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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 functions, it suffices to know previously a basis of solutions of the corresponding 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 consequence 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 verifying $U_0(x) = 1$, $U_1(x) = 2x$ and the recurrence law

$$U_{n+2}(x) = 2\,xU_{n+1}(x) - U_n(x), \quad \text{for each } \; n \in \mathbb{Z}. \tag{1}$$

It is easy to prove that: $U_{-n} = -U_{n-2}$ 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, $\mathcal{P}_n$. Moreover, we can suppose without loss of generality that the set of vertices of $\mathcal{P}_n$ is $\{0, \dots, n+1\} \subset \mathbb{N}$. Along the paper F will denote the vertex subset $F = \{1, \dots, n\}$. Therefore, the *boundary of* F is $\delta(F) = \{0, n+1\}$ and the *closure of* F is $\bar{F} = \{0, \dots, n+1\}$, the vertex set of $\mathcal{P}_n$.

For any $s \in \bar{F}$, ε_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 $u \colon \bar{F} \longrightarrow \mathbb{R}$ that vanish on $\bar{F} \setminus Q$. For each $q \in \mathbb{R}$, the linear operator $\mathcal{L}_q \colon \mathcal{C}(\bar{F}) \longrightarrow \mathcal{C}(F)$ defined for each $u \in \mathcal{C}(\bar{F})$ as

$$\mathcal{L}_q(u)(k) = 2qu(k) - u(k+1) - u(k-1), \qquad k \in F, \tag{2}$$

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 $u, v \in \mathcal{C}(\bar{F})$ the *wronskian of* u *and* v, $w[u, v] \in \mathcal{C}(\bar{F})$ is defined as,

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

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 *casoratian of* u *and* v, see for instance [1].

We will call *Green function of the Schrödinger equation* the function $g_p \in \mathcal{C}(\bar{F} \times \bar{F})$ 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 $s = 0, \dots, n$ 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* $u, v \in \mathcal{C}(\bar{F})$ *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 $f \in \mathcal{C}(F)$ *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 *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 *(linear) boundary condition on* F *with coefficients* a, b, c *and* d the linear map $\mathcal{U}: \mathcal{C}(\bar{F}) \longrightarrow \mathbb{R}$ determined by the expression

(4) $$\mathcal{U}(u) = au(0) + bu(1) + cu(n) + du(n+1), \quad \text{for any } u \in \mathcal{C}(\bar{F}).$$

Let $\mathcal{U}_1, \mathcal{U}_2 : \mathcal{C}(\bar{F}) \longrightarrow \mathbb{R}$ 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

$$(5) \qquad \begin{bmatrix} \mathcal{U}_1(u) \\ \mathcal{U}_2(u) \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \begin{bmatrix} u(0) \\ u(1) \end{bmatrix} + \begin{bmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{bmatrix} \begin{bmatrix} u(n) \\ u(n+1) \end{bmatrix}.$$

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 $\boldsymbol{\mathcal{U}} : \mathcal{C}(\bar{F}) \longrightarrow \mathbb{R}^2$ whose components are $\mathcal{U}_1$ and $\mathcal{U}_2$ is surjective or equivalently, iff* $\operatorname{rg}[A, B] = 2$.

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

$$(6) \qquad \mathcal{L}_q(u) = f, \ \text{ on } \ F, \quad \mathcal{U}_1(u) = g_1 \ \text{ and } \ \mathcal{U}_2(u) = g_2,$$

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 $f \in \mathcal{C}(\bar{F})$, 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*

$$\begin{aligned} W(q, A, B) = {} & (a_{11}b_{22} - a_{21}b_{12})U_n(q) + (a_{12}b_{21} - a_{22}b_{11})U_{n-2}(q) \\ & + (a_{11}b_{21} + a_{12}b_{22} - a_{21}b_{11} - a_{22}b_{12})U_{n-1}(q) + \det A + \det B. \end{aligned}$$

Then, the pair $(\mathcal{U}_1, \mathcal{U}_2)$ *is regular iff* $W(q, A, B) \neq 0$ *and when this condition is satisfied, for each data* $f \in \mathcal{C}(F)$ *the boundary vale problem* $\mathcal{L}_q(u) = f$ *on* F*,* $\mathcal{U}_1(u) = \mathcal{U}_2(u) = 0$ *has a unique solution.*

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

$$\begin{bmatrix} \mathcal{U}_1(u) & \mathcal{U}_1(v) \\ \mathcal{U}_2(u) & \mathcal{U}_2(v) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Clearly, the pair $(\mathcal{U}_1, \mathcal{U}_2)$ is regular iff $\mathcal{U}_1(u)\mathcal{U}_2(v) - \mathcal{U}_1(v)\mathcal{U}_2(u) \neq 0$. Keeping in mind that

$$\begin{bmatrix} \mathcal{U}_1(u) & \mathcal{U}_1(v) \\ \mathcal{U}_2(u) & \mathcal{U}_2(v) \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & b_{11} & b_{12} \\ a_{21} & a_{22} & b_{21} & b_{22} \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \\ U_{n-1}(q) & U_{n-2}(q) \\ U_n(q) & U_{n-1}(q) \end{bmatrix},$$

the application of the *Binet-Cauchy formula* conclude that

$$\begin{aligned} \mathcal{U}_1(u)\mathcal{U}_2(v) - \mathcal{U}_1(v)\mathcal{U}_2(u) &= \det A + \Big(U_{n-1}(q)^2 - U_n(q)U_{n-2}(q)\Big)\det B \\ &+ (a_{11}b_{21} - a_{21}b_{11})U_{n-1}(q) + (a_{11}b_{22} - a_{21}b_{12})U_n(q) \\ &+ (a_{12}b_{21} - a_{22}b_{11})U_{n-2}(q) \\ &+ (a_{12}b_{22} - a_{22}b_{12})U_{n-1}(q) = W(q, A, B), \end{aligned}$$

since $U_{n-1}^2(q) - U_n(q)U_{n-2}(q) = w[u, v](n) = 1$. Therefore, the pair $(\mathcal{U}_1, \mathcal{U}_2)$ is regular iff $W(q, A, B) \neq 0$.

