Regular Boundary Value Problems on a Path throughout Chebyshev Polynomials

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Abstract

In this work we study the different types 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 addition, we study the periodic boundary value problem that corresponds to the Poisson equation in a cycle. In any case, the Green functions are given in terms of Chebyshev polynomials since they verify a recurrence law similar to the one verified by the Schödinger operator on a path.

Key words: 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 second order difference equations with constant coefficients associated with the Schrödinger operator on a finite path. Our study runs in parallel to 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.

The boundary value problems here considered are of three types that correspond to the cases in which the boundary has two, one or no vertices. In any

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case it is essential to describe the solutions of the Schröndinger equation on the interior nodes of the path. In this particular situation, it is possible to obtain explicitly such solutions in terms of second kind Chebyshev 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 in terms of Chebyshev polynomials.

In the literature the most studied boundary value problems are those known as Sturm-Liouville boundary value problems, that we obtain here as a particular case, since in this work we analyze general boundary conditions. A survey on Sturm-Liouville boundary value problems can be found in (4), see also (1). In addition, when the boundary conditions are of Dirichlet type the expression of the Green function for the Schrödinger operator was already obtained in (2; 3), using techniques different to the ones we will use here. We also treat with the Poisson equation on a cycle and we show that this problem can be seen as a two-point boundary value problem on a path by introducing the so-called periodic boundary conditions.

To end this section, we will describe some basic properties of the so-called *Chebyshev Polynomials*, that will be useful in this work. For all the results given here we refer to the reader to (5).

A sequence of complex polynomials $\{Q_n\}_{n=-\infty}^{+\infty}$ is called *Chebyshev sequence* if it verifies the recurrence law

$$Q_{n+2}(z) = 2zQ_{n+1}(z) - Q_n(z), \quad \text{for each } n \in \mathbb{Z}. \tag{1}$$

The recurrence law (1) shows that any Chebyshev sequence is univocally determined by the choice of the corresponding zero and one order Chebyshev polynomials. In particular, the sequences $\{T_n\}_{n=-\infty}^{+\infty}$, $\{U_n\}_{n=-\infty}^{+\infty}$ and $\{V_n\}_{n=-\infty}^{+\infty}$ of *first, second and third kind Chebyshev polynomials* are obtained when we choose $T_0(z) = U_0(z) = V_0(z) = 1$, $T_1(z) = z$, $U_1(z) = 2z$ and $V_1(z) = 2z - 1$.

The different kinds of Chebyshev polynomials are closely related. The next results show the properties and relations that we will use along the paper, see (5). Moreover, these relationships display the relevance of the second kind Chebyshev polynomials.

Lemma 1.1 *It is verified that* $T_{n+1}(z) = zU_n(z) - U_{n-1}(z)$, $U_{-n}(z) = -U_{n-2}(z)$ *and* $V_n(z) = U_n(z) - U_{n-1}(z)$, $n \in \mathbb{Z}$. *In particular,* $U_{-1} = 0$.

Lemma 1.2 *For each* $n \in \mathbb{N}^*$ *the roots of the* n*-order Chebyshev polynomial of second kind are real, simple and belong to the interval* $(-1, 1)$ *and are given by* $u_{n,k} = \cos\left(\frac{k\pi}{n+1}\right)$, $k = 1, \ldots, n$. *In addition,* $T_{n+1}(z) = 1$ *iff either* $z = 1$ *or* $z = u_{n,2k}$, $k = 1, \ldots, \lceil \frac{n}{2} \rceil$.

2 The Schrödinger equation on a path

Our purpose 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 $H \subset \bar{F}$, we will denote by $\mathcal{C}(H)$ the vector space of functions $u\colon \bar{F} \longrightarrow \mathbb{C}$ that vanish on $\bar{F} \setminus H$.

For each $q \in \mathbb{C}$, the operator $\mathcal{L}_q\colon \mathcal{C}(\bar{F}) \longrightarrow \mathcal{C}(\bar{F})$ defined for each $u \in \mathcal{C}(\bar{F})$ as

$$\begin{aligned}
\mathcal{L}_q(u)(0) &= (2q-1)u(0) - u(1)\\
\mathcal{L}_q(u)(k) &= 2qu(k) - u(k+1) - u(k-1), \qquad k \in F, \\
\mathcal{L}_q(u)(n+1) &= (2q-1)u(n+1) - u(n),
\end{aligned} \tag{2}$$

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 combinatorial Laplacian of $\mathcal{P}_n$.

For each $f \in \mathcal{C}(F)$, we will call *Schrödinger equation on F 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 on F*.

If $u, v \in \mathcal{C}(\bar{F})$ the *wronskian of u and v*, denoted by $w[u,v] \in \mathcal{C}(\bar{F})$, see (4), is defined as,

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

and $w[u,v](n+1) = w[u,v](n)$. Note that in some works function $w[u,v]$ is called *casoratian of u and v*, see for instance (1).

We 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 Schödinger equation on a path of some well-known facts in the context of difference equations and they will be useful throughout the paper, see (1).

Proposition 2.1 *If $u,v\in\mathcal{C}(\bar F)$ are solutions of the homogeneous Schrödinger equation on F then $w[u,v]$ is constant. Moreover u and v are linearly independent iff $w[u,v]\neq 0$ and then,*

$$g_q(k,s)=\frac{1}{w[u,v]}\Big[v(s)\,u(k)-u(s)\,v(k)\Big],\qquad k,s\in\bar F$$

and for any $x_0,x_1\in\mathbb{C}$ and $f\in\mathcal{C}(F)$ the function

$$x(k)=\frac{1}{w[u,v]}\Big[\Big(x_0v(1)-x_1v(0)\Big)u(k)-\Big(x_0u(1)-x_1u(0)\Big)v(k)\Big]+\sum_{s=0}^{k}g_q(k,s)f(s),$$

is the unique solution of the Schrödinger equation on F with data f verifying that $x(0)=x_0$ and $x(1)=x_1$.

