(k-1).$$

In the sequel F denotes the subset $F = \{1, \dots, n\}$ and hence its boundary is $\delta(F) = \{0, n+1\}$. Given $f \in \mathcal{C}(V)$ the Schrödinger equation on F with data f is the equation $\mathcal{L}_q(u)(k) = f(k)$, $k \in F$, whereas the equation $\mathcal{L}_q(u)(k) = 0$, $k \in F$, is the corresponding homogeneous Schrödinger equation on F. When $u \in \mathcal{C}(V)$ satisfies the above identities u is named a solution of the equation. Observe that $\mathcal{L}_q$ is a self-adjoint operator and therefore we can solve the equation by using the usual techniques for solving second order difference equations (see for instance [1]).

Given two solutions $u, v \in \mathcal{C}(V)$ of the homogeneous Schrödinger equation on F, their wronskian is $w[u, v] \in \mathcal{C}(V)$ defined as

$$w[u, v](k) = u(k)v(k+1) - v(k)u(k+1), \quad 0 \le k \le n,$$

and as $w[u, v](n+1) = w[u, v](n)$. It is well–known that $c \cdot w[u, v]$ is constant because $\mathcal{L}_q$ is self-adjoint and moreover, u and v are linearly dependent iff their wronskian is null.

It is well-known that every initial value problem for the Schrödinger equation on F has a unique solution. The Green function of the homogeneous Schrödinger equation on F is the function $g_q \in \mathcal{C}(V \times V)$, defined for any $s \in V$ as $g_q(\cdot, s)$, the unique solution of the initial value problem with conditions $g_q(s,s)=0$ and $g_q(s+1,s)=-\dfrac{1}{c(s)}$.

Lemma 1. *If $u,v\in\mathcal{C}(V)$ are two linearly independent solutions of the homogeneous Schrödinger equation on F, then*

$$g_q[k,s]=\frac{1}{c(0)w[u,v](0)}[u(k)v(s)-u(s)v(k)],\quad 0\le k,s\le n+1.$$

Proposition 2. *Given a function $f\in\mathcal{C}(V)$, the function $y\in\mathcal{C}(V)$ such that*

$$y(0)=0,\quad y(k)=\sum_{s=1}^{k}g_q[k,s]f(s),\quad \textit{for}\quad 1\le k\le n+1,$$

is the unique solution of the problem $\mathcal{L}_q(y)=f$, with initial conditions $y(0)=0$, $y(1)=0$.

Proof. We just have to prove that $\mathcal{L}_q(y)(k)=f(k)$, for any $1\le k\le n$

$$\begin{aligned}\mathcal{L}_q(y)(k)&=c(k+1)[y(k)-y(k+1)]+c(k-1)[y(k)-y(k-1)]+q(k)y(k)\\&=c(k+1)\Big[\sum_{j=1}^{k}g_q[k,j]f(j)-\sum_{j=1}^{k+1}g_q[k+1,s]f(j)\Big]\\&+c(k-1)\Big[\sum_{j=1}^{k}g_q[k,j]f(j)-\sum_{j=1}^{k-1}g_q[k-1,s]f(j)\Big]+q(k)\sum_{j=1}^{k}g_q[k,j]f(j)\\&=c(k+1)(-g_q[k+1,k])f(k)=f(k).\end{aligned}$$

Finally $y(1)=g_q[1,1]f(1)=0$. ∎

3 Schŕodinger operators and orthogonal polynomials

Let $\{A_n\}_{n=0}^{\infty}$ be a real positive sequence and $\{B_n\}_{n=0}^{\infty}$ a real sequence. Consider $\{\mathcal{R}_n\}_{n=0}^{\infty}$ be a sequence of real orthogonal polynomials satisfying that $\deg(R_n)=n$ and the following recurrence relation

$$\mathcal{R}_n(x)=(A_nx+B_n)\mathcal{R}_{n-1}(x)-C_n\mathcal{R}_{n-2}(x),\ n\ge 2,\tag{1}$$

where $C_n=\frac{A_n}{A_{n-1}}$. If k_n denotes the leading coefficient of $\mathcal{R}_n(x)$, then $A_n=\frac{k_n}{k_{n-1}}$, $C_n=\frac{k_nk_{n-2}}{k_{n-1}^2}$, for $n\ge 1$ and $\Pi_{i=1}^{n}C_i=\frac{A_n}{A_0}$.

