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EIGENVALUES, EIGENFUNCTIONS AND GREEN'S FUNCTIONS ON A PATH VIA CHEBYSHEV POLYNOMIALS

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In this work we analyze the boundary value problems on a path associated with Schrödinger operators with constant ground state. These problems include the cases in which the boundary has two, one or none vertices. In addition, we study the periodic boundary value problem that corresponds to the Poisson equation in a cycle. Moreover, we obtain the Green's function for each regular problem and the eigenvalues and their corresponding eigenfunctions otherwise. In each case, the Green's functions, the eigenvalues and the eigenfunctions are given in terms of first, second and third kind Chebyshev polynomials.

1. INTRODUCTION

In this work we analyze linear boundary value problems on a finite path associated with Schrödinger operators with constant ground state. These problems model for instance the equations of motion for a finite atom lattice with nearest–neighbour interactions, see [**11**]. In that context, the Green's function contains all the physical information of the system and it admits an interpretation as an input–output response function, see [**9**].

In spite of its relevance the Green's 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 [**1–5**, **7**, **8**, **10**]. Moreover, a wide variety of techniques is used among which we mention the discrete Fourier transform, eigenvalues and eigenfunctions or contour integration. In some cases a closed–form of Green's functions has been obtained using Chebyshev

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polynomials. In this work, we concentrate on determining explicit expressions, via Chebyshev polynomials, for the Green's function associated with any regular boundary value problem on a path. Our study is similar to what is known for boundary value problems associated with ordinary differential equations, [**6**, Chapters 7, 11, 12]. When the boundary value problem is singular, the eigenvalues and eigenfunctions can be seen as eigenvalues and eigenfunction of the combinatorial Laplacian with the same boundary conditions. So, we take advantage of the previous study to determine the eigenvalues and eigenfunctions in term of Chebyshev polynomials. It is worth to mention that in the discrete setting, a similar structure to the continuous and non–selfadjoint case appears; that is, there exist boundary value problems without eigenvalues and problems for which any complex value is an eigenvalue.

The boundary value problems here considered are of three types that correspond to the cases in which the boundary has either two, one or none side. A preliminary study of two–side regular boundary value problems on a path was developed by the authors in [**4**] under the denomination of two–point boundary value problems. 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 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's function, as well as the eigenvalues and the eigenfunctions for the non–regular case, in terms of Chebyshev polynomials. We also deal with the Poisson equation on a cycle and we show that this problem can be seen as a two–side boundary value problem on a path by introducing the so–called *periodic boundary conditions.*

2. THE SCHRÖDINGER EQUATION ON A PATH

Our purpose in this section is to formulate the difference equations related with Schrödinger operators on a connected subset of the finite path of $n+2$ vertices, $\mathcal{P}_{n+2}$. We can suppose without loss of generality that the set of vertices of $\mathcal{P}_{n+2}$ is $V = \{0, \dots, n+1\}$ and we define F as the subset of vertices $F = \{1, \dots, n\}$.

For any $s \in V$, ε_s stands for the Dirac function on s. Moreover, $\mathcal{C}(V)$ is the vector space of functions $u\colon V \to \mathbb{C}$. For each $q \in \mathbb{C}$, the operator $\mathcal{L}_q\colon \mathcal{C}(V) \to \mathcal{C}(V)$ defined as

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

is called a *Schrödinger operator on* $\mathcal{P}_{n+2}$ and 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 but the combinatorial Laplacian of $\mathcal{P}_{n+2}$ and, in this case, we omit the subindex.

For each $f \in \mathcal{C}(V)$, we call a *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, is called a *homogeneous Schrödinger equation on F*.

If $u, v \in \mathcal{C}(V)$ the *Wronskian* (or *Casoratian*) of u and v, which is denoted by $w[u, v] \in \mathcal{C}(V)$, is defined as

$$w[u,v](k) = u(k)v(k+1) - u(k+1)v(k), \quad k = 0, \dots, n \tag{2}$$

and $w[u, v](n + 1) = w[u, v](n)$, see [**1**, **10**].

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**, **10**].

Lemma 2.1. *The set of solutions of the homogeneous Schrödinger equation on F is a two–dimensional vector space. Moreover, if $u, v \in \mathcal{C}(V)$ are solutions of the homogeneous Schrödinger equation on F then $w[u, v]$ is constant on V and this value is non–zero iff u and v are linearly independent.*

To end this section, we describe some basic properties of the so–called *Chebyshev Polynomials* that will be useful in this work; see [**12**]. A sequence of complex polynomials $\{Q_n\}_{n=-\infty}^{+\infty}$ is called a *Chebyshev sequence* if it satisfies the recurrence law

$$Q_{n+2}(z) = 2zQ_{n+1}(z) - Q_n(z), \quad \text{for each } n \in \mathbb{Z}. \tag{3}$$

The recurrence law (3) shows that any linear combination of Chebyshev sequences is a Chebyshev sequence and that if $\{Q_k\}_{k=-\infty}^{\infty}$ is a Chebyshev sequence, then $\{Q_{k-m}\}_{k=-\infty}^{\infty}$ also is, for any $m \in \mathbb{Z}$. In adddition, any Chebyshev sequence is uniquely 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 by choosing $T_0(z) = U_0(z) = V_0(z) = 1$, $T_1(z) = z$, $U_1(z) = 2z$ and $V_1(z) = 2z - 1$, respectively. The different kinds of Chebyshev polynomials are closely related. Moreover, these relationships display the relevance of the second kind Chebyshev polynomials.

Lemma 2.2. *For any $n \in \mathbb{Z}$ and any $z \in \mathbb{C}$, $T_{n+1}(z) = zU_n(z) - U_{n-1}(z)$, $U_{-n}(z) = -U_{n-2}(z)$ and $V_n(z) = U_n(z) - U_{n-1}(z)$. In particular, for any $z \in \mathbb{C}$, $U_{-1}(z) = 0$ and for any $k, m, r \in \mathbb{Z}$*

$$U_{m+r}(z)U_{k-r}(z) - U_m(z)U_k(z) = U_{r-1}(z)U_{k-m-r-1}(z).$$

Lemma 2.3. *For each $n \in \mathbb{N}^*$ the roots of the n-th order Chebyshev polynomial of second kind are $q_k = \cos\left(\dfrac{k\pi}{n+1}\right)$, $k = 1, \dots, n$. Moreover, $T_{n+1}(z) = 1$ iff $z = q_{2k}$, $k = 0, \dots, \left\lceil \dfrac{n}{2} \right\rceil$, and for any $m \in \mathbb{Z}$ and $k = 1, \dots, \left\lceil \dfrac{n}{2} \right\rceil$, $U_{n-m}(q_k) = (-1)^{k+1}U_{m-1}(q_k)$ and $T_{n+2-m}(q_k) = (-1)^k T_{m-1}(q_k)$.*

The close relationship between the homogeneous Schrödinger equation on F and Chebyshev polynomials is well–known and has been widely used either explicitly or implicitly at previous works, see for instance [**3**, **5**, **8**]. This relation appears clearly from the Equality (3) and it is contained in the following result.

Lemma 2.4. *A function $u \in \mathcal{C}(V)$ is a solution of the homogeneous Schrödinger equation on F iff there exists a Chebyshev sequence $\{Q_k\}_{k=-\infty}^{\infty}$ such that $u(k) = Q_k(q)$ for any $k \in F$. In particular, if for any $k \in V$ we define $u(k) = U_{k-1}(q)$ and $v(k) = U_{k-2}(q)$, then $w[u,v] = 1$ and hence $\{u,v\}$ are a basis of the space of solution of the homogeneous Schrödinger equation on F. Moreover, any solution of the Schrödinger equation on F with data $f \in \mathcal{C}(V)$ is determined by $u(k) = y(k) + \sum\limits_{s=1}^{k} U_{s-k-1}(q)f(s)$, $k \in V$, where y is a solution of the homogeneous Schrödinger equation on F.*

3. TWO–SIDE BOUNDARY VALUE PROBLEMS

Our aim in this section is to analyze the boundary value problems on $F = \{1,\dots,n\}$ associated with a Schrödinger operator. As a typical boundary condition involves vertices at each side of the path, namely the vertices $0, 1, n$ and $n+1$, these problems are generally named *two–side boundary value problems*.