On the other hand, given $f \in \mathcal{C}(F)$ consider $u_p \in \mathcal{C}(\bar{F})$ such that $\mathcal{L}_q(u_p) = f$ on F. Hence, $z = a\,u + b\,v + u_p$ where $a, b \in \mathbb{R}$ is a solution of the semihomogeneous boundary value problem iff

$$\begin{bmatrix} \mathcal{U}_1(u) & \mathcal{U}_1(v) \\ \mathcal{U}_2(u) & \mathcal{U}_2(v) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = - \begin{bmatrix} \mathcal{U}_1(u_p) \\ \mathcal{U}_2(u_p) \end{bmatrix}.$$

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 $\mathcal{L}_q$ we can express all formulae in terms of Chebyshev polynomials.

If we suppose that the pair $(\mathcal{U}_1, \mathcal{U}_2)$ is regular, according with Proposition 3.3, for any $f \in \mathcal{C}(F)$ the boundary value problem $\mathcal{L}_q(u) = f$ on F and $\mathcal{U}_1(u) = \mathcal{U}_2(u) = 0$ has a unique solution. In these conditions we will call *Green function for the semihomogenoeus boundary value problem* $\mathcal{L}_q(u) = f$ *on* F, $\mathcal{U}_1(u) = \mathcal{U}_2(u) = 0$ the function $G_q \in \mathcal{C}(\bar{F} \times F)$ characterized by verifying for any $s \in F$

$$\mathcal{L}_q(G_q(\cdot, s)) = \varepsilon_s \text{ on } F, \quad \mathcal{U}_1(G_q(\cdot, s)) = \mathcal{U}_2(G_q(\cdot, s)) = 0. \tag{7}$$

Therefore, applying Proposition 2.1, we obtain that

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

where z satisfies that $\mathcal{L}_q(z) = 0$ on F, and

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

Proposition 4.1 *Let* $\mathcal{U}_1$ *and* $\mathcal{U}_2$ *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* $\mathcal{L}_q(z) = f$ *on* F *and* $\mathcal{U}_1(z) = \mathcal{U}_2(z) = 0$ *is given by the identity*

$$
\begin{aligned}
G_q(k,s) = {} & \frac{u(k)}{W(q,A,B)}\Big[a_{21}U_{s-1}(q) + a_{22}U_{s-2}(q)\Big] \\
& - \frac{v(k)}{W(q,A,B)}\Big[b_{11}U_{n-s-1}(q) + b_{12}U_{n-s}(q)\Big] \\
& - \frac{1}{W(q,A,B)}\begin{cases} u(k)v(s), \; 0 \le k \le s \le n, \\ v(k)u(s), \; 1 \le s \le k \le n+1. \end{cases}
\end{aligned}
$$

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 $u = \mathcal{U}_1(u_1)v_1 - \mathcal{U}_1(v_1)u_1$ and $v = \mathcal{U}_2(u_1)v_1 - \mathcal{U}_2(v_1)u_1$, 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,

$$
\begin{aligned}
u(k) = {} & (a_{12} + b_{11}U_{n-1}(q) + b_{12}U_n(q))U_{k-2}(q) \\
& + (a_{11} - b_{11}U_{n-2}(q) - b_{12}U_{n-1}(q))U_{k-1}(q) \\
& = a_{11}U_{k-1}(q) + a_{12}U_{n-2}(q) + b_{11}(U_{n-1}(q)U_{k-2}(q) - U_{n-2}(q)U_{k-1}(q)) \\
& + b_{12}(U_n(q)U_{k-2}(q) - U_{n-1}(q)U_{k-1}(q)).
\end{aligned}
$$

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

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

The proof finishes observing that as $\{u,v\}$ is a basis of the homogeneous

Scrödinger equation, then $-U_{k-s-1}(q) = \dfrac{1}{w[u,v]}\Big(v(s)u(k) - v(k)u(s)\Big)$. ∎

The boundary value problem

(8) $$\mathcal{L}_q(u) = f \ \text{ on } F \quad au(0) + bu(1) = cu(n) + du(n+1) = 0,$$

where $(a^2+b^2)(c^2+d^2) > 0$ is called *Sturm-Liouville problem.* Observe that these boundary conditions are determined by $A = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix}$ and $B = \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix}$.

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

$$G_q(k,s) = \begin{cases} \dfrac{\Big(aU_{k-1}(q) + bU_{k-2}(q)\Big)\Big(cU_{n-s-1}(q) + dU_{n-s}(q)\Big)}{adU_n(q) + (ac+bd)U_{n-1}(q) + bcU_{n-2}(q)}, & 0 \le k \le s \le n, \\ \dfrac{\Big(aU_{s-1}(q) + bU_{s-2}(q)\Big)\Big(cU_{n-k-1}(q) + dU_{n-k}(q)\Big)}{adU_n(q) + (ac+bd)U_{n-1}(q) + bcU_{n-2}(q)}, & 1 \le s \le k \le n+1. \end{cases}$$

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