Choosing a pair of initial polynomials $\mathcal{R}_0(x)$ and $\mathcal{R}_1(x)$, the recurrence relation in Equation (1) leads to a family of orthogonal polynomials and allows us to extend the recurrence relation for $n=1$. For instance, the families

$\{P_n\}_{n=0}^{\infty}$ and $\{Q_n\}_{n=0}^{\infty}$, such that $Q_0(x) = P_0(x) = 1$, $Q_1(x) = A_1x + B_1$ and $P_1(x) = \frac{A_0}{A_0+A_1}Q_1(x)$, satisfy that $P_{-1}(x) = P_1(x)$ and $Q_{-1}(x) = 0$. From now on, the families $\{P_n\}_{n=0}^{\infty}$ and $\{Q_n\}_{n=0}^{\infty}$, will be called *first kind and second kind orthogonal polynomials*, respectively, as for $A_n = 2$, $B_n = 0$, $n \geq 0$, they are the well-known Chebyshev polynomials of first and second kind.

Thus, for a fixed $x \in \mathbb{R}$, if we consider the recurrence relation of Equation (1) and we choose the concuctance $c(k) = A_0/A_{k+1}$ for each $k \in V$ and the potential $q_x(k) = A_0(A_{k+1}x + B_{k+1} - 1)/A_{k+1} - A_0/A_k$ for each $k \in V$, the corresponding Schrödinger operator is given by

$$\begin{aligned}
\mathcal{L}_{q_x}(u)(0) &= \Big[\frac{A_0(A_1x + B_1)}{A_1} - 1\Big]u(0) - \frac{A_0}{A_1}u(1),\\
\mathcal{L}_{q_x}(u)(k) &= \frac{A_0(A_{k+1}x + B_{k+1})}{A_{k+1}}u(k) - \frac{A_0}{A_{k+1}}u(k+1) - \frac{A_0}{A_k}u(k-1), \quad k \in F,\\
\mathcal{L}_{q_x}(u)(n+1) &= \frac{A_0(A_{n+2}x + B_{n+2} - 1)}{A_{n+2}}u(n+1) - \frac{A_0}{A_{n+1}}u(n),
\end{aligned}$$

for any $u \in \mathcal{C}(V)$.

From now on, we consider only $x \neq -\frac{B_1}{A_1}$; i.e, such that $P_1(x) \neq 0$.

Lemma 3. *The functions $u(k) = P_k(x)$ and $v(k) = Q_k(x)$ for any $k \in V$, form a basis of the solution space of the homogeneous Schrödinger equation. Moreover, the Green function of the homogenous Schrödinger equation is*

$$g_x[k,s] = \frac{1}{P_1(x)}[P_k(x)Q_s(x) - P_s(x)Q_k(x)], \quad k,s \in V. \tag{2}$$

Therefore, the general solution of the Schrödinger equation on F with data $f \in \mathcal{C}(V)$ is determined by

$$u(k) = \alpha P_k(x) + \beta Q_k(x) + \sum_{s=1}^{k} g_x[k,s]f(s), \quad k \in V, \quad \textit{where} \quad \alpha, \beta \in \mathbb{R}.$$

Proof. As $P_k(x)$ and $Q_k(x)$, $k \in V$, satisfy the recurrence relation (1) it is easy to verify that they are solution of the homogeneous Schrödinger equation. Then their associated wronskian is:

$$\begin{aligned}
w[u,v](k) &= P_k(x)Q_{k+1}(x) - P_{k+1}(x)Q_k(x) = C_{k+1}w[u,v](k-1) = \cdots =\\
&= \left(\prod_{i=2}^{k+1} C_i\right) \cdot w[u,v](0) = \left(\prod_{i=2}^{k+1} C_i\right)\frac{A_1}{A_0}P_1(x) = \left(\prod_{i=1}^{k+1} C_i\right)P_1(x)\\
&= \frac{A_{k+1}}{A_0}P_1(x) \neq 0.
\end{aligned}$$

Thus they are independent and the general solution of the homogeneous Schrödinger equation will be given by $y(k) = \alpha P_k(x) + \beta Q_k(x)$, for α, $\beta \in \mathbb{R}$, $k \in V$. Besides, the general solution of the general Schrödinger equation on F is the sum of $y(k)$ plus a particular solution of the general Schrödinger equation on F. We can take as a particular solution the one obtained in Proposition (2), i.e., $y(k) = \sum_{s=1}^{k} g_q[k,s]f(s)$ for any $k \in F$, and then the result holds. ∎

If the coefficients $A_n = A$, $B_n = B$ are constants we can consider a different basis as in the case of Chebyshev polynomial, see [4], and hence we can obtain the following result.