Given $a, b, c, d \in \mathbb{C}$ non-simultaneously zero, the linear map $\mathcal{B}\colon \mathcal{C}(V) \to \mathbb{C}$ determined by the expression

$$\mathcal{B}(u) = au(0) + bu(1) + cu(n) + du(n+1), \qquad \text{for any } u \in \mathcal{C}(V) \tag{4}$$

is called *linear two–side boundary condition on F with coefficients a, b, c and d.* If $\mathcal{B}_1, \mathcal{B}_2$ are the boundary conditions on F with coefficients $c_{11}, c_{12}, c_{13}, c_{14}$ and $c_{21}, c_{22}, c_{23}, c_{24}$, respectively, then for any $u \in \mathcal{C}(V)$ it is verified that

$$\begin{bmatrix} \mathcal{B}_1(u) \\ \mathcal{B}_2(u) \end{bmatrix} = \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix} \begin{bmatrix} u(0) \\ u(1) \end{bmatrix} + \begin{bmatrix} c_{13} & c_{14} \\ c_{23} & c_{24} \end{bmatrix} \begin{bmatrix} u(n) \\ u(n+1) \end{bmatrix} \tag{5}$$

and $\mathcal{B}_1$ and $\mathcal{B}_2$ are called *boundary conditions determined by the matrix $C = (c_{ij})$*. In addition, if for any $1 \le i < j \le 4$ we consider the matrix $C_{ij} = \begin{bmatrix} c_{1i} & c_{1j} \\ c_{2i} & c_{2j} \end{bmatrix}$ and $d_{ij} = \det C_{ij}$, then the polynomial

$$P_{C}(z) = d_{14}U_n(z) + (d_{13} + d_{24})U_{n-1}(z) + d_{23}U_{n-2}(z) + d_{12} + d_{34} \tag{6}$$

is called *boundary polynomial determined by C.*

Lemma 3.1. *If $\mathcal{B}_1$ and $\mathcal{B}_2$ are the boundary conditions determined by the matrix $C \in \mathcal{M}_{2\times 4}(\mathbb{R})$, then they are linearly independent iff* $\operatorname{rank} C = 2$; *that is, iff $d_{ij} \neq 0$ for some $1 \le i < j \le 4$.*

In the sequel we suppose that the boundary conditions (5) are fixed and $\operatorname{rank} C = 2$. Then, a *boundary value problem on F* consists in finding $u \in \mathcal{C}(V)$ such that

$$\mathcal{L}_q(u) = f, \quad \text{on} \quad F, \qquad \mathcal{B}_1(u) = g_1 \quad \text{and} \quad \mathcal{B}_2(u) = g_2 \tag{7}$$

for given $f \in \mathcal{C}(V)$ and $g_1, g_2 \in \mathbb{C}$. The problem is called *semi–homogeneous* when $g_1 = g_2 = 0$ and *homogeneous* if, in addition, $f = 0$. We say that the boundary value problem (7) is *regular* if the corresponding homogenous boundary value problem has the null function as its unique solution. It follows by standard arguments that the boundary value problem (7) is regular iff for any data $f \in \mathcal{C}(V)$, $g_1, g_2 \in \mathbb{C}$ it has a unique solution. The following result shows that we can restrict our analysis of two–side boundary value problems to the study of the semi–homogeneous ones.

Lemma 3.2. *Consider $\alpha, \beta, \gamma, \delta \in \mathbb{C}$ such that $c_{j1}\alpha + c_{j2}\beta + c_{j3}\gamma + c_{j4}\delta = g_j$, $j = 1, 2$. Then $u \in \mathcal{C}(V)$ verifies that $\mathcal{L}_q(u) = f$ on F, $\mathcal{B}_1(u) = g_1$ 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 $\mathcal{L}_q(v) = f + (\alpha - 2q\beta)\varepsilon_1 + \beta\varepsilon_2 + \gamma\varepsilon_{n-1} + (\delta - 2q\gamma)\varepsilon_n$ on F and moreover that $\mathcal{B}_1(v) = \mathcal{B}_2(v) = 0$.*

A pair of boundary conditions $(\widehat{\mathcal{B}}_1, \widehat{\mathcal{B}}_2)$ determined by $\widehat{C} \in \mathcal{M}_{2\times 4}(\mathbb{C})$ is called *equivalent* to the pair $(\mathcal{B}_1, \mathcal{B}_2)$ if there exists a non–singular matrix $M \in \mathcal{M}_2(\mathbb{C})$ such that $\widehat{C} = MC$. Clearly $P_{\widehat{C}}(z) = (\det M) P_C(z)$, Lemma 3.1 implies that $\widehat{\mathcal{B}}_1$ and $\widehat{\mathcal{B}}_2$ are linearly independent and moreover, a function $v \in \mathcal{C}(V)$ verifies $\mathcal{B}_1(v) = \mathcal{B}_2(v) = 0$ iff $\widehat{\mathcal{B}}_1(v) = \widehat{\mathcal{B}}_2(v) = 0$. Therefore, the semi–homogeneous boundary value problem $\mathcal{L}_q(u) = f$ on F, $\widehat{\mathcal{B}}_1(u) = \widehat{\mathcal{B}}_2(u) = 0$ is equivalent to the semi–homogeneous boundary value problem associated with (7), since both have the same solutions. As a consequence a boundary value problem is regular iff any equivalent boundary value problem is also regular.

Our first objective is to obtain the solution of any regular semi–homogeneous boundary value problem by considering its resolvent kernel. Specifically, if we suppose that the boundary value problem (7) is regular, then for any $f \in \mathcal{C}(V)$, the function $G_q \in \mathcal{C}(V \times F)$ characterized by

$$\mathcal{L}_q(G_q(\cdot, s)) = \varepsilon_s \quad \text{on} \quad F, \qquad \mathcal{B}_1(G_q(\cdot, s)) = \mathcal{B}_2(G_q(\cdot, s)) = 0, \quad s \in F \tag{8}$$

is called *Green's function for the boundary value problem* (7). Then, if $f \in \mathcal{C}(V)$ the function $u(k) = \sum\limits_{s=1}^{n} G_q(k, s)\, f(s)$, $k \in V$, is the unique solution of the semi–homogeneous boundary value problem with data f.

Theorem 3.3. *The boundary value problem* (7) *is regular iff $P_C(q) \neq 0$ and then its Green's function for any $1 \leq s \leq n$ and any $0 \leq k \leq s$ is given by*

$$\begin{aligned} G(k, s) = {} & \frac{1}{P_C(q)} \Big[d_{14} U_{n-s}(q) + d_{13} U_{n-s-1}(q) \Big] U_{k-1}(q) \\ + {} & \frac{1}{P_C(q)} \Big[d_{24} U_{n-s}(q) + d_{23} U_{n-s-1}(q) \Big] U_{k-2}(q) - \frac{d_{34}}{P_C(q)} U_{|k-s|-1}(q) \end{aligned}$$

and for any $1 \leq s \leq n$ and any $s \leq k \leq n+1$ by

$$\begin{aligned} G(k, s) = {} & \frac{1}{P_C(q)} \Big[d_{14} U_{n-k}(q) + d_{13} U_{n-k-1}(q) \Big] U_{s-1}(q) \\ + {} & \frac{1}{P_C(q)} \Big[d_{24} U_{n-k}(q) + d_{23} U_{n-k-1}(q) \Big] U_{s-2}(q) - \frac{d_{12}}{P_C(q)} U_{|k-s|-1}(q). \end{aligned}$$

Proof. Throughout the proof we systematically use the last identity in Lemma 2.2.