The above proposition is true for any second order difference equation on F. Now, the special characteristics of the Schrödinger equation we have raised here allow us to describe its solutions in terms of Chebyshev polynomials. First, observe that Identity (1) implies that if $\{Q_k\}_{k=-\infty}^{\infty}$ is a Chebyshev sequence, then for any $m\in\mathbb{Z}$ the function $u\in\mathcal{C}(\bar F)$ defined as $u(k)=Q_{k-m}(q)$ for $k\in\bar F$ is a solution of the homogeneous Schrödinger equation on F. The following result shows the importance of the second kind Chebyshev polynomials.

Proposition 2.2 *Consider the functions $u,v\in\mathcal{C}(\bar F)$ given by $u(k)=U_{k-1}(q)$ and $v(k)=U_{k-2}(q)$, $k\in\bar F$. Then, $w[u,v]=1$ and for any $x_0,x_1\in\mathbb{C}$ the function*

$$x(k)=x_1U_{k-1}(q)-x_0U_{k-2}(q),\qquad k\in\bar F,$$

is the unique solution of the homogeneous Schrödinger equation on F verifying that $x(0)=x_0$ and $x(1)=x_1$. In addition the Green function of the Schrödinger equation on F is given by

$$g_q(k,s)=-U_{k-s-1}(q),\qquad k,s\in\bar F.$$

Proof. Of course, u and v are solutions of the homogeneous Schrödinger equation and hence

$$w[u,v]=w[u,v](0)=-U_0(q)U_{-2}(q)=U_0(q)^2=1.$$

In conclusion, $\{u,v\}$ is a basis of solutions of the homogeneous Schrödinger equation and for any $x_0,x_1\in\mathbb{C}$, $x(k)=x_1U_{k-1}(q)-x_0U_{k-2}(q)$ is the unique solution of the homogeneous Schrödinger equation such that $x(0)=x_0$ and $x(1)=x_1$. In particular, $-U_{k-1}(q)$ is precisely the unique solution of the homogeneous Schrödinger equation such that $x(0)=0$ and $x(1)=-1$. Therefore, for each $s\in\bar F$, the unique solution of the homogeneous Schrödinger equation such that $x(s)=0$ and $x(s)=-1$ is given by $-U_{k-s-1}(q)$, so $g_q(k,s)=-U_{k-s-1}(q)$ for any $k,s\in\bar F$. ∎

From the above proposition and taking into account the expression for the Green function given in Proposition 2.1 in terms of a basis, we can deduce the following identity

$$U_{k-s-1}(q)=U_{s-1}(q)U_{k-2}(q)-U_{k-1}(q)U_{s-2}(q),\qquad k,s\in\bar F. \tag{4}$$

3 Two-point boundary value problems

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*. 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.

Given $a,b,c,d\in\mathbb{C}$ non simultaneously null, we will call *(linear) boundary condition on F with coefficients a,b,c and d* the linear map $\mathcal{U}\colon\mathcal{C}(\bar F)\longrightarrow\mathbb{C}$ determined by the expression

$$\mathcal{U}(u)=au(0)+bu(1)+cu(n)+du(n+1),\qquad \text{for any } u\in\mathcal{C}(\bar F). \tag{5}$$

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

$$\begin{bmatrix}\mathcal{U}_1(u)\\ \mathcal{U}_2(u)\end{bmatrix}=\begin{bmatrix}a_{11}&a_{12}\\ a_{21}&a_{22}\end{bmatrix}\begin{bmatrix}u(0)\\ u(1)\end{bmatrix}+\begin{bmatrix}b_{11}&b_{12}\\ b_{21}&b_{22}\end{bmatrix}\begin{bmatrix}u(n)\\ u(n+1)\end{bmatrix}. \tag{6}$$

As we want to assure that the boundary conditions are linearly independent and that the vertices 0 and $n+1$ are always involved, we need to impose that $a_{11}b_{22}\neq a_{21}b_{12}$. Then, it is easy to verify that there exists $a,b,c,d\in\mathbb{C}$ such that the above boundary conditions are equivalent to the following ones:

$$\mathcal{U}_1(u)=u(0)+au(1)+bu(n)\ \text{ and }\ \mathcal{U}_2(u)=cu(1)+du(n)+u(n+1). \tag{7}$$

In particular, when $b = c = 0$ the above pair of boundary conditions are called *Sturm-Liouville conditions*.

We also consider the so-called *periodic boundary conditions* on $\mathcal{P}_n$,

$$\mathcal{U}_1(u) = u(0) - u(n+1) \quad \text{and} \quad \mathcal{U}_2(u) = 2qu(0) - u(1) - u(n), \tag{8}$$

that when $q \neq 0$ are equivalent to conditions (7) for $a = b = c = d = -\frac{1}{2q}$.

The periodic boundary conditions appear associated with the so-called *Poisson equation* for the Schrödinger operator on the cycle $\mathcal{C}_n$ with $n+1$ vertices. If we suppose that the vertex set of $\mathcal{C}_n$ is $\{0, \ldots, n\}$, then

$$\begin{aligned} \mathcal{L}_q(u)(0) &= 2qu(0) - u(1) - u(n) = f(0) \\ \mathcal{L}_q(u)(k) &= 2qu(k) - u(k+1) - u(k-1) = f(k), \quad k = 1, \ldots, n-1, \\ \mathcal{L}_q(u)(n) &= 2qu(n) - u(n-1) - u(0) = f(n) \end{aligned} \tag{9}$$

where f is defined on $\{0, \ldots, n\}$. The equivalence between the two problems is carried out by duplicating vertex 0 and labeling the new vertex as $n+1$, as is shown in Figure 1.