Lemma 4. *Consider the functions $u(k) = Q_k(x)$ and $v(k) = Q_{k-1}(x)$ for any $k \in V$. Then, $w[u,v](s) = 1$ for any $k \in V$ and hence $\{u,v\}$ is a basis of the solution space of the homogeneous Schrödinger equation on F. Therefore, any solution of the Schrödinger equation on F with data $f \in \mathcal{C}(V)$ is determined by*

$$u(k) = y(k) + \sum_{s=1}^{k} [Q_{s-1}(x)Q_k(x) - Q_s(x)Q_{k-1}(x)]f(s), \quad k \in F.$$

4 Two side boundary value problems

Given $d_i \in \mathbb{R}$, $i \in \partial F = \{0, 1, n, n+1\}$, a linear boundary condition on F with coefficients d_i is a linear map $\mathcal{B} : \mathcal{C}(V) \to \mathbb{R}$ such that

$$\mathcal{B}(u) = d_0 u(0) + d_1 u(1) + d_n u(n) + d_{n+1} u(n+1), \text{ for any } u \in \mathcal{C}(V).$$

A *two side boundary value problem on F* consists in finding $u \in \mathcal{C}(V)$ such that

$$\mathcal{L}_{q_x}(u) = f \text{ on } F, \quad \mathcal{B}_1(u) = g_1, \quad \mathcal{B}_2(u) = g_2, \tag{3}$$

for given $f \in \mathcal{C}(V)$ and $g_1, g_2 \in \mathbb{R}$, where the boundary conditions $\mathcal{B}_1$ and $\mathcal{B}_2$ are linearly independent. The problem is *semi–homogeneous* when $g_1 = g_2 = 0$, and *homogeneous* if besides $f = 0$. Problem (3) is *regular* if the corresponding homogenous boundary value problem has the null function as its unique solution.

A function $y \in \mathcal{C}(V)$ is a solution of the homogeneous boundary value problem iff $y = \alpha u + \beta v$, where $\alpha, \beta \in \mathbb{R}$ and $\{u, v\}$ is a basis of solutions of the homogeneous equation on V, satisfies

$$\begin{pmatrix} \mathcal{B}_1(u) & \mathcal{B}_1(v) \\ \mathcal{B}_2(u) & \mathcal{B}_2(v) \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Therefore Problem (3) is regular iff $\mathcal{B}_1(u)\mathcal{B}_2(v) - \mathcal{B}_2(u)\mathcal{B}_1(v) \neq 0$ and hence, it also holds that the boundary value problem is regular iff for any data $f \in \mathcal{C}(V)$, $g_1, g_2 \in \mathbb{R}$ it has a unique solution. Moreover, for $u(k) = P_k(x)$ and $v(k) = Q_k(x)$, $k \in V$, the boundary polynomial is

$$P_{\mathcal{B}}(x) = \mathcal{B}_1(u)\mathcal{B}_2(v) - \mathcal{B}_2(u)\mathcal{B}_1(v) = \sum_{i,j \in \partial F} p_{ij} u(i) v(j),$$

where $p_{ij} = d_{1i}d_{2j} - d_{2i}d_{1j}$ for all $i, j \in \partial F$. Observe that $p_{ii} = 0$ and $p_{ij} = -p_{ji}$ for all $i, j \in \partial F$. Therefore,

$$P_{\mathcal{B}}(x) = \quad P_1(x) \sum_{\substack{i<j \\ i,j\in\partial F}} p_{i,j} g_x[i, j],$$

where g_x is the Green function defined in Equation (2).

The following lemma shows that two side boundary problems can be restricted to the study of the semi–homogeneous ones.

Lemma 5. *Consider $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ such that $d_{j1}\alpha + d_{j2}\beta + d_{j3}\gamma + d_{j4}\delta = g_j$, for $j = 1, 2$, then $u \in \mathcal{C}(V)$ verifies the Schrödinger equation $\mathcal{L}_{q_x}(u) = f$ on F, together with the boundary conditions $\mathcal{B}_1(u) = g_1$ and $\mathcal{B}_2(u) = g_2$, iff the function $v = u - \alpha\varepsilon_0 - \beta\varepsilon_1 - \gamma\varepsilon_n - \delta\varepsilon_{n+1}$ verifies that*

$$\begin{aligned} \mathcal{L}_{q_x}(v) &= f + \left(\frac{A_0}{A_1}\alpha - \frac{A_0}{A_2}(A_2 x + B_2)\beta\right)\varepsilon_1 + \frac{A_0}{A_2}\beta\varepsilon_2 + \frac{A_0}{A_n}\gamma\varepsilon_{n-1} \\ &\quad + \left(\frac{A_0}{A_{n+1}}\delta - \frac{A_0}{A_{n+1}}(A_{n+1}x + B_{n+1})\gamma\right)\varepsilon_n \end{aligned}$$

on F and $\mathcal{B}_1(u) = \mathcal{B}_2(u) = 0$.