If $u(k) = U_{k-1}(q)$ and $v(k) = U_{k-2}(q)$, applying Lemma 2.4, a function $y \in \mathcal{C}(V)$ is a solution of the homogeneous boundary value problem iff $y = \alpha u + \beta v$ where $\alpha, \beta \in \mathbb{C}$ verify

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

Therefore, the boundary value problem is regular iff $\mathcal{B}_1(u)\mathcal{B}_2(v) - \mathcal{B}_2(u)\mathcal{B}_1(v) \neq 0$ and hence, the first claim follows from the identity $P_{_C}(q) = \mathcal{B}_1(u)\mathcal{B}_2(v) - \mathcal{B}_2(u)\mathcal{B}_1(v)$.

For a fixed $s \in F$, from Lemma 2.4 we get that for any $k \in V$,

$$G_q(k,s) = y_s(k) + \sum_{r=1}^{k} U_{r-k-1}(q)\varepsilon_s(r) = y_s(k) + \begin{cases} 0, & \text{if } k \leq s, \\ U_{s-k-1}(q), & \text{if } k \geq s, \end{cases}$$

where y_s satisfies that $\mathcal{L}_q(y_s) = 0$ on F and $\mathcal{B}_j(y_s) = c_{j3}U_{n-s-1}(q) + c_{j4}U_{n-s}(q),\ j = 1, 2$. Hence, if $y_s(k) = a(s)u(k) + b(s)v(k)$, it holds

$$\begin{bmatrix} a(s) \\ b(s) \end{bmatrix} = \begin{bmatrix} \mathcal{B}_1(u) & \mathcal{B}_1(v) \\ \mathcal{B}_2(u) & \mathcal{B}_2(v) \end{bmatrix}^{-1} \begin{bmatrix} c_{13}U_{n-s-1}(q) + c_{14}U_{n-s}(q) \\ c_{23}U_{n-s-1}(q) + c_{24}U_{n-s}(q) \end{bmatrix}$$

and therefore

$$\begin{aligned} P_{_C}(q)a(s) &= d_{13}U_{n-s-1}(q) + d_{14}U_{n-s}(q) - d_{34}U_{s-2}(q), \\ P_{_C}(q)b(s) &= d_{23}U_{n-s-1}(q) + d_{24}U_{n-s}(q) + d_{34}U_{s-1}(q). \end{aligned}$$

Consequently, we obtain that

$$\begin{aligned} P_{_C}(q)y_s(k) = {} & \big(d_{13}U_{n-s-1}(q) + d_{14}U_{n-s}(q)\big)U_{k-1}(q) \\ & + \big(d_{23}U_{n-s-1}(q) + d_{24}U_{n-s}(q)\big)U_{k-2}(q) - d_{34}U_{s-k-1}(q). \end{aligned}$$

On the other hand, for $k \geq s$

$$\begin{aligned} P_{_C}(q)\big(y_s(k) + U_{s-k-1}(q)\big) &= d_{13}\big(U_{n-s-1}(q)U_{k-1}(q) - U_{n-1}(q)U_{k-s-1}(q)\big) \\ &\quad + d_{14}\big(U_{n-s}(q)U_{k-1}(q) - U_n(q)U_{k-s-1}(q)\big) \\ &\quad + d_{23}\big(U_{n-s-1}(q)U_{k-2}(q) - U_{n-2}(q)U_{k-s-1}(q)\big) \\ &\quad + d_{24}\big(U_{n-s}(q)U_{k-2}(q) - U_{n-1}(q)U_{k-s-1}(q)\big) \\ &\qquad + d_{12}U_{s-k-1}(q) \\ &= \big(d_{13}U_{n-1-k}(q) + d_{14}U_{n-k}(q)\big)U_{s-1}(q) \\ &\quad + \big(d_{23}U_{n-1-k}(q) + d_{24}U_{n-k}(q)\big)U_{s-2}(q) \\ &\qquad - d_{12}U_{k-s-1}(q) \end{aligned}$$

and the expression for the Green's function follows. $\square$

In view of the above result, we say that $q \in \mathbb{C}$ is *a regular value* of the boundary value problem (7) if $P_C(q) \neq 0$ and *a singular value* of the boundary value problem, otherwise. Observe that q is a singular value iff $2(1-q)$ is an eigenvalue of the following boundary eigenvalue problem

$$\mathcal{L}(u) = \lambda u, \quad \text{on} \quad F; \quad \mathcal{B}_1(u) = \mathcal{B}_2(u) = 0. \tag{9}$$

If $\lambda \in \mathbb{C}$ is an eigenvalue, the dimension of its associated eigenfunction subspace is either 1, in which case λ is called a *simple eigenvalue*, or 2, in which case λ is called a *double eigenvalue*.

Proposition 3.4. *If $\lambda = 2(1-q)$, λ is a double eigenvalue of* (9) *iff*

$$\begin{aligned} c_{11} &= c_{13}U_{n-2}(q) + c_{14}U_{n-1}(q), \qquad & c_{12} &= -c_{13}U_{n-1}(q) - c_{14}U_n(q), \\ c_{21} &= c_{23}U_{n-2}(q) + c_{24}U_{n-1}(q), \qquad & c_{22} &= -c_{23}U_{n-1}(q) - c_{24}U_n(q). \end{aligned}$$

Therefore, $P_C(z) = d_{34}\Big(U_{n-2}(q)U_n(z) - 2U_{n-1}(q)U_{n-1}(z) + U_n(q)U_{n-2}(z) + 2\Big)$, $d_{34} \neq 0$ *and hence the pair of boundary conditions are equivalent to*

$$\begin{aligned} \widehat{\mathcal{B}}_1(u) &= U_{n-2}(q)u(0) - U_{n-1}(q)u(1) + u(n), \\ \widehat{\mathcal{B}}_2(u) &= U_{n-1}(q)u(0) - U_n(q)u(1) + u(n+1). \end{aligned}$$

Proof. It is clear that $\lambda = 2(1-q)$ is a double eigenvalue of (7) iff any solution of the homogeneous Schrödinger equation, $\mathcal{L}_q(v) = 0$ on F, verifies the boundary conditions. Therefore, if $u(k) = U_{k-1}(q)$ and $v(k) = U_{k-2}(q)$, then λ is a double eigenvalue iff $\mathcal{B}_1(u) = \mathcal{B}_2(u) = \mathcal{B}_1(v) = \mathcal{B}_2(v) = 0$, which imply the identities for the coefficients of the boundary conditions. These identities imply that $d_{12} = d_{34}$, $d_{13} = d_{24} = -d_{34}U_{n-1}(q)$, $d_{14} = d_{34}U_{n-2}(q)$ and $d_{23} = d_{34}U_n(q)$, and hence $d_{34} \neq 0$ since $\operatorname{rank} C = 2$. The last conclusion follows taking into account that $\widehat{\mathcal{B}}_1$ and $\widehat{\mathcal{B}}_2$ are the boundary conditions determined by the matrix $C_{34}^{-1}C$. $\square$

Proposition 3.5. *If $\lambda = 2(1-q)$ is a simple eigenvalue of* (9), *then*

$$\begin{aligned} u(k) &= c_{21}U_{k-1}(q) + c_{22}U_{k-2}(q) - c_{23}U_{n-k-1}(q) - c_{24}U_{n-k}(q) \\ v(k) &= c_{11}U_{k-1}(q) + c_{12}U_{k-2}(q) - c_{13}U_{n-k-1}(q) - c_{14}U_{n-k}(q), \end{aligned}$$

are linearly dependent eigenfunctions corresponding to λ. Moreover, u is non–null except when $c_{21} = c_{23}U_{n-2}(q) + c_{24}U_{n-1}(q)$ and $c_{22} = -c_{23}U_{n-1}(q) - c_{24}U_n(q)$ in which case v is non–null.

