Regular two-point boundary value problems for the Schrödinger operator on a path

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Abstract
In this work we study the different type of regular boundary value problems on a path associated with the Schrödinger operator. In particular, we obtain the Green function for each problem and we emphasize the case of Sturm-Liouville boundary conditions. In any case, the Green function is given in terms of second kind Chebyshev polynomials since they verify a recurrence law similar to the one verified by the Schödinger operator on a path.

Keywords: Discrete Schrödinger operator, Path, Boundary value problems, Green function, Chebyshev polynomials.

1 Introduction

In this work, we analyze the linear boundary value problem in the context of the second order difference equation with constant coefficients associated with the Schrödinger operator on a finite path. Our study runs in parallel to

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the known for boundary value problems associated with ordinary differential
equations. In particular we concentrate on determining explicit expressions
for the Green function associated with regular boundary value problems on a
path.

We show that, like its continuous counterpart, to determine these func-
tions, it suffices to know previously a basis of solutions of the correspond-
ing homogenous equation. As the difference equation considered here is the
Schrödinger equation in a path, it is possible to obtain explicitly one such
basis in terms of second kind Chebyshev polynomials. As a immediate conse-
quence of this property, we obtain that the Green function of any boundary
value problem can be expressed easily in terms of Chebyshev polynomials.

The second kind Chebyshev polynomials are defined as the sequence veri-
fying
\[ U_0(x) = 1, \quad U_1(x) = 2x \]
and the recurrence law
\[ U_{n+2}(x) = 2xU_{n+1}(x) - U_n(x), \quad \text{for each } n \in \mathbb{Z}. \] (1)
It is easy to prove that: \( U_{-n} = -U_n \) for all \( n \in \mathbb{Z} \) which, in particular, implies that \( U_{-1} = 0 \), see [5].

2 The Schrödinger equation on a path

Our propose in this section is to formulate the difference equations related
with the Schrödinger operator on a connected subset of the finite path of
\( n + 2 \) vertices, \( P_n \). Moreover, we can suppose without loss of generality that
the set of vertices of \( P_n \) is \( \{0, \ldots, n + 1\} \subset \mathbb{N} \). Along the paper \( F \) will
denote the vertex subset \( F = \{1, \ldots, n\} \). Therefore, the boundary of \( F \) is
\( \delta(F) = \{0, n + 1\} \) and the closure of \( F \) is \( \bar{F} = \{0, \ldots, n + 1\} \), the vertex set of \( P_n \).

For any \( s \in \bar{F}, \varepsilon_s \) will stand for the Dirac delta on \( s \). Moreover, if \( Q \subset \bar{F} \),
we will denote by \( \mathcal{C}(Q) \) the vector space of functions \( u: \bar{F} \rightarrow \mathbb{R} \) that vanish
on \( \bar{F} \setminus Q \). For each \( q \in \mathbb{R} \), the linear operator \( \mathcal{L}_q: \mathcal{C}(\bar{F}) \rightarrow \mathcal{C}(F) \) defined for
each \( u \in \mathcal{C}(\bar{F}) \) as
\[ \mathcal{L}_q(u)(k) = 2qu(k) - u(k+1) - u(k-1), \quad k \in F, \] (2)
will be called Schrödinger operator on \( \bar{F} \). Moreover the value \( 2(q - 1) \) is
usually called the potential or ground state associated with \( \mathcal{L}_q \). Observe that
the Schrödinger operator with null ground state is nothing else that the so-
called combinatorial Laplacian on \( F \).