The solution of any regular semi–homogeneous boundary problem can be obtained by considering its resolvent kernel; *i.e.*, the function $G_{q_x} \in \mathcal{C}(V \times F)$ such that

$$\mathcal{L}_{q_x}(G_{q_x}(\cdot, s)) = \varepsilon_s \text{ on } F, \quad \mathcal{B}_1(G_{q_x}(\cdot, s)) = \mathcal{B}_2(G_{q_x}(\cdot, s)) = 0, \quad s \in F.$$

This function is called the *Green function* for Problem (3). Therefore, for any $f \in \mathcal{C}(V)$ the unique solution of the semi–homogeneous boundary problem with data f is the function

$$u(k) = \sum_{s=1}^{n} G_{q_x}(k, s) f(s).$$

Theorem 6. *The boundary value problem (3) is regular iff $P_{\mathcal{B}}(x) \neq 0$. In this case, the Green function is given, for any $1 \leq s \leq n$ and $0 \leq k \leq n+1$, by*

$$\begin{aligned} G_{q_x}(k, s) = \frac{P_1(x)}{P_{\mathcal{B}}(x)} &\left[p_{n,n+1}\frac{A_{n+1}}{A_0} g_x[s, k] + \sum_{i=0}^{1}\sum_{j=n}^{n+1} p_{i,j} g_x[k, i] g_x[j, s]\right] \\ &+ \begin{cases} 0, & k \leq s \\ g_x[k, s], & k \geq s. \end{cases} \end{aligned}$$

Proof. The unique solution of the BVP can be expressed as the sum of the general solution of the homogenous Schrödinger equation plus a particular solution of the problem : $x = x_h + x_p$. The general solution of the homogeneous Schrödinger equation x_h is given by Lemma (3) and we can also consider as x_p the same computed in Lemma (3), that is, $x_p(k) = \sum_{s=1}^{k} g_x[k, s] f(s)$ for $k \in V$.

On the other hand $x_h = au + bv$, where $u(k) = P_k(x)$ and $v(k) = Q_k(x)$, $k \in V$, and we just have to impose the boundary conditions to obtain the value of the parameters a, $b \in \mathbb{R}$ of the unique solution of the BVP. Observe from Lemma (3) that for a fixed $s \in F$, $k \in V$, the Green function G_{q_x} of the BVP (3) is given by

$$G_{q_x}(k,s) = a(s)p_k(x) + b(s)r_k(x) + \begin{cases} 0 & \text{if} \quad k < s, \\ g_x[k,s] & \text{if} \quad k \geq s. \end{cases}$$

Therefore for a fixed $s \in F$ we just have to solve the system

$$\begin{pmatrix} \mathcal{B}_1(u) & \mathcal{B}_1(v) \\ \mathcal{B}_2(u) & \mathcal{B}_2(v) \end{pmatrix} \begin{pmatrix} a(s) \\ b(s) \end{pmatrix} = - \begin{pmatrix} \mathcal{B}_1(g_x[k,s]) \\ \mathcal{B}_2(g_x[k,s]) \end{pmatrix},$$

and thus

$$\begin{aligned} P_{\mathcal{B}}(x)a(s) &= \mathcal{B}_1(v)\mathcal{B}_2(g_x[k,s]) - \mathcal{B}_2(v)\mathcal{B}_1(g_x[k,s]), \\ P_{\mathcal{B}}(x)b(s) &= \mathcal{B}_2(u)\mathcal{B}_1(g_x[k,s]) - \mathcal{B}_1(u)\mathcal{B}_2(g_x[k,s]). \end{aligned}$$