Proof. If we consider $z_1(k) = U_{k-1}(q)$ and $z_2(k) = U_{k-2}(q)$, then $u = Az_1 + Bz_2$ verifies $\mathcal{B}_1(u) = \mathcal{B}_2(u) = 0$ iff

$$\begin{bmatrix} \mathcal{B}_1(z_1) & \mathcal{B}_1(z_2) \\ \mathcal{B}_2(z_1) & \mathcal{B}_2(z_2) \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}.$$

The above matrix is singular since $P_C(q) = 0$ and non–null since $2(1-q)$ is a simple eigenvalue. When the first row is non–null, if we can choose $A = -\mathcal{B}_1(z_2)$

and $B=\mathcal{B}_1(z_1)$, then u is a non–null eigenfunction, whereas when the second row is non–null, the choice $A=-\mathcal{B}_2(z_2)$ and $B=\mathcal{B}_2(z_1)$ determines that u is non–null. Taking into account the identities

$$\mathcal{B}_1(z_1)=c_{12}+c_{13}U_{n-1}(q)+c_{14}U_n(q),\ \mathcal{B}_1(z_2)=-c_{11}+c_{13}U_{n-2}(q)+c_{14}U_{n-1}(q),$$
$$\mathcal{B}_2(z_1)=c_{22}+c_{23}U_{n-1}(q)+c_{24}U_n(q),\ \mathcal{B}_2(z_2)=-c_{21}+c_{23}U_{n-2}(q)+c_{24}U_{n-1}(q),$$

when either $\mathcal{B}_2(z_1)\neq 0$ or $\mathcal{B}_2(z_2)\neq 0$, we obtain that

$$\begin{aligned}u(k)&=c_{21}U_{k-1}(q)+c_{22}U_{k-2}(q)+c_{23}\big(U_{n-1}(q)U_{k-2}(q)-U_{n-2}(q)U_{k-1}(q)\big)\\&\qquad+c_{24}\big(U_n(q)U_{k-2}(q)-U_{n-1}(q)U_{k-1}(q)\big)\\&=c_{21}U_{k-1}(q)+c_{22}U_{k-2}(q)-c_{23}U_{n-k-1}(q)-c_{24}U_{n-k}(q).\end{aligned}$$

When either $\mathcal{B}_1(z_1)\neq 0$ or $\mathcal{B}_1(z_2)\neq 0$, the same reasoning determines the expression for the non–null function $v(k)=-\mathcal{B}_1(z_2)U_{k-1}(q)+\mathcal{B}_2(z_1)U_{k-2}(q)$. $\square$

Our next objective is to determine the different eigenvalues and eigenfunctions for the eigenvalue problem (9) for each pair of boundary conditions. So, we classify the boundary conditions depending on whether they involve vertices on the interior or exterior boundary of F. The *inner boundary* and the *outer boundary* of F are defined as $\delta_-(F)=\{1,n\}$ and $\delta_+(F)=\{0,n+1\}$, respectively. Then, we say that the pair $(\mathcal{B}_1,\mathcal{B}_2)$ is *of inner type* iff there exists an equivalent pair whose boundary conditions involves only vertices in $\delta_-(F)$; we say that the pair $(\mathcal{B}_1,\mathcal{B}_2)$ is *of outer type* iff each boundary condition of every equivalent pair involves the value of functions in at least one vertex of $\delta_+(F)$, and we say that the pair $(\mathcal{B}_1,\mathcal{B}_2)$ is *of in–outer type*, otherwise.

Proposition 3.6. *The following results hold*:

(i) *The pair $(\mathcal{B}_1,\mathcal{B}_2)$ is of inner type iff $C_{14}=0$ and hence it is equivalent to the pair*
$$\widehat{\mathcal{B}}_1(u)=u(1)\quad\textit{and}\quad\widehat{\mathcal{B}}_2(u)=u(n).$$

(ii) *The pair $(\mathcal{B}_1,\mathcal{B}_2)$ is of outer type iff $d_{14}\neq 0$ and then, there exist $a,b,c,d\in\mathbb{C}$ such that it is equivalent to the pair*
$$\widehat{\mathcal{B}}_1(u)=u(0)+au(1)+bu(n)\quad\textit{and}\quad\widehat{\mathcal{B}}_2(u)=cu(1)+du(n)+u(n+1).$$

(iii) *The pair $(\mathcal{B}_1,\mathcal{B}_2)$ is of in–outer type iff $C_{14}\neq 0$ but $d_{14}=0$. Then, there exist $a,b,c,d,\alpha,\beta\in\mathbb{C}$ with $(|a|+|d|)(|\alpha|+|\beta|)>0$ and such that $(\mathcal{B}_1,\mathcal{B}_2)$ is equivalent to the pair*
$$\widehat{\mathcal{B}}_1(u)=au(0)+bu(1)+cu(n)+du(n+1)\quad\textit{and}\quad\widehat{\mathcal{B}}_2(u)=\alpha u(1)+\beta u(n).$$

Proof. The pair is of inner type iff there exists a non singular matrix M such that $MC_{14}=0$; that is, iff $C_{14}=0$. Moreover, in this case necessarily $d_{23}\neq 0$, since $\operatorname{rank} C = 2$ and hence $\widehat{\mathcal{B}}_1$ and $\widehat{\mathcal{B}}_2$ are the boundary conditions determined by $C_{23}^{-1}C$.

If $d_{14} \neq 0$, then, for any non singular matrix M, we get that $\det(MC_{14}) \neq 0$, which implies that each row of MC_{14} is non null and hence the boundary condition are of outer type. In addition, $\widehat{\mathcal{B}}_1$ and $\widehat{\mathcal{B}}_2$ are the boundary conditions determined by $C_{14}^{-1}C$.

Conversely, if $d_{14} = 0$ but $C_{14} \neq 0$, then there exists a non singular matrix M such that the second row of MC_{14} is null and hence the pair $(\mathcal{B}_1, \mathcal{B}_2)$ is of in–outer type and moreover $\widehat{\mathcal{B}}_1$ and $\widehat{\mathcal{B}}_2$ are the boundary conditions determined by MC. □

Proposition 3.7. *The eigenvalues of the inner boundary eigenvalue problem*

$$\mathcal{L}u = \lambda u, \quad \textit{on } F, \quad u(1) = u(n) = 0$$

are simple and given by $\lambda_j = 2(1 - q_j)$ *where* $q_j = \cos\left(\dfrac{j\pi}{n-1}\right)$, $j = 1, \dots, n-2$. *Moreover,* $U_{k-2}(q_j)$ *is an eigenfunction associated with* λ_j, *for any* $j = 1, \dots, n-2$.

Proof. The expression of the eigenvalues is a straightforward consequence of being $U_{n-2}(z)$ the boundary polynomial of the inner boundary value problem. Moreover, applying Proposition 3.4, λ_j is simple since $0 = c_{22} \neq -c_{23}U_{n-1}(q_j) - c_{24}U_n(q_j) = -U_{n-1}(q_j) = (-1)^{j+1}$. Finally, the expression for the eigenfunction follows from Proposition 3.5. □

Proposition 3.8. *Given* $a, b, c, d \in \mathbb{C}$, *the eigenvalues of the outer boundary eigenvalue problem*

$$\mathcal{L}(u) = \lambda u \quad \textit{on } F, \quad u(0) + au(1) + bu(n) = cu(1) + du(n) + u(n+1) = 0$$

are $\{2(1 - q_j)\}_{j=1}^n$ *where* q_j, $j = 1, \dots, n$ *are the zeros of the polynomial*

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

Moreover, the following properties hold:

(i) $\lambda = 2(1 - q)$ *is a double eigenvalue iff* $U_{n-2}(q) \neq 0$ *and moreover* $b = c = \dfrac{1}{U_{n-2}(q)}$ *and* $a = d = -\dfrac{U_{n-1}(q)}{U_{n-2}(q)}$.