For each \( f \in \mathcal{C}(F) \), we will call Schrödinger equation with data \( f \) the identity
\( \mathcal{L}_q(u) = f \) on \( F \). In particular \( \mathcal{L}_q(u) = 0 \) on \( F \), will be called homogeneous
Schrödinger equation.
If \( u, v \in C(\bar{F}) \) the \textit{wronskian} of \( u \) and \( v \), \( w[u, v] \in C(\bar{F}) \) is defined as,
\[
w[u, v](k) = u(k)v(k+1) - u(k+1)v(k), \quad k = 0, \ldots, n
\]
and \( w[u, v](n+1) = w[u, v](n) \), see [4,6]. Note that in some works the function \( w[u, v] \) is called the \textit{casoratian} of \( u \) and \( v \), see for instance [1].

We will call \textit{Green function} of the Schrödinger equation the function \( g_p \in C(\bar{F} \times \bar{F}) \) such that for any \( s \in \bar{F} \), \( g_q(\cdot, s) \) is the unique solution of the homogeneous Schrödinger equation verifying that \( g_q(s, s) = 0 \) and \( g_q(s+1, s) = -1 \) when \( s = 0, \ldots, n \) and \( g_q(n+1, n+1) = 0 \) and \( g_q(n, n+1) = 1 \).

The following results are the reformulation, for the Schrödinger equation on a path, of some well-known results in the context of difference equations and they will be useful throughout the paper, [1].

**Proposition 2.1** Let \( \{U_k\}_{k=-\infty}^{\infty} \) be the sequence of second kind Chebyshev polynomials and consider the functions \( u, v \in C(\bar{F}) \) defined as \( u(k) = U_{k-1}(q) \) and \( v(k) = U_{k-2}(q), \) \( k \in \bar{F} \). Then, \( w[u, v] = 1 \), the Green function of the Schrödinger equation is given by
\[
g_q(k, s) = -U_{k-s-1}(q), \quad k, s \in \bar{F}
\]
and for any \( f \in C(F) \) and \( x_0, x_1 \in \mathbb{R} \) the unique solution of the Schrödinger equation with data \( f \) verifying that \( x(0) = x_0 \) and \( x(1) = x_1 \).
\[
x(k) = x_1 U_{k-1}(q) - x_0 U_{k-2}(q) - \sum_{s=1}^{k} U_{k-s-1}(q)f(s), \quad k \in \bar{F}.
\]

**3 Two-point boundary value problems on a path**

Our aim in this section is to analyze the different boundary value problems on \( F \) associated with the Schrödinger operator. As \( \delta(F) \) has exactly two points, these problems are generally known as \textit{two-point boundary value problems on} \( F \). Our analysis runs in a parallel way to the two-point boundary value problems for ordinary differential equations and many techniques and results are the same in the discrete setting. Therefore, we will omit the proofs that follow the same guidelines that its continuous counterpart and will remit to the reader to the fundamental reference [3, Chapters 7,11].

Given \( a, b, c, d \in \mathbb{R} \) non simultaneously null, we will call \textit{(linear) boundary condition} on \( F \) with coefficients \( a, b, c \) and \( d \) the linear map \( U: C(\bar{F}) \rightarrow \mathbb{R} \) determined by the expression
\[
U(u) = au(0) + bu(1) + cu(n) + du(n+1), \quad \text{for any} \ u \in C(\bar{F}).
\]
Let \( \mathcal{U}_1, \mathcal{U}_2 : \mathcal{C}(\bar{F}) \rightarrow \mathbb{R} \) be boundary conditions on \( F \) with coefficients \( a_{11}, a_{12}, b_{11}, b_{12} \) and \( a_{21}, a_{22}, b_{21}, b_{22} \), respectively. Then, for any \( u \in \mathcal{C}(\bar{F}) \) it is verified that
\[
\begin{bmatrix}
\mathcal{U}_1(u) \\
\mathcal{U}_2(u)
\end{bmatrix} = \begin{bmatrix}
a_{11} & a_{12} \\
a_{21} & a_{22}
\end{bmatrix} \begin{bmatrix}
u(0) \\
u(1)
\end{bmatrix} + \begin{bmatrix}
b_{11} & b_{12} \\
b_{21} & b_{22}
\end{bmatrix} \begin{bmatrix}
u(n) \\
u(n+1)
\end{bmatrix}.
\]

With the above notations \( \mathcal{U}_1 \) and \( \mathcal{U}_2 \) are called boundary conditions determined by the matrices \( A = (a_{ij}) \) and \( B = (b_{ij}) \).