From Proposition 2 we have that for $i = 1, 2$

$$\mathcal{B}_i(g_x[k,s]) = d_{in} g_x[n,s] + d_{in+1} g_x[n+1,s].$$

And thus

$$\begin{aligned} P_{\mathcal{B}}(x)a(s) &= \sum_{i=0}^{1} \sum_{j=n}^{n+1} p_{ij} g_x[j,s] Q_i(x) - p_{nn+1} g_x[n,n+1] Q_s(x), \\ P_{\mathcal{B}}(x)b(s) &= -\sum_{i=0}^{1} \sum_{j=n}^{n+1} p_{ij} g_x[j,s] P_i(x) + p_{nn+1} g_x[n,n+1] P_s(x). \end{aligned}$$

Finally we obtain

$$\begin{aligned} \frac{P_{\mathcal{B}}(x)}{P_1(x)} \left[a(s)P_k(x) + b(s)Q_k(x) \right] &= p_{nn+1} g_x[n,n+1] p_{ij} g_x[s,k] \\ &+ \sum_{i=0}^{1} g_x[i,k] \left(\sum_{j=n}^{n+1} p_{ij} g_x[s,j] \right). \end{aligned}$$

∎

In what follows we study the more usual boundary value problems appearing in the literature with proper name; that is, unilateral, Dirichlet and Neumann problems, or more generally, Sturm-Liouville problems.

The pair of boundary conditions $(\mathcal{B}_1, \mathcal{B}_2)$ is called *unilateral* if either $d_{1,j} = d_{2,j} = 0$, for any $j \in \{n, n+1\}$ (initial value problem) or $d_{1,i} = d_{2,i} = 0$, for any $i \in \{0,1\}$ (final value problem). Any unilateral pair verifies that $p_{0j} = p_{1_j} = 0$, for $j \in \{n, n+1\}$, and thus $P_{\mathcal{B}}(x) = \frac{P_1(x)}{A_0}(A_1 p_{0,1} + A_{n+1} p_{n,n+1})$. In addition, either $p_{n,n+1} = 0$ and $p_{0,1} \neq 0$ or $p_{n,n+1} \neq 0$ and $p_{0,1} = 0$, since the boundary conditions are linearly independent, which implies that unilateral boundary problems are regular. Therefore, any unilateral pair is equivalent to either $(u(0), u(1))$ for initial value problems, or $(u(n), u(n+1))$ for final value problems.

Corollary 7. *The Green function for the initial boundary value problem is given by* $G_{q_x}(k,s) = \begin{cases} 0, & k \leq s, \\ g_x[k,s], & k \geq s. \end{cases}$ *Whereas the Green function for the final boundary value problem is* $G_{q_x}(k,s) = \begin{cases} g_x[s,k], & k \leq s, \\ 0, & k \geq s, \end{cases}$ *for any* $1 \leq s \leq n$, $0 \leq k \leq n+1$.

The boundary conditions are called *Sturm-Liouville conditions*, when $d_{1j} = d_{2i} = 0$, for $i \in \{0,1\}$, $j \in \{n, n+1\}$; that is, when

$$\mathcal{B}_1(u) = au(0) + bu(1) \quad \text{and} \quad \mathcal{B}_2(u) = cu(n) + du(n+1), \tag{4}$$

where $a, b, c, d \in \mathbb{R}$ are such that $(|a| + |b|)(|c| + |d|) > 0$. The most popular Sturm-Liouville conditions are the so-called *Dirichlet boundary conditions*, that correspond to take $b = c = 0$, and *Neumann boundary conditions*, that correspond to take $b = -a$ and $d = -c$.

Corollary 8. *Given* $a, b, c, d \in \mathbb{R}$ *such that* $(|a| + |b|)(|c| + |d|) > 0$ *and the Sturm-Liouville boundary conditions, then*

$$\begin{aligned} P_{\mathcal{B}}(x) = \; & a\Big[d\big(Q_{n+1}(x) - P_{n+1}(x)\big) + c\big(Q_n(x) - P_n(x)\big)\Big] + \\ & b\Big[P_1(x)\big(dQ_{n+1}(x) + cQ_n(x)\big) - Q_1(x)\big(dP_{n+1}(x) + cP_n(x)\big)\Big] \end{aligned}$$

and the Green function for the Sturm-Liouville boundary value problem is

$$\begin{aligned} G_{q_x}(k,s) \; &= \frac{1}{P_1(x)P_{\mathcal{B}}(x)}\Big[a\big(P_k(x) - Q_k(x)\big) + b\big(Q_1(x)P_k(x) - Q_k(x)P_1(x)\big)\Big] \\ &\times \; \Big[c\big(P_s(x)Q_n(x) - P_n(x)Q_s(x)\big) + d\big(P_s(x)Q_{n+1}(x) - P_{n+1}(x)Q_s(x)\Big] \end{aligned}$$