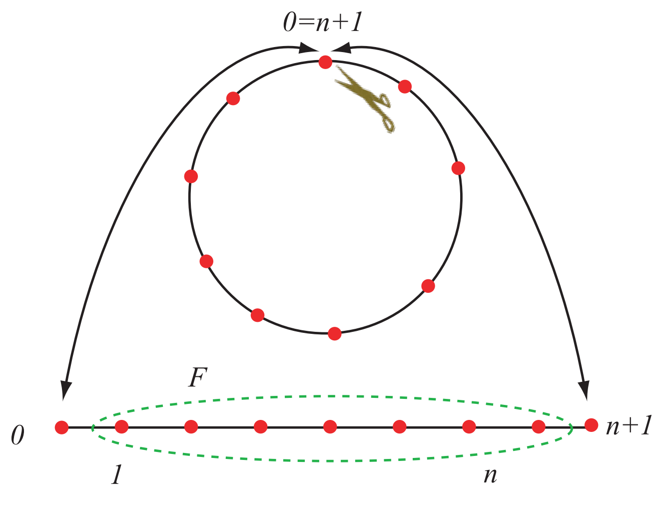

Fig. 1. Periodic boundary conditions

Then the first equation in (8) corresponds to a continuity condition, the second one is the first of (9), whereas the last equation in (9), corresponds to the equality $\mathcal{L}_q(u)(n) = f(n)$ on the path, since $u(0) = u(n+1)$.

In the sequel we will suppose that the boundary conditions (7) are fixed. Then, a *boundary value problem on* F consists in finding $u \in \mathcal{C}(\bar{F})$ such that

$$\mathcal{L}_q(u) = f, \quad \text{on} \quad F, \qquad \mathcal{U}_1(u) = g_1 \quad \text{and} \quad \mathcal{U}_2(u) = g_2, \tag{10}$$

for any $f \in \mathcal{C}(F)$ and $g_1, g_2 \in \mathbb{C}$. In particular, the problem is called *semihomogeneous* when $g_1 = g_2 = 0$, whereas it is called *homogeneous* when $f = 0$ and $g_1 = g_2 = 0$.

Clearly, the homogeneous problem has the null function as a solution. We will say that the boundary value problem (10) is *regular* if the corresponding homogenous boundary value problem has the null function as its unique solution.

The following result shows that we can restrict our analysis of two-point boundary value problems to the study of the semihomogeneous ones.

Lemma 3.1 *Given* $g_1, g_2 \in \mathbb{C}$ *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* $v = u - g_1\varepsilon_0 - g_2\varepsilon_{n+1}$ *satisfies that* $\mathcal{L}_q(v) = f + g_1\varepsilon_1 + g_2\varepsilon_n$ *on* F *and* $\mathcal{U}_1(v) = \mathcal{U}_2(v) = 0$*.*

Proposition 3.2 *Consider the* n*-order polynomial*

$$W(z) = U_n(z) + (a+d)U_{n-1}(z) + (ad - bc)U_{n-2}(z) + b + c.$$

Then the boundary value problem (10) is regular iff $W(q) \neq 0$ *and this condition is equivalent to the fact that any boundary value problem has a unique solution.*

Proof. If $\{u, v\}$ is a basis of solutions of the homogeneous Schrödinger equation, then $y \in \mathcal{C}(\bar{F})$ is a solution of the homogeneous boundary value problem iff there exists $\alpha, \beta \in \mathbb{C}$ such that $y = \alpha u + \beta v$ and it is verified that

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

Therefore, the problem is regular iff $\mathcal{U}_1(u)\mathcal{U}_2(v) - \mathcal{U}_1(v)\mathcal{U}_2(u) \neq 0$.

If we consider the basis given in Proposition 2.2, *i.e.* $u(k) = U_{k-1}(q)$ and $v(k) = U_{k-2}(q)$, then

$$\begin{bmatrix} \mathcal{U}_1(u) & \mathcal{U}_1(v) \\ \mathcal{U}_2(u) & \mathcal{U}_2(v) \end{bmatrix} = \begin{bmatrix} a + bU_{n-1}(q) & bU_{n-2}(q) - 1 \\ c + dU_{n-1}(q) + U_n & dU_{n-2}(q) + U_{n-1}(q) \end{bmatrix}.$$

Hence,

$$\mathcal{U}_1(u)\mathcal{U}_2(v)-\mathcal{U}_1(v)\mathcal{U}_2(u)=U_n(q)+(a+d)U_{n-1}(q)+(ad-bc)U_{n-2}(q)+c$$
$$+\,b\Big(U_{n-1}^2(q)-U_n(q)U_{n-2}(q)\Big)=W(q),$$

since $U_{n-1}^2(q)-U_n(q)U_{n-2}(q)=w[u,v](n)=1$.

The last claim follows by standard arguments. ∎

We aim now to tackle the resolution of any regular semihomogeneous boundary value problem by considering its resolvent kernel, that is, the Green's function associated with the problem. Moreover, since we are studying problems that involve the Schrödinger operator $\mathcal{L}_q$ on a path we can express all formulae in terms of Chebyshev polynomials.