**Lemma 3.1** Let \( \mathcal{U}_1 \) and \( \mathcal{U}_2 \) be the boundary conditions determined by \( A, B \in \mathcal{M}_2(\mathbb{R}) \). Then, \( \mathcal{U}_1 \) and \( \mathcal{U}_2 \) are linearly independent iff the map \( \mathcal{U} : \mathcal{C}(\bar{F}) \rightarrow \mathbb{R}^2 \) whose components are \( \mathcal{U}_1 \) and \( \mathcal{U}_2 \) is surjective or equivalently, iff \( \text{rg}(A, B) = 2 \).

Fixed \( (\mathcal{U}_1, \mathcal{U}_2) \) a pair of linearly independent boundary conditions, a boundary value problem on \( F \) consists in finding \( u \in \mathcal{C}(\bar{F}) \) such that
\[
\mathcal{L}_q(u) = f, \quad \text{on } F, \quad \mathcal{U}_1(u) = g_1 \quad \text{and} \quad \mathcal{U}_2(u) = g_2,
\]
for any \( f \in \mathcal{C}(F) \) and \( g_1, g_2 \in \mathbb{R} \). In particular, the boundary value problem is called semihomogeneous when \( g_1 = g_2 = 0 \), whereas it is called homogeneous when \( f = 0 \) and \( g_1 = g_2 = 0 \).

The following result applies Lemma 3.1 to show that we can restrict our analysis of boundary value problems on \( F \) to the case of semihomogeneous problems.

**Lemma 3.2** Given \( \mathcal{U}_1, \mathcal{U}_2 \) linearly independent boundary conditions and \( g_1, g_2 \in \mathbb{R} \), consider \( u_p \in \mathcal{C}(\bar{F}) \) such that \( \mathcal{U}_1(u_p) = g_1 \) and \( \mathcal{U}_2(u_p) = g_2 \). Then for any \( f \in \mathcal{C}(F) \), the function \( u \in \mathcal{C}(\bar{F}) \) satisfies that \( \mathcal{L}_q(u) = f \) on \( F \), \( \mathcal{U}_1(u) = g_1 \) and \( \mathcal{U}_2(u) = g_2 \) iff the function \( v = u - u_p \) satisfies that \( \mathcal{L}_q(v) = f - \mathcal{L}_q(u_p) \) on \( F \) and \( \mathcal{U}_1(v) = \mathcal{U}_2(v) = 0 \).

Clearly, the homogeneous problem has the null function as solution. We will say that the pair \( (\mathcal{U}_1, \mathcal{U}_2) \) is regular if the corresponding homogenous boundary value problem has the null function as its unique solution. Next we characterize the regularity of a pair of boundary conditions.

**Proposition 3.3** Let \( \mathcal{U}_1 \) and \( \mathcal{U}_2 \) be the linearly independent boundary conditions determined by the matrices \( A = (a_{ij}) \) and \( B = (b_{ij}) \) and consider the value
\[
W(q, A, B) = (a_{11}b_{22} - a_{21}b_{12})U_n(q) + (a_{12}b_{21} - a_{22}b_{11})U_{n-2}(q) \\
+ (a_{11}b_{21} + a_{12}b_{22} - a_{21}b_{11} - a_{22}b_{12})U_{n-1}(q) + \det A + \det B.
\]
Then, the pair \((U_1, U_2)\) is regular iff \(W(q, A, B) \neq 0\) and when this condition is satisfied, for each data \(f \in C(F)\) the boundary value problem \(L_q(u) = f\) on \(F\), \(U_1(u) = U_2(u) = 0\) has a unique solution.