(ii) *There exists at most a unique double eigenvalue except when* $a = d = 0$ *and either* $b = c = -1$, *in which case* $2 - 2\cos\left(\dfrac{2j\pi}{n}\right)$, $j = 1, \dots, \left\lfloor \dfrac{n-1}{2} \right\rfloor$ *are the double eigenvalues, or* $b = c = 1$, *in which case* $2 - 2\cos\left(\dfrac{(2j-1)\pi}{n}\right)$, $j = 1, \dots, \left\lceil \dfrac{n-1}{2} \right\rceil$ *are the double eigenvalues.*

(iii) *If* $\lambda = 2(1 - q)$ *is a simple eigenvalue, then* $U_{k-1}(q) + aU_{k-2}(q) - bU_{n-k-1}(q)$ *is a non–null eigenfunction corresponding to* λ, *except when* $U_{n-2}(q) \neq 0$, $b = \dfrac{1}{U_{n-2}(q)}$ *and* $a = -\dfrac{U_{n-1}(q)}{U_{n-2}(q)}$ *in which case* $U_{n-k}(q) + dU_{n-k-1}(q) - cU_{k-2}(q)$ *is a non–null eigenfunction corresponding to* λ.

Proof. Note first that $P(z)$ is the boundary polynomial corresponding to the outer boundary value problem.

(i) From Proposition 3.4, $\lambda = 2(1-q)$ is a double eigenvalue iff $1 = bU_{n-2}(q)$, $a = -bU_{n-1}(q)$, $0 = dU_{n-2}(q) + U_{n-1}(q)$ and $c = -dU_{n-1}(q) - U_n(q)$, which is equivalent to be $U_{n-2}(q) \neq 0$, $b = c = \dfrac{1}{U_{n-2}(q)}$ and $a = d = -\dfrac{U_{n-1}(q)}{U_{n-2}(q)}$.

(ii) If $2(1-q)$ and $2(1-\hat{q})$ are two double eigenvalues, from (i) we get that $U_{n-2}(q) = U_{n-2}(\hat{q})$ and $U_{n-1}(q) = U_{n-1}(\hat{q})$. In addition, $P(q) = P(\hat{q}) = 0$ imply that $U_n(q) = U_n(\hat{q})$. Therefore, by applying the equation (3), it is verified that $2(q-\hat{q})U_{n-1}(q) = 0$. Hence, either $q = \hat{q}$ or $U_{n-1}(q) = 0$. In this case, $U_{n-2}(q) = \pm 1$ and hence the result follows.

(iii) Taking into account the identities obtained in part (i), the result is a straightforward consequence of Proposition 3.5. □

Proposition 3.9. *Given $a, b, c, d, \alpha, \beta \in \mathbb{C}$ such that $(|a|+|d|)(|\alpha|+|\beta|) > 0$, then $\lambda = 2(1-q)$ is an eigenvalue of the in–outer boundary eigenvalue problem*

$$\mathcal{L}(u) = \lambda u \quad \textit{on } F, \quad au(0) + bu(1) + cu(n) + du(n+1) = \alpha u(1) + \beta u(n) = 0,$$

iff $(a\beta - d\alpha)U_{n-1}(q) + (b\beta - c\alpha)U_{n-2}(q) + a\alpha - d\beta = 0$. Moreover, the following properties hold:

(i) *All eigenvalues are simple except when either $a = d$, $b = -(c + 2dq)$ and $\alpha = -\beta$, in which case $2 - 2\cos\left(\dfrac{2j\pi}{n-1}\right)$, $j = 1, \dots, \left\lfloor \dfrac{n-2}{2} \right\rfloor$ are the double eigenvalues, or $a = -d$, $b = c + 2dq$ and $\alpha = \beta$, in which case $2 - 2\cos\left(\dfrac{(2j-1)\pi}{n-1}\right)$, $j = 1, \dots, \left\lceil \dfrac{n-2}{2} \right\rceil$ are the double eigenvalues.*

(ii) *If $2(1-q)$ is a simple eigenvalue, then $\alpha U_{k-2}(q) - \beta U_{n-k-1}(q)$ is a corresponding non–null eigenfunction, except when $q = \cos\left(\dfrac{2j\pi}{n-1}\right)$, $j = 1, \dots, \left\lfloor \dfrac{n-2}{2} \right\rfloor$ and $\alpha = -\beta$, in which case $(a-d)U_{k-1}(q) + (b + c + 2qd)U_{k-2}(q)$ is a non–null eigenfunction, or $q = \cos\left(\dfrac{(2j-1)\pi}{n-1}\right)$, $j = 1, \dots, \left\lceil \dfrac{n-2}{2} \right\rceil$ and $\alpha = \beta$, in which case $(a+d)U_{k-1}(q) + (b - c - 2qd)U_{k-2}(q)$ is a non–null eigenfunction.*

(iii) *If $a\beta - d\alpha = 0$ and $b\beta - c\alpha \neq 0$, then all eigenvalues are simple, there exist at most $n-2$ different eigenvalues and the boundary conditions are equivalent to*

$$\widehat{\mathcal{B}}_1(u) = au(0) + bu(1) + cu(n) + du(n+1) \quad \textit{and} \quad \widehat{\mathcal{B}}_2(u) = au(1) + du(n).$$

(iv) *If $a\beta - d\alpha = b\beta - c\alpha = 0$ and $a \neq \pm d$, then the boundary conditions are equivalent to*

$$\widetilde{\mathcal{B}}_1(u) = au(0) + du(n+1) \quad \textit{and} \quad \widetilde{\mathcal{B}}_2(u) = au(1) + du(n)$$

and eigenvalues do not exist .

(v) *If $a\beta - d\alpha = b\beta - c\alpha = 0$ and $a = \pm d$, then the boundary conditions are equivalent to*

$$\widetilde{\mathcal{B}}_1(u) = u(0) \pm u(n+1) \quad \text{and} \quad \widetilde{\mathcal{B}}_2(u) = u(1) \pm u(n)$$

and any complex value is a simple eigenvalue. Moreover, $U_{k-2}(q) \mp U_{n-k-1}(q)$ is a corresponding non–null eigenfunction, except when $a = d$ and $q = \cos\left(\frac{(2j-1)\pi}{n-1}\right)$, $j = 1, \dots, \left\lfloor \frac{n-2}{2} \right\rfloor$ or when $a = -d$ and $q = \cos\left(\frac{2j\pi}{n-1}\right)$, $j = 1, \dots, \left\lceil \frac{n-2}{2} \right\rceil$. In both cases, $T_{k-1}(q)$ is a non–null eigenfunction.

Proof. In this case, the boundary polynomial is

$$P(z) = (a\beta - d\alpha)U_{n-1}(z) + (b\beta - c\alpha)U_{n-2}(z) + a\alpha - d\beta,$$

and hence $2(1-q)$ is an eigenvalue iff $P(q) = 0$.

(i) Applying Proposition 3.4, $2(1-q)$ is a double eigenvalue iff $a = cU_{n-2}(q) + dU_{n-1}(q)$, $b = -cU_{n-1}(q) - dU_n(q)$, $0 = \beta U_{n-2}(q)$ and $\alpha = -\beta U_{n-1}(q)$. Then, as $\beta \neq 0$ since $|\alpha| + |\beta| > 0$, we obtain that $U_{n-2}(q) = 0$, which in turns implies that $U_{n-1}(q) = \pm 1$ and $U_n(q) = \pm 2q$. Definitely, $2(1-q)$ is a double eigenvalue iff $U_{n-2}(q) = 0$, $a = \pm d$, $b = \mp(c + 2dq)$ and $\alpha = \mp\beta$ and the expression for the double eigenvalues follows from Lemma 2.3.