If we suppose that the boundary value problem (10) is regular, according with the above proposition, 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 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 the following equalities

$$\mathcal{L}_q(G_q(\cdot,s))=\varepsilon_s\ \text{ on }\ F,\quad \mathcal{U}_1(G_q(\cdot,s))=\mathcal{U}_2(G_q(\cdot,s))=0,\ \ s\in F. \tag{11}$$

Therefore, given $f\in\mathcal{C}(F)$ the function $u(k)=\sum\limits_{s=1}^{n}G_q(k,s)\,f(s)$, $k\in\bar F$ is the unique solution of the semihomogeneous boundary value problem.

Fixed $s\in F$, from Propositions 2.1 and 2.2 we get that for any $k\in\bar F$,

$$G_q(k,s)=z(k)-\sum_{r=0}^{k}U_{k-r-1}(q)\varepsilon_s(r)=z(k)-\begin{cases}0, & \text{if } k\le s\\ U_{k-s-1}(q), & \text{if } k\ge s.\end{cases} \tag{12}$$

where z satisfies that $\mathcal{L}_q(z)=0$ on F. So, for any regular boundary value problem the determination of its Green function is reduced to obtain, for fixed $s\in F$, the function z. In consequence, it will be useful to assign to a given regular boundary problem an specific basis of the homogeneous Schrödinger equation.

Lemma 3.3 *The functions $u, v \in \mathcal{C}(\bar{F})$ defined for any $k \in \bar{F}$ as*

$$u(k) = U_{k-1}(q) + aU_{k-2}(q) - bU_{n-k-1}(q)$$

$$v(k) = U_{n-k}(q) + dU_{n-k-1}(q) - cU_{k-2}(q)$$

verify that $\mathcal{U}_1(u) = \mathcal{U}_2(v) = 0$ and $-w[u,v] = \mathcal{U}_1(v) = \mathcal{U}_2(u) = W(q)$.

Proof. If we take $u_1(k) = U_{k-1}(q)$ and $v_1(k) = U_{k-2}(q)$, $k \in \bar{F}$, then the functions $u(k) = \mathcal{U}_1(u_1)v_1(k) - \mathcal{U}_1(v_1)u_1(k)$ and $v(k) = \mathcal{U}_2(v_1)u_1(k) - \mathcal{U}_2(u_1)v_1(k)$, $k \in \bar{F}$, verify that $\mathcal{U}_1(u) = \mathcal{U}_2(v) = 0$ and moreover

$$-w[u,v] = \mathcal{U}_1(v) = \mathcal{U}_2(u) = \mathcal{U}_1(u_1)\mathcal{U}_2(v_1) - \mathcal{U}_2(u_1)\mathcal{U}_1(v_1) = W(q),$$

since $w[u_1, v_1] = 1$. On the other hand,

$$\begin{aligned} u(k) &= \Big(a + bU_{n-1}(q)\Big)U_{k-2}(q) + \Big(1 - bU_{n-2}(q)\Big)U_{k-1}(q) \\ &= U_{k-1}(q) + aU_{k-2}(q) - b\Big(U_{n-2}(q)U_{k-1}(q) - U_{n-1}(q)U_{k-2}(q)\Big) \\ &= U_{k-1}(q) + aU_{k-2}(q) - bU_{n-k-1}(q), \end{aligned}$$

since $U_{n-k-1}(q) = U_{n-2}(q)U_{k-1}(q) - U_{n-1}(q)U_{k-2}(q)$, from Proposition 2.2. The same arguments work for v. ∎

Theorem 3.4 *If $W(q) \neq 0$, then the Green function for the semihomogeneous boundary value problem $\mathcal{L}_q(z) = f$ on F and $\mathcal{U}_1(z) = \mathcal{U}_2(z) = 0$ is given by*

$$\begin{aligned} G_q(k,s) = & \frac{bU_{k-s-1}(q) - bcU_{n-s-1}(q)U_{k-2}(q)}{U_n(q) + (a+d)U_{n-1}(q) + (ad-bc)U_{n-2}(q) + b + c} \\ & + \frac{\Big(U_{k-1}(q) + aU_{k-2}(q)\Big)\Big(dU_{n-s-1}(q) + U_{n-s}(q)\Big)}{U_n(q) + (a+d)U_{n-1}(q) + (ad-bc)U_{n-2}(q) + b + c} \end{aligned}$$

for $1 \leq s \leq n$ and $0 \leq k \leq s$ and

$$\begin{aligned} G_q(k,s) = & \frac{cU_{s-k-1}(q) - bcU_{n-k-1}(q)U_{s-2}(q)}{U_n(q) + (a+d)U_{n-1}(q) + (ad-bc)U_{n-2}(q) + b + c} \\ & + \frac{\Big(U_{s-1}(q) + aU_{s-2}(q)\Big)\Big(dU_{n-k-1}(q) + U_{n-k}(q)\Big)}{U_n(q) + (a+d)U_{n-1}(q) + (ad-bc)U_{n-2}(q) + b + c} \end{aligned}$$

for $1 \leq s \leq n$ and $s \leq k \leq n+1$.