**Proof.** If we consider \(u(k) = U_{k-1}(q)\) and \(v(k) = U_{k-2}(q)\), then \(z \in C(\bar{F})\) is a solution of the homogeneous value problem iff there exist \(a, b \in \mathbb{R}\) such that \(z = au + bv\) and verifying

\[
\begin{bmatrix}
U_1(u) & U_1(v) \\
U_2(u) & U_2(v)
\end{bmatrix}
\begin{bmatrix}
a \\
b
\end{bmatrix}
= \begin{bmatrix}
0 \\
0
\end{bmatrix}.
\]

Clearly, the pair \((U_1, U_2)\) is regular iff \(U_1(u)U_2(v) - U_1(v)U_2(u) \neq 0\). Keeping in mind that

\[
\begin{bmatrix}
U_1(u) & U_1(v) \\
U_2(u) & U_2(v)
\end{bmatrix}
\begin{bmatrix}
a_{11} & a_{12} & b_{11} & b_{12} \\
a_{21} & a_{22} & b_{21} & b_{22}
\end{bmatrix}
\begin{bmatrix}
0 & -1 \\
1 & 0 \\
U_{n-1}(q) & U_{n-2}(q) \\
U_n(q) & U_{n-1}(q)
\end{bmatrix}
= \begin{bmatrix}
0 \\
0 \\
0 \\
0
\end{bmatrix}.
\]

the application of the Binet-Cauchy formula conclude that

\[
U_1(u)U_2(v) - U_1(v)U_2(u) = \det A + \left(U_{n-1}(q)^2 - U_n(q)U_{n-2}(q)\right)\det B
\]

\[
+ (a_{11}b_{21} - a_{21}b_{11})U_{n-1}(q) + (a_{12}b_{21} - a_{22}b_{11})U_n(q)
\]

\[
+ (a_{12}b_{21} - a_{21}b_{12})U_{n-2}(q)
\]

\[
+ (a_{12}b_{22} - a_{22}b_{12})U_{n-1}(q) = W(q, A, B),
\]

since \(U_{n-1}^2(q) - U_n(q)U_{n-2}(q) = w[u, v](n) = 1\). Therefore, the pair \((U_1, U_2)\) is regular iff \(W(q, A, B) \neq 0\).

On the other hand, given \(f \in C(F)\) consider \(u_p \in C(\bar{F})\) such that \(L_q(u_p) = f\) on \(F\). Hence, \(z = au + bv + u_p\) where \(a, b \in \mathbb{R}\) is a solution of the semi-homogeneous boundary value problem iff

\[
\begin{bmatrix}
U_1(u) & U_1(v) \\
U_2(u) & U_2(v)
\end{bmatrix}
\begin{bmatrix}
a \\
b
\end{bmatrix}
= \begin{bmatrix}
U_1(u_p) \\
U_2(u_p)
\end{bmatrix}.
\]
When the pair is regular, the determinant of the coefficient matrix of the above system is non null which implies that the system has a unique solution. □

4 The Green function for a regular two-point boundary value problem on a path

The aim of this section is to tackle the resolution, in a closed form, of the semihomogeneous boundary value problems. Moreover, since we are considering problems that involve the Schrödinger operator $L_q$ we can express all formulae in terms of Chebyshev polynomials.