(ii) From Proposition 3.4, $\alpha U_{k-2}(q) - \beta U_{n-k-1}(q)$ is a non–null eigenfunction, except when $0 = \beta U_{n-2}(q) = \alpha + \beta U_{n-1}(q)$. Taking into account that $\beta \neq 0$, we get that $U_{n-2}(q) = 0$ and the results follow from Proposition 2.3.

(iii) Under the hypotheses, the degree of $P(z)$ is $n-2$ and hence there exists at most $n-2$ different eigenvalues. Moreover, there exists $\mu \neq 0$ such that $\alpha = \mu a$ and $\beta = \mu d$, which implies that the inner boundary condition $\alpha u(1) + \beta u(n) = 0$ is equivalent to $\widetilde{\mathcal{B}}_2$. In addition, each eigenvalue must be simple since $a = \pm d$ and $\alpha = \mp\beta$ would imply that $a = d = \alpha = \beta = 0$, a contradiction with the hypothesis $(|a| + |d|)(|\alpha| + |\beta|) > 0$.

(iv) In this case, the boundary polynomial is constant and non–null, which implies that the boundary value problem does not have eigenvalues. Moreover, the equality $b\beta - c\alpha = 0$ implies that there exists $\nu \neq 0$ such that $b = \nu\alpha = \nu\mu a$ and $c = \nu\beta = \nu\mu d$ and hence the pair of boundary conditions is equivalent to $(\widetilde{\mathcal{B}}_1, \widetilde{\mathcal{B}}_2)$.

(v) In this case, the boundary polynomial is null and then any complex number is an eigenvalue. Moreover, reasoning as in part (iii) we get that any eigenvalue is simple. From, Proposition 3.5, $U_{k-2}(q) \mp U_{n-k-1}(q)$ is a non–null eigenfunction, except when $0 = U_{n-2}(q)$ and $1 = \mp U_{n-1}(q)$ and then, $U_{k-1}(q) - U_{k-3}(q) = 2T_{k-1}(q)$ is a non–null eigenfunction. $\square$

The boundary value problems above considered encompass the different two–side boundary value problems that appear in the literature with proper name. To end this section we specify the more usual ones; that is, unilateral, Sturm–Liouville, specially Dirichlet and Neumann problems, and periodic problems.

The pair of boundary conditions $(\mathcal{B}_1,\mathcal{B}_2)$ is called *unilateral* if either $C_{34}=0$, and then (7) is named *initial value problem*, or $C_{12}=0$, and then (7) is named *final value problem*. Any unilateral pair verifies that $d_{14}=d_{13}=d_{23}=d_{24}=0$ and hence its boundary polynomial is $P_n(q)=d_{12}+d_{34}$. In addition, either $d_{34}=0$ and $d_{12}\neq 0$ or $d_{12}=0$ and $d_{34}\neq 0$ since $\operatorname{rank} C=2$, which implies that unilateral boundary value problems are regular. Therefore, any unilateral pair is of in–outer type and equivalent to either $\big(u(0),u(1)\big)$, for initial value problems, or $\big(u(n),u(n+1)\big)$ for final value problems.

Corollary 3.10. *The Green's function for the initial value problem is*

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

whereas the Green's function for the final value problem is

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

When $c_{13}=c_{14}=c_{21}=c_{22}=0$, $\mathcal{B}_1$ and $\mathcal{B}_2$ are called *Sturm-Liouville conditions*; that is,

$$\mathcal{B}_1(u)=au(0)+bu(1)\quad\text{and}\quad \mathcal{B}_2(u)=cu(n)+du(n+1), \tag{10}$$

where $a,b,c,d\in\mathbb{C}$ are such that $(|a|+|b|)(|c|+|d|)>0$. Observe that any boundary conditions of inner type are equivalent to the Sturm–Liouville conditions $u(1)$ and $u(n)$, that are named *inner Dirichlet conditions*. On the other hand, the Sturm-Liouville pair (10) is of outer type iff $ad\neq 0$ and hence it is equivalent to the pair

$$\widehat{\mathcal{B}}_1(u)=u(0)+\widehat{b}u(1)\quad\text{and}\quad \widehat{\mathcal{B}}_2(u)=\widehat{c}u(n)+u(n+1),\qquad \widehat{b},\widehat{c}\in\mathbb{C}.$$

The most popular outer Sturm-Liouville conditions are the so–called *outer Dirichlet conditions*, that correspond to take $\widehat{b}=\widehat{c}=0$, and the *Neumann conditions*, that correspond to take $\widehat{b}=\widehat{c}=-1$. Finally, the Sturm-Liouville pair (10) is of in–outer type when $ad=0$ and $|a|+|d|>0$. Therefore, any in–outer Sturm-Liouville pair is equivalent to either the pair

$$\widehat{\mathcal{B}}_1(u)=u(1)\quad\text{and}\quad \widehat{\mathcal{B}}_2(u)=\widehat{c}u(n)+u(n+1),\qquad \widehat{c}\in\mathbb{C}$$

or the pair

$$\widehat{\mathcal{B}}_1(u)=u(0)+\widehat{b}u(1)\quad\text{and}\quad \widehat{\mathcal{B}}_2(u)=u(n),\qquad \widehat{b}\in\mathbb{C}.$$

Corollary 3.11. *Given $a,b,c,d\in\mathbb{C}$ such that $(|a|+|d|)(|c|+|d|)>0$ and the Sturm–Liouville boundary conditions*

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

its boundary polynomial is $P(z) = adU_n(z) + (ac+bd)U_{n-1}(z) + bcU_{n-2}(z)$ *and then when* $P(q) \neq 0$, *its Green function is given by*

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

where $1 \le s \le n$. *On the other hand, when* $P(q) = 0$, *then* $2(1-q)$ *is a simple eigenvalue and* $u(k) = aU_{k-1}(q) + bU_{k-2}(q)$ *is a corresponding non–null eigenfunction.*

As a consequence, the boundary polynomial for the outer Dirichlet problem is $U_n(z)$ and hence it is regular iff $q \neq \cos\left(\dfrac{k\pi}{n+1}\right)$, $k = 1, \ldots, n$, in which case its Green function is given by

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

where $1 \le s \le n$. Therefore, the eigenvalues of the outer Dirichlet problem are given by $\lambda_j = 2 - 2\cos\left(\dfrac{k\pi}{n+1}\right)$ whose corresponding eigenfunctions are multiple of $U_{k-1}(q_j)$, $j = 1, \ldots, n$.

On the other hand, the boundary polynomial for the Neumann problem is

$$U_n(z) - 2U_{n-1}(z) + U_{n-2}(z) = 2(q-1)U_{n-1}(z)$$

and hence it is regular iff $q \neq \cos\left(\dfrac{k\pi}{n}\right)$, $k = 0, \ldots, n-1$, in which case its Green function is given by

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

where $1 \le s \le n$. Therefore, the eigenvalues of the Neumann problem are given by $\lambda_0 = 0$, whose eigenfunctions are constant and $\lambda_j = 2 - 2\cos\left(\dfrac{k\pi}{n}\right)$ whose corresponding eigenfunctions are multiple of $V_{k-1}(q_j)$, $j = 1, \ldots, n-1$.

We remark that a more intricate expression for the above Green functions in terms of first and second kind Chebyshev polynomials can be found in [**3**]. Obviously, both expression are equivalent via some additional properties of the Chebyshev polynomials. In addition, for the outer Dirichlet problem the above expression was obtained in [**5**].