Proof. As $W(q) \neq 0$, Lemma 3.3 assures that the functions

$$u(k) = U_{k-1}(q) + aU_{k-2}(q) - bU_{n-k-1}(q),$$
$$v(k) = U_{n-k}(q) + dU_{n-k-1}(q) - cU_{k-2}(q)$$

are a basis of solutions of the homogeneous Schrödinger equation on F. Therefore, taking into account Identity (12), there exist $\alpha, \beta \in \mathcal{C}(F)$ such that for any $k \in \bar{F}$ and any $s \in F$

$$G_q(k,s) = \alpha(s)\, u(k) + \beta(s)\, v(k) - \begin{cases} 0, & \text{if } k \leq s \\ U_{k-s-1}(q), & \text{if } k \geq s \end{cases}$$

which implies that

$$\mathcal{U}_1(G_q(\cdot,s)) = \beta(s)W(q) - bU_{n-s-1}(q),$$
$$\mathcal{U}_2(G_q(\cdot,s)) = \alpha(s)W(q) - dU_{n-s-1}(q) - U_{n-s}(q).$$

Therefore, to verify that $\mathcal{U}_1(G_q(\cdot,s)) = \mathcal{U}_2(G_q(\cdot,s)) = 0$ for any $s \in F$, the functions α and β must satisfy the equalities

$$\beta(s) = \frac{bU_{n-s-1}(q)}{W(q)} \quad \text{and} \quad \alpha(s) = \frac{dU_{n-s-1}(q) + U_{n-s}(q)}{W(q)}$$

On the other hand, from Proposition 2.1 we know that

$$-U_{k-s-1}(q) = \frac{1}{w[u,v]}\Big(v(s)u(k) - u(s)v(k)\Big) = \frac{1}{W(q)}\Big(u(s)v(k) - v(s)u(k)\Big),$$

which implies that

$$G_q(k,s) = \begin{cases} \dfrac{\Big(dU_{n-s-1}(q) + U_{n-s}(q)\Big)u(k) + bU_{n-s-1}(q)v(k)}{W(q)}, & \text{if } k \leq s, \\[2ex] \dfrac{cU_{s-2}(q)u(k) + \Big(U_{s-1}(q) + aU_{s-2}(q)\Big)v(k)}{W(q)}, & \text{if } k \geq s. \end{cases}$$

Finally, for $0 \le k \le s \le n$ we get that

$$
\begin{aligned}
&\Big(U_{n-s}(q) + dU_{n-s-1}(q)\Big)u(k) + bU_{n-s-1}(q)v(k) \\
&= \Big(U_{k-1}(q) + aU_{k-2}(q)\Big)\Big(dU_{n-s-1}(q) + U_{n-s}(q)\Big) \\
&+ b\Big(U_{n-s-1}(q)U_{n-k}(q) - U_{n-k-1}(q)U_{n-s}(q) - cU_{n-s-1}(q)U_{k-2}(q)\Big) \\
&= \Big(U_{k-1}(q) + aU_{k-2}(q)\Big)\Big(dU_{n-s-1}(q) + U_{n-s}(q)\Big) \\
&+ b\Big(U_{k-s-1}(q) - cU_{n-s-1}(q)U_{k-2}(q)\Big),
\end{aligned}
$$

where the last equality follows from Identity (4). The case $1 \le s \le k \le n+1$ follows by similar arguments. ∎

Corollary 3.5 *The Sturm-Liouville problem is regular iff*

$$U_n(q) + (a+d)U_{n-1}(q) + adU_{n-2}(q) \neq 0$$

in which case the Green function is given by

$$
G_q(k,s) = \begin{cases} \dfrac{\Big(U_{k-1}(q) + aU_{k-2}(q)\Big)\Big(dU_{n-s-1}(q) + U_{n-s}(q)\Big)}{U_n(q) + (a+d)U_{n-1}(q) + adU_{n-2}(q)}, & 0 \le k \le s \le n, \\[2ex] \dfrac{\Big(U_{s-1}(q) + aU_{s-2}(q)\Big)\Big(dU_{n-k-1}(q) + U_{n-k}(q)\Big)}{U_n(q) + (a+d)U_{n-1}(q) + adU_{n-2}(q)}, & 1 \le s \le k \le n+1. \end{cases}
$$

The most popular Sturm-Liouville problems are the so-called Dirichlet and Neumann problems that correspond to take $a = d = 0$ and $a = d = -1$, respectively. Therefore, the Dirichlet problem is regular iff $q \neq \cos\left(\frac{k\pi}{n+1}\right)$, $k = 1, \ldots, n$ in which case the Green function is given by

$$
G_q(k,s) = \frac{1}{U_n(q)} \begin{cases} U_{k-1}(q)\, U_{n-s}(q), \text{ si } 0 \le k \le s \le n, \\[1ex] U_{s-1}(q)\, U_{n-k}(q), \text{ si } 1 \le s \le k \le n+1, \end{cases}
$$

whereas the Neumann problem is regular iff $q \neq \cos\left(\frac{k\pi}{n}\right)$, $k = 0, \ldots, n-1$ in which case the Green function is given by

$$
G_q(k,s) = \frac{1}{2(q-1)\, U_{n-1}(q)} \begin{cases} V_{k-1}(q)\, V_{n-s}(q), \text{ si } 0 \le k \le s \le n, \\[1ex] V_{s-1}(q)\, V_{n-k}(q), \text{ si } 1 \le s \le k \le n+1. \end{cases}
$$

Proposition 3.6 *The periodic boundary value problem is regular iff it is verified that* $q \neq \cos\left(\frac{2k\pi}{n+1}\right)$, $k = 0, \ldots, \lceil \frac{n+1}{2} \rceil$, *in which case the Green function is* *given by*

$$G_q(k,s) = \frac{U_{n-|k-s|}(q) + U_{|k-s|-1}(q)}{2(T_{n+1}(q)-1)}.$$

Proof. If $u(k) = U_{k-1}(q)$ and $v(k) = U_{k-2}(q)$, then using the same reasoning than in Proposition 4.2 we obtain that the periodic boundary value problem is regular iff $\mathcal{U}_1(u)\mathcal{U}_2(v) - \mathcal{U}_1(v)\mathcal{U}_2(u) \neq 0$, where $\mathcal{U}_1$ and $\mathcal{U}_2$ are the periodic boundary conditions. As $\mathcal{U}_1(u) = -U_n(q)$, $\mathcal{U}_1(v) = \mathcal{U}_2(u) = -1 - U_{n-1}(q)$ and $\mathcal{U}_2(v) = -2q - U_{n-2}(q)$, we get that

$$\mathcal{U}_1(u)\mathcal{U}_2(v) - \mathcal{U}_1(v)\mathcal{U}_2(u) = 2\Big(qU_n(q) - U_{n-1}(q) - 1\Big) = 2(T_{n+1}(q)-1).$$