for any $0 \leq k \leq s \leq n$ *and* $1 \leq s$*; whereas*

$$\begin{aligned} G_{q_x}(k,s) \; &= \frac{1}{P_1(x)P_{\mathcal{B}}(x)}\Big[a\big(P_s(x) - Q_s(x)\big) + b\big(Q_1(x)P_s(x) - Q_s(x)P_1(x)\big)\Big] \\ &\times \; \Big[c\big(P_k(x)Q_n(x) - P_n(x)Q_k(x)\big) + d\big(P_k(x)Q_{n+1}(x) - P_{n+1}(x)Q_k(x)\Big] \end{aligned}$$

for any $n+1 \geq k \geq s \geq 1$ *and* $s \leq n$.

As a consequence, the boundary polynomial for the Dirichlet problem is

$$P_{\mathcal{B}}(x) = ad\big(Q_{n+1}(x) - P_{n+1}(x)\big)$$

and hence it is regular iff $Q_{n+1}(x) \neq P_{n+1}(x)$, and the Green's function is given by

$$G_{q_x}(k,s) = \begin{cases} \dfrac{\big(P_k(x)-Q_k(x)\big)\big(Q_{n+1}(x)P_s(x)-P_{n+1}(x)Q_s(x)\big)}{P_1(x)\big(Q_{n+1}(x)-P_{n+1}(x)\big)}, & k \le s \\[2ex] \dfrac{\big(P_s(x)-Q_s(x)\big)\big(Q_{n+1}(x)P_k(x)-P_{n+1}(x)Q_k(x)\big)}{P_1(x)\big(Q_{n+1}(x)-P_{n+1}(x)\big)}, & k \ge s. \end{cases}$$

Finally, for Neumann boundary problem, the boundary polynomial is

$$P_{\mathcal{B}}(x) = ac\Big[\big(1-Q_1(x)\big)\big(P_{n+1}(x)-P_n(x)\big) - \big(1-P_1(x)\big)\big(Q_{n+1}(x)-Q_n(x)\big)\Big]$$

and the Green function, $G_{q_x}(k,s)$, for the Neumann problem is

$$\frac{\Big[(1-Q_1(x))P_k(x) - \big(1-P_1(x)\big)Q_k(x)\Big]\Big[Q_s(x)\big(P_{n+1}(x)-P_n(x)\big) - P_s(x)\big(Q_{n+1}(x)-Q_n(x)\big)\Big]}{P_1(x)\Big[\big(1-Q_1(x)\big)\big(P_{n+1}(x)-P_n(x)\big) - \big(1-P_1(x)\big)\big(Q_{n+1}(x)-Q_n(x)\big)\Big]}$$

for any $0 \le k \le s \le n$ and $1 \le s$; whereas

$$\frac{\Big[(1-Q_1(x))P_s(x) - \big(1-P_1(x)\big)Q_s(x)\Big]\Big[Q_k(x)\big(P_{n+1}(x)-P_n(x)\big) - P_k(x)\big(Q_{n+1}(x)-Q_n(x)\big)\Big]}{P_1(x)\Big[\big(1-Q_1(x)\big)\big(P_{n+1}(x)-P_n(x)\big) - \big(1-P_1(x)\big)\big(Q_{n+1}(x)-Q_n(x)\big)\Big]}$$

for any $n+1 \ge k \ge s \ge 1$ and $s \le n$.

5 One side boundary value problems

In this section we analyze one side boundary value problems; i.e, the boundary conditions are located at one side of the path P_{n+2}. So if we consider the vertex subset $\widehat{F} = \{0,1,\dots,n\}$, the linear map $\mathcal{B} : \mathcal{C}(V) \to \mathbb{R}$ such that

$$\mathcal{B}(u) = au(n) + bu(n+1), \text{ for any } u \in \mathcal{C}(V)$$

is a *linear one side boundary condition on* $\widehat{F}$ with coefficients $a, b \in \mathbb{R}$, wherever $|a|+|b|>0$. Moreover, an *one side boundary value problem on* $\widehat{F}$ consists in finding $u \in \mathcal{C}(V)$ such that

$$\mathcal{L}_{q_x}(u) = f \text{ on } \widehat{F}, \quad \mathcal{B}(u) = g, \tag{5}$$