The last two–side boundary value problem we analyze here corresponds to the so–called *periodic boundary conditions for the Schrödinger operator* $\mathcal{L}_q$ on $\mathcal{P}_{n+2}$,

$$\mathcal{B}_1(u) = u(0) - u(n+1) \quad \text{and} \quad \mathcal{B}_2(u) = 2qu(0) - u(1) - u(n). \tag{11}$$

The periodic boundary conditions are of in–outer type when $q = 0$ and of outer type otherwise. In fact, when $q \neq 0$ they are equivalent to the conditions

$$\widehat{\mathcal{B}}_1(u) = u(0) - \frac{1}{2q}\,u(1) - \frac{1}{2q}\,u(n) \quad \text{and} \quad \widehat{\mathcal{B}}_2(u) = -\frac{1}{2q}\,u(1) - \frac{1}{2q}\,u(n) + u(n+1).$$

The periodic boundary conditions appear associated with the so–called *Poisson equation* for the Schrödinger operator $\mathcal{L}_q$ on the cycle $\mathcal{C}_n$ with $n+1$ vertices. Specifically, if we suppose that the vertex set of $\mathcal{C}_n$ is $\{0,\dots,n\}$ and f is defined on $\{0,\dots,n\}$, then the Poisson equation on $\mathcal{C}_n$ is

$$\begin{aligned} \mathcal{L}_q(u)(0) &= \;\; 2qu(0) - u(1) - u(n) = f(0) \\ \mathcal{L}_q(u)(k) &= \;\; 2qu(k) - u(k+1) - u(k-1) = f(k), \quad k = 1,\dots,n-1, \\ \mathcal{L}_q(u)(n) &= \;\; 2qu(n) - u(n-1) - u(0) = f(n). \end{aligned} \tag{12}$$

The equivalence between the two problems is carried out by duplicating vertex 0 and labeling the new vertex as $n+1$, as it is shown in Figure 1.

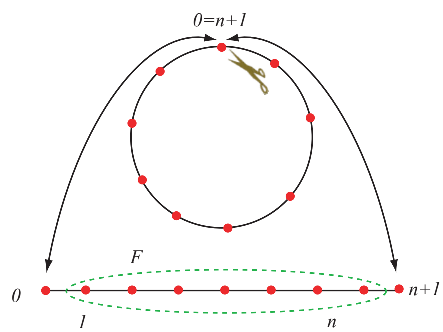

Figure 1. Periodic boundary conditions.

The first equation in (11) corresponds to a continuity condition, the second one is the first of (12), whereas the last equation in (12), corresponds to the equality $\mathcal{L}_q(u)(n) = f(n)$ on the path, since $u(0) = u(n+1)$.

Proposition 3.12. *The periodic boundary value problem is regular iff*

$$q \neq \cos\left(\frac{2k\pi}{n+1}\right),\; k = 0,\dots,\left\lceil \frac{n}{2} \right\rceil$$

and then its Green's function is given by

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

where $1 \le s \le n$ *and* $0 \le k \le n+1$.

Proof. The boundary polynomial is $P(z) = 2qU_n(z) - 2U_{n-1}(z) - 2 = 2\big(T_{n+1}(q) - 1\big)$ from Lemma 2.2. Therefore, the periodic boundary problem is regular iff $q \neq \cos\left(\frac{2k\pi}{n+1}\right)$, for any $k = 0,\dots,\left\lceil \frac{n}{2} \right\rceil$. Moreover, applying now Theorem 3.3, for

$k \leq s$ we obtain that

$$\begin{aligned} G_q(k,s) &= \frac{1}{P(q)}\Big[2qU_{n-s}(q) - U_{n-1-s}(q)\Big]U_{k-1}(q) \\ &\qquad\qquad - \frac{1}{P(q)}\Big[U_{n-s}(q)U_{k-2}(q) - U_{s-1-k}(q)\Big] \\ &= \frac{1}{P(q)}\Big[U_{n+1-s}(q)U_{k-1}(q) - U_{n-s}(q)U_{k-2}(q) + U_{s-k-1}(q)\Big] \\ &= \frac{1}{P(q)}\Big[U_{n-|k-s|}(q) + U_{|k-s|-1}(q)\Big] \end{aligned}$$

where we have take into account that

$$\begin{aligned} U_{n-s}(q)U_{k-2}(q) &= U_{n+1-s}(q)U_{k-1}(q) - U_0(q)U_{n+k-s}(q) \\ &= U_{n+1-s}(q)U_{k-1}(q) - U_{n+k-s}(q) \end{aligned}$$

and the same reasoning can be applied in the case $s \leq k$. □

Proposition 3.13. *If $2(1-q)$ is an eigenvalue of the periodic eigenvalue problem*

$$\mathcal{L}(u) = \lambda u \quad \text{on } F, \quad u(0) - u(n+1) = 2u(0) - u(1) - u(n) = 0,$$

then it is simple and either $q = \cos\left(\dfrac{2k\pi}{n+1}\right)$, $k = 1, \dots, \left\lfloor \dfrac{n}{2} \right\rfloor$ with $U_{k-1}(q)$ as an eigenfunction, or $q = \cos\left(\dfrac{2k\pi}{n}\right)$, $k = 0, \dots, \left\lfloor \dfrac{n-1}{2} \right\rfloor$ with $V_{k-1}(q)$ as an eigenfunction.

Proof. The boundary polynomial is $P(z) = 2(U_n(z) - U_{n-1}(z) - 1) = 2(V_n(z) - 1)$. Therefore, $2(1-q)$ is an eigenvalue iff $V_n(q) = 1$ and hence the expression for the eigenvalues follows. From part (i) of Proposition 3.8, we get that $\lambda = 2(1-q)$ is a double eigenvalue iff $U_{n-2}(q) = -2$ and $U_{n-1}(q) = -1$. Then, $0 = P(q) = 2U_n(q)$ which can not happen and hence any eigenvalue is simple. Moreover, from part (iii) of Proposition 3.8, $2U_{k-1}(q) - U_{k-2}(q) + U_{n-k-1}(q)$ is a non–null eigenfunction corresponding to λ and from Lemma 2.3 the above function is a multiple of either $U_{k-1}(q)$ or $V_{k-1}(q)$. □

4. ONE–SIDE BOUNDARY VALUE PROBLEMS

Our aim in this section is to analyze the so–called *one–side boundary value problems*; that is, the boundary value problems associated with the Schrödinger operator on a subset of a finite path whose boundary is located at one side of the path. Such a subset is denoted by $\widehat{F}$ and we can suppose without loss of generality that $\widehat{F} = \{0, 1, \dots, n\}$, which implies that its inner boundary is $\delta_-(\widehat{F}) = \{n\}$, whereas its outer boundary is $\delta_+(\widehat{F}) = \{n+1\}$.

Given $a, b \in \mathbb{C}$ such that $|a|+|b| > 0$, the linear map $\mathcal{B}\colon \mathcal{C}(V) \to \mathbb{C}$ determined by the expression

$$\mathcal{B}(u) = au(n) + bu(n+1), \qquad \text{for any } u \in \mathcal{C}(V) \tag{13}$$

is called *linear one–side boundary condition on* $\widehat{F}$ *with coefficients* a *and* b. In addition,

$$P(z) = bV_{n+1}(z) + aV_n(z) \tag{14}$$

is called *one–side boundary polynomial determined by* a *and* b.

For fixed $\mathcal{B}$ and given $f \in \mathcal{C}(V)$ and $g \in \mathbb{C}$, an *one–side boundary value problem problem on* $\widehat{F}$ consists in finding $u \in \mathcal{C}(V)$ such that

$$\mathcal{L}_q(u) = f, \quad \text{on} \quad \widehat{F}, \qquad \mathcal{B}(u) = g. \tag{15}$$

The problem is called *semi–homogeneous* when $g = 0$ and *homogeneous* if in addition $f = 0$.