When $q \neq 0$, then the periodic boundary conditions are equivalent to conditions (7) for $a = b = c = d = -\frac{1}{2q}$ and hence we can apply the result of Theorem 3.4. Firstly, $W(q) = \frac{1}{q}\left(qU_n(q) - U_{n-1}(q) - 1\right) = \frac{1}{q}\left(T_{n+1}(q) - 1\right)$. Moreover,

$$\Big(U_{k-1}(q) + aU_{k-2}(q)\Big)\Big(dU_{n-s-1}(q) + U_{n-s}(q)\Big) = \frac{1}{4q^2}\,U_k(q)U_{n+1-s}(q),$$

whereas

$$bU_{k-s-1}(q) - bcU_{n-s-1}(q)U_{k-2}(q) = \frac{-1}{4q^2}\Big(2qU_{k-s-1}(q) + U_{n-s-1}(q)U_{k-2}(q)\Big).$$

In addition,

$$\begin{aligned} U_k(q)U_{n+1-s}(q) - U_{n-s-1}(q)U_{k-2}(q) &= 2qU_{k-1}(q)U_{n+1-s}(q) - U_{k-2}U_{n+1-s}(q) \\ - U_{n-s-1}(q)U_{k-2}(q) &= 2q\Big(U_{k-1}(q)U_{n+1-s}(q) - U_{k-2}(q)U_{n-s}(q)\Big) = 2qU_{n+k-s}(q) \end{aligned}$$

which implies that $G(k,s) = \dfrac{U_{n+k-s}(q) - U_{k-s-1}(q)}{2(T_{n+1}(q)-1)}$ for $k \leq s$. The result for $s \leq k$ follows analogously.

To conclude, keeping in mind that $T_{n+1}(0) = -U_{n-1}(0)$, it is easy to prove that when $q = 0$, for any $s = 1,\ldots,n$ the function

$$G_0(k,s) = \frac{U_{n-|k-s|}(0) + U_{|k-s|-1}(0)}{2(T_{n+1}(0)-1)}$$

verifies that $G_0(0,s) - G_0(n+1,s) = G_0(1,s) + G_0(n,s) = 0$, and also that $\mathcal{L}_0(G_q(\cdot,s)) = \varepsilon_s$ on F. ∎

4 One-point boundary value problems

Our aim in this section is to analyze the boundary value problems associated with the Schrödinger operator on a subset of a finite path with exactly one vertex on its boundary. Such a subset will be denoted by $\hat{F}$ and we can suppose without loss of generality that $\hat{F} = \{0, 1, \dots, n\}$, which implies that its boundary is $\delta(\hat{F}) = \{n+1\}$. The case when $\hat{F} = \{1, \dots, n+1\}$ and hence $\delta(\hat{F}) = \{0\}$ can be carried out with obvious modifications.

In this scenario a boundary condition on $\hat{F}$ is given by

$$\mathcal{U}(u) = au(n) + bu(n+1), \quad \text{for any } u \in \mathcal{C}(\bar{F}) \tag{13}$$

where we must impose that $b \neq 0$ in order that the condition involves the vertex on the boundary. Therefore, we can assume without loss of generality that

$$\mathcal{U}(u) = au(n) + u(n+1), \quad \text{for any } u \in \mathcal{C}(\bar{F}) \text{ where } a \in \mathbb{C}. \tag{14}$$

Fixed the boundary condition $\mathcal{U}$, given in (14), a *boundary value problem problem on* $\hat{F}$ consists in finding $u \in \mathcal{C}(\bar{F})$ such that

$$\mathcal{L}_q(u) = f, \text{ on } \hat{F}, \quad \mathcal{U}(u) = g, \tag{15}$$

for any $f \in \mathcal{C}(\hat{F})$ and $g \in \mathbb{C}$. In particular, the boundary value problem is called *semihomogeneous* when $g = 0$, whereas it is called *homogeneous* when $f = 0$ and $g = 0$.

We will say that the boundary value problem (15) is *regular* if the corresponding homogenous boundary value problem $\mathcal{L}_q(u) = 0$ on $\hat{F}$ and $\mathcal{U}(u) = 0$ has the null function as its unique solution.

Analogously to the two-point boundary value problems, we can reduce the study of boundary value problems on $\hat{F}$ to the study of the semihomogeneous ones.