for a given $f \in \mathcal{C}(V)$ and $g \in \mathbb{R}$. The problem is semi–homogeous when $g = 0$ and homogeneous if, in addition, $f = 0$. Again, the one side boundary value problem is regular if the corresponding homogeneous problem has the null function as its unique solution; equivalently, (5) is regular iff for any data $f \in \mathcal{C}(V)(V)$ and $g \in \mathcal{R}$ it has a unique solution. In this case, the *Green function for the one side boundary value problem (5)* is the function $G_{q_x} \in \mathcal{C}(V \times \widehat{F})$ characterized by

$$\mathcal{L}_{q_x}(G_{q_x}(\cdot,s)) = \varepsilon_s \text{ on } \widehat{F}, \quad \mathcal{B}(G_{q_x}(\cdot,s)) = 0, \quad \text{for any } s \in \widehat{F}. \tag{6}$$

The analysis of one side boundary value problems can be easily derived from the study of two side boundary value problems by observing that (5) can be re–written as the following two side Sturm–Liouville problem

$$\mathcal{L}_{q_x}(u) = f, \text{ on } F, \quad \Big[A_0Q_1(x) - A_1\Big]u(0) - A_0u(1) = A_1f(0), \; \mathcal{B}(u) = g. \quad (7)$$

Therefore, we can reduce the analysis of one side boundary value problems to the analysis of semi–homogeneous Sturm-Liouville problems.

Lemma 9. *Given $g \in \mathcal{R}$, then for any $f \in \mathcal{C}(V)$ the function $u \in \mathcal{C}(V)$ satisfies that $\mathcal{L}_{q_x}(u) = f$ on $\widehat{F}$ and $\mathcal{B}(u) = g$ iff the function $v = u + \frac{A_1}{A_0}f(0)\varepsilon_1 - \dfrac{g(a\varepsilon_n + b\varepsilon_{n+1})}{a^2+b^2}$ satisfies $\Big[A_0Q_1(x) - A_1\Big]v(0) - A_0v(1) = \mathcal{B}(v) = 0$ and on F*

$$\begin{aligned}\mathcal{L}_{q_x}(v) = &\quad f + \frac{A_1f(0)}{A_2}\big((A_2x+B_2)\varepsilon_1 - \varepsilon_2\big)\\ + &\quad \frac{A_0g}{(a^2+b^2)}\Big(\big(a(A_{n+1}x+B_{n+1}) - b\big)\frac{\varepsilon_n}{A_{n+1}} - a\frac{\varepsilon_{n-1}}{A_n}\Big).\end{aligned}$$

Corollary 10. *Given the one side boundary value problem (5), then*

$$P_{\mathcal{B}}(x) = \quad A_1\Big[\big(P_1(x)-1\big)\big(bQ_{n+1}(x) + aQ_n(x)\big) + bP_{n+1}(x) + aP_n(x)\Big]$$

and the Green function is

$$\begin{aligned}G_{q_x}(k,s) = &\quad \frac{\Big[Q_k(x)\big(1-P_1(x)\big) - P_k(x)\Big]}{P_1(x)\Big[\big(P_1(x)-1\big)\big(bQ_{n+1}(x)+aQ_n(x)\big) + bP_{n+1}(x) + aP_n(x)\Big]}\\ \times &\quad \Big[\big(bQ_{n+1}(x)+aQ_n(x)\big)P_s(x) - \big(bP_{n+1}(x)+aP_n(x)\big)Q_s(x)\Big]\end{aligned}$$

for any $0 \le k \le s \le n$; whereas

$$\begin{aligned}G_{q_x}(k,s) = &\quad \frac{\Big[Q_s(x)\big(1-P_1(x)\big) - P_s(x)\Big]}{P_1(x)\Big[\big(P_1(x)-1\big)\big(bQ_{n+1}(x)+aQ_n(x)\big) + bP_{n+1}(x) + aP_n(x)\Big]}\\ \times &\quad \Big[\big(bQ_{n+1}(x)+aQ_n(x)\big)P_k(x) - \big(bP_{n+1}(x)+aP_n(x)\big)Q_k(x)\Big]\end{aligned}$$

for any $n+1 \ge k \ge s \ge 0$ and $s \le n$.