If we suppose that the pair $(U_1, U_2)$ is regular, according with Proposition 3.3, for any $f \in \mathcal{C}(F)$ the boundary value problem $L_q(u) = f$ on $F$ and $U_1(u) = U_2(u) = 0$ has a unique solution. In these conditions we will call Green function for the semihomogeneous boundary value problem $L_q(u) = f$ on $F$, $U_1(u) = U_2(u) = 0$ the function $G_q \in \mathcal{C}(\bar{F} \times F)$ characterized by verifying for any $s \in F$

\[(7) \quad L_q(G_q(\cdot, s)) = \varepsilon_s \quad \text{on} \quad F, \quad U_1(G_q(\cdot, s)) = U_2(G_q(\cdot, s)) = 0.\]

Therefore, applying Proposition 2.1, we obtain that

\[G_q(k, s) = z(k) + K_q(k, s), \quad \text{for any} \quad k \in \bar{F},\]

where $z$ satisfies that $L_q(z) = 0$ on $F$, and

\[K_q(k, s) = -\sum_{r=1}^{k} U_{k-r-1}(q) \varepsilon_s(r) = \begin{cases} 0, & \text{if} \quad 0 \leq k \leq s \leq n, \\ -U_{k-s-1}(q), & \text{if} \quad 1 \leq s \leq k \leq n+1. \end{cases}\]

**Proposition 4.1** Let $U_1$ and $U_2$ be the linearly independent boundary conditions determined by $A, B \in \mathcal{M}_2(\mathbb{R})$ and consider $u, v \in \mathcal{C}(\bar{F})$ defined for any $k \in \bar{F}$ as

\[u(k) = a_{11} U_{k-1}(q) + a_{12} U_{k-2}(q) - b_{11} U_{n-k-1}(q) - b_{12} U_{n-k}(q),\]
\[v(k) = a_{21} U_{k-1}(q) + a_{22} U_{k-2}(q) - b_{21} U_{n-k-1}(q) - b_{22} U_{n-k}(q).\]

If $W(q, A, B) \neq 0$, the Green function for the boundary value problem $L_q(z) = f$ on $F$ and $U_1(z) = U_2(z) = 0$ is given by the identity
\[ G_q(k, s) = \frac{u(k)}{W(q, A, B)} \left[ a_{21} U_{s-1}(q) + a_{22} U_{s-2}(q) \right] - \frac{v(k)}{W(q, A, B)} \left[ b_{11} U_{n-s-1}(q) + b_{12} U_{n-s}(q) \right] - \frac{1}{W(q, A, B)} \left\{ \begin{array}{l} u(k)v(s), \quad 0 \leq k \leq s \leq n, \\
 v(k)u(s), \quad 1 \leq s \leq k \leq n + 1. \end{array} \right\} \]

**Proof.** If we take \( u_1(k) = U_{k-1}(q) \) and \( v_1(k) = U_{k-2}(q) \), \( k \in \bar{F} \), then we know that \( w[u_1, v_1] = 1 \). On the other hand, if we consider the functions defined as \( u = U_1(u_1)v_1 - U_1(v_1)u_1 \) and \( v = U_2(u_1)v_1 - U_2(v_1)u_1 \), then \( \mathcal{U}_1(u) = \mathcal{U}_2(v) = 0 \), \( -\mathcal{U}_1(v) = \mathcal{U}_2(u) = \mathcal{U}_1(u_1)\mathcal{U}_2(v_1) - \mathcal{U}_2(u_1)\mathcal{U}_1(v_1) \) and moreover, \( w[u, v] = W(q, A, B) \).

In addition, \( \mathcal{U}_1(u_1) = a_{12} + b_{11} U_{n-1}(q) + b_{12} U_{n}(q) \), \( \mathcal{U}_2(u_1) = a_{22} + b_{21} U_{n-1}(q) + b_{22} U_{n}(q) \), whereas \( \mathcal{U}_1(v_1) = -a_{11} + b_{11} U_{n-2}(q) + b_{12} U_{n-1}(q) \), \( \mathcal{U}_2(v_1) = -a_{21} + b_{21} U_{n-2}(q) + b_{22} U_{n-1}(q) \). Therefore,

\[
\begin{align*}
u(k) &= (a_{12} + b_{11} U_{n-1}(q) + b_{12} U_{n}(q)) U_{k-2}(q) \\
&\quad + (a_{11} - b_{11} U_{n-2}(q) - b_{12} U_{n-1}(q)) U_{k-1}(q) \\
&= a_{11} U_{k-1}(q) + a_{12} U_{n-2}(q) + b_{11} (U_{n-1}(q) U_{k-2}(q) - U_{n-2}(q) U_{k-1}(q)) \\
&\quad + b_{12} (U_{n}(q) U_{k-2}(q) - U_{n-1}(q) U_{k-1}(q)).
\end{align*}
\]