Lemma 4.1 *Given $g \in \mathbb{C}$, then for any $f \in \mathcal{C}(\hat{F})$ the function $u \in \mathcal{C}(\bar{F})$ satisfies that $\mathcal{L}_q(u) = f$ on $\hat{F}$ and $\mathcal{U}(u) = g$ iff $v = u - g\varepsilon_{n+1}$ satisfies that $\mathcal{L}_q(v) = f + g\varepsilon_n$ on $\hat{F}$ and $\mathcal{U}(v) = 0$.*

Proposition 4.2 *Let the $(n+1)$-order polynomial $\hat{W}(z) = V_{n+1}(z) + aV_n(z)$. Then the boundary value problem (15) is regular iff $\hat{W}(q) \neq 0$ and this condition is equivalent to the fact that any boundary value problem has a unique solution.*

Proof. If $y \in \mathcal{C}(\bar{F})$ is a solution of the homogeneous boundary value problem, then y is a solution of the homogeneous Schrödinger equation on F. Therefore, there exist $\alpha, \beta \in \mathbb{C}$ such that $y(k) = \alpha U_{k-1}(q) + \beta U_{k-2}(q)$ for any $k \in \bar{F}$. Moreover, as $\mathcal{L}_q(y)(0) = \mathcal{U}(y) = 0$, α and β must verify

$$\begin{bmatrix} -1 & 1-2q \\ U_n(q) + aU_{n-1}(q) & U_{n-1}(q) + aU_{n-2}(q) \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Therefore, the problem is regular iff

$$\begin{aligned} 0 &\neq (2q-1)U_n(q) + \Big[a(2q-1) - 1\Big]U_{n-1}(q) - aU_{n-2}(q) \\ &= U_{n+1}(q) + U_{n-1}(q) - U_n(q) + aU_n(q) + aU_{n-2}(q) \\ &- (1+a)U_{n-1}(q) - aU_{n-2}(q) = \hat{W}(q). \end{aligned}$$

Newly, the last claim follows by standard arguments. ∎

When the problem is regular we define the *Green function for the boundary value problem* $\mathcal{L}_q(u) = f$ *on* $\hat{F}$, $\mathcal{U}(u) = 0$ as the function $G_q \in \mathcal{C}(\bar{F} \times \hat{F})$ characterized by

$$\mathcal{L}_q(G_q(\cdot, s)) = \varepsilon_s \;\text{ on } \hat{F}, \quad \mathcal{U}(G_q(\cdot, s)) = 0, \quad \text{for any } s \in \hat{F}. \tag{16}$$

We can derive expressions for the Green function in terms of Chebyshev polynomials.

Proposition 4.3 *If* $\hat{W}(q) \neq 0$, *the Green function for the semihomogeneous boundary value problem* $\mathcal{L}_q(u) = f$ *on* $\hat{F}$, $\mathcal{U}(u) = 0$ *is given by*

$$G_q(k,s) = \begin{cases} \dfrac{V_k(q)\Big(aU_{n-s-1}(q) + U_{n-s}(q)\Big)}{V_{n+1}(q) + aV_n(q)}, & \text{if } 0 \le k \le s \le n, \\[2ex] \dfrac{\Big(aU_{n-k-1}(q) + U_{n-k}(q)\Big)V_s(q)}{V_{n+1}(q) + aV_n(q)}, & \text{if } 0 \le s \le k \le n+1. \end{cases}$$

Proof. For each $s \in \hat{F}$, $G_q(\cdot, s)$ is, in particular, a solution of a Schrödinger equation on F and hence there exist $\alpha, \beta \in \mathcal{C}(\hat{F})$ such that for any $k \in \bar{F}$ and any $s \in F$

$$G_q(k,s) = \alpha(s)U_{k-1}(q) + \beta(s)U_{k-2}(q) - \begin{cases} 0, & \text{if } k \le s \\ U_{k-s-1}(q), & \text{if } k \ge s \end{cases}$$

whereas for any $k \in \bar{F}$, $G_q(k,0) = \alpha(0)U_{k-1}(q) + \beta(0)U_{k-2}(q)$.

On the other hand, for any $s \in F$, we get that

$$\begin{aligned} \mathcal{L}_q(G_q(\cdot,s))(0) &= \beta(s)(1-2q) - \alpha(s) \\ \mathcal{U}(G_q(\cdot,s)) &= \alpha(s)\Big(U_n(q) + aU_{n-1}(q)\Big) + \beta(s)\Big(U_{n-1}(q) + aU_{n-2}(q)\Big) \\ &\quad - \Big(U_{n-s}(q) + aU_{n-s-1}(q)\Big). \end{aligned}$$

Therefore, to verify that $\mathcal{L}_q(G_q(\cdot,s))(0) = \mathcal{U}(G_q(\cdot,s)) = 0$, $\alpha(s)$ and $\beta(s)$ must satisfy the equalities

$$\beta(s) = -\frac{U_{n-s}(q) + aU_{n-s-1}(q)}{\hat{W}(q)} \quad \text{and} \quad \alpha(s) = (2q-1)\frac{U_{n-s}(q) + aU_{n-s-1}(q)}{\hat{W}(q)}$$

and hence

$$G_q(k,s) = \frac{1}{\hat{W}(q)} \begin{cases} V_k(q)\Big(aU_{n-s-1}(q) + U_{n-s}(q)\Big), \; k \le s, \\ \\ \Big(aU_{n-k-1}(q) + U_{n-k}(q)\Big)V_s(q), \; s \le k. \end{cases}$$

Finally,

$$\begin{aligned} \mathcal{L}_q(G_q(\cdot,0))(0) &= \beta(0)(1-2q) - \alpha(0) = 1 \\ \mathcal{U}(G_q(\cdot,0)) &= \alpha(0)\Big(U_n(q) + aU_{n-1}(q)\Big) + \beta(0)\Big(U_{n-1}(q) + aU_{n-2}(q)\Big) = 0, \end{aligned}$$

which implies that $\alpha(0)$ and $\beta(0)$ are given by

$$\beta(0) = -\frac{U_n(q) + aU_{n-1}(q)}{\hat{W}(q)} \quad \text{and} \quad \alpha(0) = \frac{U_{n-1}(q) + aU_{n-2}(q)}{\hat{W}(q)}$$

and hence $G_q(k,0) = \dfrac{U_{n-k}(q) + aU_{n-k-1}(q)}{\hat{W}(q)}$. ∎

5 Poisson equation

In this section we study the Poisson equation associated with the Schrödinger operator on the finite path $\mathcal{P}_n$. The *Poisson equation on* $\bar{F}$ consists in finding $u \in \mathcal{C}(\bar{F})$ such that $\mathcal{L}_q(u) = f$ on $\bar{F}$ for any $f \in \mathcal{C}(\bar{F})$ and it is called *regular* if the corresponding homogeneous problem $\mathcal{L}_q(u) = 0$ on $\bar{F}$ has the null function as its unique solution.