6 The Poisson equation

Finally we study the Poisson equation associated with the Schrödinger operator on the finite path P_{n+2}, which consists in finding $u \in \mathcal{C}(V)$ such that $\mathcal{L}_{q_x}(u) = f$ on V for any $f \in \mathcal{C}(V)$. Analogously to the previous problems, it is called regular if the corresponding homogeneous problem $\mathcal{L}_{q_x}(u) = 0$ on V has the null function as its unique solution, i.e., if $\mathcal{L}_{q_x}(u) = f$ has a unique solution for any data f. In addition, $P_{\mathcal{B}}(x)$ is named the Poisson polynomial. Then the Green's funtion for the Poisson equation is denoted by $G_{q_x} \in \mathcal{C}(V \times V)$, and characterized by

$$\mathcal{L}_{q_x}(G_{q_x}(\cdot, s)) = \varepsilon_s \text{ on } F, \quad \text{for any} \quad s \in V. \tag{8}$$

The analysis of the Poisson equation can be also derived from the study of two-side boundary value problems, since the Poisson equation can be re-written as the following two-side Sturm-Liouville problem

$$\begin{aligned}
\mathcal{L}_{q_x}(G_{q_x}(\cdot, s)) &= \varepsilon_s \text{ on } F, s \in V, \\
\mathcal{B}_1(u) &= (A_0 Q_1(x) - A_1)u(0) - A_0 u(1) = A_1 f(0) \\
\mathcal{B}_2(u) &= -A_0 u(n) + A_0(A_{n+2}x + B_{n+2} - 1)u(n+1) = A_{n+2} f(n+1).
\end{aligned}$$

Thus, as a Sturm-Liouville problem the boundary polynomial is

$$\begin{aligned}
P_{\mathcal{B}}(x) &= A_0(A_0 Q_1(x) - A_1)\Big[(A_{n+2}x + B_{n+2} - 1)\big[Q_{n+1}(x) - P_{n+1}(x)\big] \\
&\qquad + \big[P_n(x) - Q_n(x)\big]\Big] \\
&-A_0^2\Big[(A_{n+2}x + B_{n+2} - 1)\big[Q_{n+1}(x)P_1(x) - P_{n+1}(x)Q_1(x)\big] \\
&\qquad + \big[P_n(x)Q_1(x) - Q_n(x)P_1(x)\big]\Big],
\end{aligned}$$

and the Green function for the Poisson equation is

$$\begin{aligned}
G_{q_x}(k, s) &= \frac{A_0}{P_1(x)P_{\mathcal{B}}(x)}\Big[(A_0 Q_k(x)\big(P_1(x) - Q_1(x)\big) - A_1\big(P_k(x) - Q_k(x)\big)\Big] \\
&\times\Big[\big(P_n(x)Q_s(x) - P_s(x)Q_n(x)\big) + \\
&\qquad (A_{n+2}x + B_{n+2} - 1)\big(P_s(x)Q_{n+1}(x) - P_{n+1}(x)Q_s(x)\Big]
\end{aligned}$$

for any $0 \le k \le s \le n$ and $1 \le s$; whereas

$$\begin{aligned}
G_{q_x}(k, s) &= \frac{A_0}{P_1(x)P_{\mathcal{B}}(x)}\Big[(A_0 Q_k(x)\big(P_1(x) - Q_1(x)\big) - A_1\big(P_s(x) - Q_s(x)\big)\Big] \\
&\times\Big[\big(P_n(x)Q_k(x) - P_k(x)Q_n(x)\big) + \\
&\qquad (A_{n+2}x + B_{n+2} - 1)\big(P_k(x)Q_{n+1}(x) - P_{n+1}(x)Q_k(x)\Big]
\end{aligned}$$

for any $n + 1 \ge k \ge s \ge 1$ and $s \le n$.

Finally, for the Poisson equation we can also obtain the following result

Proposition 11. *Let λ be a root of $P_{n+2}(x)$, then 0 is an eigenvalue of $\mathcal{L}_{q_\lambda}$ with associated eigenfunction $u(k) = P_k(\lambda)$, for $0 \le k \le n + 1$.*

Proof. First we have the recurrence relation

$$\frac{A_0}{A_{n+2}}(A_{n+2}x + B_{n+2} - 1)P_{n+1}(x) - \frac{A_0}{A_{n+2}}P_n(x) = P_{n+2}(x).$$

Thus the last equation is verified iff $x = \lambda$ is a root of $P_{n+2}(x)$. In such case the homogeneous Poisson equation $\mathcal{L}_{q_\lambda}(u) = 0$ has as a solution the eigenfunction $u(k) = P_k(\lambda)$, for $0 \leq k \leq n+1$. ∎

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