Applying Proposition 2.1 we get that

\[ -U_{k-s-1}(q) = U_{s-2}(q) U_{k-1}(q) - U_{s-1}(q) U_{k-2}(q) \]

and hence \( u(k) = a_{11} U_{k-1}(q) + a_{12} U_{n-2}(q) - b_{11} U_{n-k-1}(q) - b_{12} U_{n-k}(q) \). The same arguments show that \( v(k) = a_{21} U_{k-1}(q) + a_{22} U_{k-2}(q) - b_{21} U_{n-k-1}(q) - b_{22} U_{n-k}(q) \).

On the other hand, as \( w[u, v] = W(q, A, B) \neq 0 \), then \( \{u, v\} \) are linearly independent. Therefore, there exist \( a, b \in \mathcal{C}(F) \) such that \( G_q(k, s) = a(s) u(k) + b(s) v(k) + K_q(k, s) \) for any \( k \in \bar{F} \) and any \( s \in F \). Moreover functions \( a \) and \( b \) are given by the following equalities

\[
\begin{align*}
b(s) &= -\frac{\mathcal{U}_1(K_q(v, s))}{\mathcal{U}_1(v)} = -\frac{1}{W(q, A, B)} \left[ b_{11} U_{n-s-1}(q) + b_{12} U_{n-s}(q) \right] \\
&= \frac{-1}{W(q, A, B)} \left[ b_{11} U_{n-s-1}(q) + b_{12} U_{n-s}(q) \right] \\
a(s) &= -\frac{\mathcal{U}_2(K_q(v, s))}{\mathcal{U}_2(u)} = \frac{1}{W(q, A, B)} \left[ b_{21} U_{n-s-1}(q) + b_{22} U_{n-s}(q) \right] \\
&= \frac{1}{W(q, A, B)} \left[ a_{21} U_{n-s-1}(q) + a_{22} U_{n-s}(q) \right] - \frac{v(s)}{W(q, A, B)}.
\end{align*}
\]

The proof finishes observing that as \( \{u, v\} \) is a basis of the homogeneous
Scrödinger equation, then
\[ -U_{k-s-1}(q) = \frac{1}{w[u, v]} \left( v(s)u(k) - v(k)u(s) \right). \]

The boundary value problem
\[ L_q(u) = f \quad \text{on } F \quad au(0) + bu(1) = cu(n) + du(n + 1) = 0, \]
where \((a^2 + b^2)(c^2 + d^2) > 0\) is called Sturm-Liouville problem. Observe that these boundary conditions are determined by
\[ A = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix}. \]

**Corollary 4.2** The Sturm-Liouville problem is regular iff
\[ adU_n(q) + (ac + bd)U_{n-1}(q) + bcU_{n-2}(q) \neq 0 \]
in which case the Green function is given by
\[ G_q(k, s) = \begin{cases} \frac{(aU_{k-1}(q) + bU_{k-2}(q))(cU_{n-s-1}(q) + dU_{n-s}(q))}{adU_n(q) + (ac + bd)U_{n-1}(q) + bcU_{n-2}(q)}, & 0 \leq k \leq s \leq n, \\ \frac{(aU_{s-1}(q) + bU_{s-2}(q))(cU_{n-k-1}(q) + dU_{n-k}(q))}{adU_n(q) + (ac + bd)U_{n-1}(q) + bcU_{n-2}(q)}, & 1 \leq s \leq k \leq n + 1. \end{cases} \]

**References**