Proposition 5.1 *The Poisson equation is regular iff $q \neq \cos\left(\frac{k\pi}{n+2}\right)$, for any $k = 0, \ldots, n+1$ and this condition is equivalent to the fact that any Poisson equation has a unique solution.*

Proof. If $y \in \mathcal{C}(\bar{F})$ is a solution of the homogeneous Poisson equation, then y is a solution of the homogeneous Schrödinger equation on F. Therefore, there exist $\alpha, \beta \in \mathbb{C}$ such that $y(k) = \alpha U_{k-1}(q) + \beta U_{k-2}(q)$ for any $k \in \bar{F}$. Moreover, as $\mathcal{L}_q(y)(0) = \mathcal{L}_q(y)(n+1) = 0$, α and β must verify

$$\begin{bmatrix} -1 & 1-2q \\ V_{n+1}(q) & V_n(q) \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

Therefore, the problem is regular iff

$$0 \neq (2q-1)V_{n+1}(q) - V_n(q) = V_{n+2}(q) - V_{n+1}(q) = 2(q-1)U_{n+1}(q).$$

Newly, the last claim follows by standard arguments. ∎

When the Poisson equation is regular we define the *Green function for the Poisson equation on* $\bar{F}$ as the function $G_q \in \mathcal{C}(\bar{F} \times \bar{F})$ characterized by

$$\mathcal{L}_q(G_q(\cdot, s)) = \varepsilon_s \text{ on } \bar{F}, \quad \text{for any } s \in \bar{F}. \tag{17}$$

Proposition 5.2 *If $q \neq \cos\left(\frac{k\pi}{n+2}\right)$, $k = 0, \ldots, n+1$, then the Green function for the Poisson equation is given by*

$$G_q(k,s) = \frac{1}{2(q-1)\,U_{n+1}(q)} \begin{cases} V_k(q)\,V_{n+1-s}(q), & \text{if } 0 \le k \le s \le n+1, \\ V_s(q)\,V_{n+1-k}(q), & \text{if } 0 \le s \le k \le n+1. \end{cases}$$

Proof. For each $s \in \bar{F}$, $G_q(\cdot, s)$ is, in particular, a solution of a Schrödinger equation on F and hence there exist $\alpha, \beta \in \mathcal{C}(\hat{F})$ such that for any $k \in \bar{F}$ and any $s \in F$

$$G_q(k,s) = \alpha(s)U_{k-1}(q) + \beta(s)U_{k-2}(q) - \begin{cases} 0, & \text{if } k \le s \\ U_{k-s-1}(q), & \text{if } k \ge s \end{cases}$$

whereas when $s = 0, n+1$, $G_q(k,s) = \alpha(s)U_{k-1}(q) + \beta(s)U_{k-2}(q)$, for any $k \in \bar{F}$.

On the other hand, for any $s \in F$, we get that

$$\mathcal{L}_q(G_q(\cdot,s))(0) = \beta(s)(1-2q) - \alpha(s)$$

$$\mathcal{L}_q(G_q(\cdot,s))(n+1) = \alpha(s)V_{n+1}(q) + \beta(s)V_n(q) - V_{n+1-s}(q).$$

Therefore, to verify that $\mathcal{L}_q(G_q(\cdot,s))(0) = \mathcal{L}_q(G_q(\cdot,s))(n+1) = 0$, $\alpha(s)$ and $\beta(s)$ must satisfy the equalities

$$\beta(s) = -\frac{V_{n+1-s}(q)}{2(q-1)U_{n+1}(q)} \quad \text{and} \quad \alpha(s) = (2q-1)\frac{V_{n+1-s}(q)}{2(q-1)U_{n+1}(q)}$$

and hence

$$G_q(k,s) = \frac{1}{2(q-1)U_{n+1}(q)} \begin{cases} V_k(q)V_{n+1-s}(q), \; k \le s, \\ \\ V_s(q)V_{n+1-k}(q), \; s \le k. \end{cases}$$

Finally, for $s = 0, n+1$ we get that

$$\mathcal{L}_q(G_q(\cdot,s))(0) = \beta(s)(1-2q) - \alpha(s) = \varepsilon_s(0)$$

$$\mathcal{L}_q(G_q(\cdot,s))(n+1) = \alpha(s)V_{n+1}(q) + \beta(s)V_n(q) = \varepsilon_s(n+1),$$

which imply that

$$\alpha(0) = \frac{V_n(q)}{2(q-1)U_{n+1}(q)}, \qquad \beta(0) = -\frac{V_{n+1}(q)}{2(q-1)U_{n+1}(q)},$$
$$\alpha(n+1) = \frac{2q-1}{2(q-1)U_{n+1}(q)}, \; \beta(n+1) = -\frac{1}{2(q-1)U_{n+1}(q)}$$

and hence $G_q(k,0) = \dfrac{V_{n+1-k}(q)}{2(q-1)U_{n+1}(q)}$ and $G_q(k,n+1) = \dfrac{V_k(q)}{2(q-1)U_{n+1}(q)}$. ∎

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