We say that the boundary value problem (15) is *regular* if the corresponding homogenous boundary value problem $\mathcal{L}_q(u) = 0$ on $\widehat{F}$ and $\mathcal{B}(u) = 0$ has the null function as its unique solution. Newly (15) is regular iff for any data $f \in \mathcal{C}(V)$ and $g \in \mathbb{C}$ it has a unique solution.

When the problem (15) is regular we define the *Green's function for the one–side boundary value problem* (15) as the function $G_q \in \mathcal{C}(V \times \widehat{F})$ characterized by

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

The analysis of one–side boundary value problems can be easily derived from the study of two–side boundary value problems by observing that (15) can be re–written as the following two–side Sturm–Liouville problem

$$\mathcal{L}_q(u) = f, \quad \text{on} \quad F, \qquad (2q-1)u(0) - u(1) = f(0) \;\; \text{and} \;\; \mathcal{B}(u) = g. \tag{17}$$

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

Lemma 4.1. *Given* $g \in \mathbb{C}$, *then for any* $f \in \mathcal{C}(V)$ *the function* $u \in \mathcal{C}(V)$ *satisfies that* $\mathcal{L}_q(u) = f$ *on* $\widehat{F}$ *and* $\mathcal{B}(u) = g$ *iff the function*

$$v = u - \varepsilon_0 - \Big(2q - 1 - f(0)\Big)\varepsilon_1 - \frac{g(\bar{a}\varepsilon_n + \bar{b}\varepsilon_{n+1})}{|a|^2 + |b|^2}$$

satisfies that

$$\mathcal{L}_q(v) = f + \varepsilon_1 + \Big(2q - 1 - f(0)\Big)(\varepsilon_2 - 2q\varepsilon_1) + \frac{g(\bar{a}\varepsilon_{n-1} + (\bar{b} - 2q\bar{a})\varepsilon_n)}{|a|^2 + |b|^2}$$

on F *and* $(2q-1)v(0) - v(1) = \mathcal{B}(v) = 0$.

Observe that the boundary polynomial determined for the above Sturm-Liouville problem is given by

$$\begin{aligned}
P(z) &= b(2q-1)U_n(z) + (a(2q-1) - b)U_{n-1}(z) - aU_{n-2}(z) \\
&= b(2q-1)U_n(z) + (a(2q-1) - b)U_{n-1}(z) + aU_n(z) - 2qaU_{n-1}(z) \\
&= bU_{n+1}(z) + bU_{n-1}(z) - bU_n(z) - (a+b)U_{n-1}(z) + aU_n(z) \\
&= bV_{n+1}(z) + aV_n(z);
\end{aligned}$$

that is, the one–side boundary polynomial determined by a, b.

Proposition 4.2. *The one–side boundary value problem* (15) *is regular iff* $bV_{n+1}(q) + aV_n(q) \neq 0$ *and then its Green function is given by*

$$G_q(k,s) = \begin{cases} \dfrac{V_k(q)\Big(aU_{n-s-1}(q) + bU_{n-s}(q)\Big)}{bV_{n+1}(q) + aV_n(q)}, & 0 \le k \le s \le n, \\ \dfrac{V_s(q)\Big(aU_{n-k-1}(q) + bU_{n-k}(q)\Big)}{bV_{n+1}(q) + aV_n(q)}, & 1 \le s < k \le n+1. \end{cases}$$

Proof. The regularity condition is a straightforward consequence of the equivalence between the one–side boundary value problem (15) and the Sturm–Liouville problem (17). In addition, if $\widehat{G}_q$ is the Green function for the Sturm–Liouville problem, the above equivalence implies that

$$G_q(k,s) = \widehat{G}_q(k,s) = \begin{cases} \dfrac{V_k(q)\Big(aU_{n-s-1}(q) + bU_{n-s}(q)\Big)}{bV_{n+1}(q) + aV_n(q)}, & k \le s, \\ \dfrac{V_s(q)\Big(aU_{n-k-1}(q) + bU_{n-k}(q)\Big)}{bV_{n+1}(q) + aV_n(q)}, & s \le k, \end{cases}$$

for any $s = 1, \dots, n$ and any $k \in V$, where we have taken into account that $(2q-1)U_{k-1}(q) - U_{k-2}(q) = V_k(q)$. Moreover, applying Lemma 4.1, we obtain that

$$G_q(k,0) = \varepsilon_0(k) + 2(q-1)\varepsilon_1(k) + \widehat{G}_q(k,1) + 2(q-1)\Big(\widehat{G}_q(k,2) - 2q\widehat{G}_q(k,1)\Big).$$

For any $k \ge 2$, we obtain that

$$G_q(k,0) = \frac{V_0(q)\Big(aU_{n-k-1}(q) + bU_{n-k}(q)\Big)}{bV_{n+1}(q) + aV_n(q)},$$

since $V_2(q) - 2qV_1(q) = -1 = -V_0(q)$ and $V_1(q) - 2(q-1) = 1 = V_0(q)$.

When $k \le 1$,

$$\widehat{G}_q(k,1) + 2(q-1)\Big(\widehat{G}_q(k,2) - 2q\widehat{G}_q(k,1)\Big) = V_k(q)\left(\frac{aU_{n-1}(q) + bU_n(q)}{aV_n(q) + bV_{n+1}(q)} - 1\right),$$

since $aU_{n-3}(q) + bU_{n-2}(q) - 2q\Big(aU_{n-2}(q) + bU_{n-1}(q)\Big) = -aU_{n-1}(q) - bU_n(q)$. Then, for $k = 0$ we obtain that

$$G_q(0,0) = \frac{V_0(q)\Big(aU_{n-1}(q) + bU_n(q)\Big)}{bV_{n+1}(q) + aV_n(q)},$$

whereas for $k = 1$, we have

$$
\begin{aligned}
G_q(1,0) &= -1 + (2q-1)\left(\frac{aU_{n-1}(q) + bU_n(q)}{aV_n(q) + bV_{n+1}(q)}\right) \\
&= \frac{a\Big[(2q-1)U_{n-1}(q) - U_n(q) + U_{n-1}(q)\Big]}{bV_{n+1}(q) + aV_n(q)} \\
&\qquad\qquad + \frac{b\Big[(2q-1)U_n(q) - U_{n+1}(q) + U_n(q)\Big]}{bV_{n+1}(q) + aV_n(q)} \\
&= \frac{V_0(q)\Big(aU_{n-2}(q) + bU_{n-1}(q)\Big)}{bV_{n+1}(q) + aV_n(q)}. \qquad \square
\end{aligned}
$$

We say that $q \in \mathbb{C}$ is *a regular value* of the boundary value problem (15) if $bV_{n+1}(q) + aV_n(q) \neq 0$ and *a singular value* of the boundary value problem, otherwise. Observe that q is a singular value iff $2(1-q)$ is an eigenvalue of the following boundary eigenvalue problem

$$
\mathcal{L}(u) = \lambda u, \quad \text{on} \quad \widehat{F}; \quad \mathcal{B}(u) = 0. \tag{18}
$$

Proposition 4.3. *The eigenvalues of the one–side boundary eigenvalue problem*

$$
\mathcal{L}u = \lambda u, \quad \textit{on } \widehat{F}, \quad au(n) + bu(n+1) = 0
$$

are simple and $\lambda = 2(1-q)$ *is one of them iff* $bV_{n+1}(q) + aV_n(q) = 0$. *Moreover,* $aU_{n-k-1}(q) + bU_{n-k}(q)$ *is a non–null eigenfunction associated with* λ.

Proof. If $\lambda = 2(1-q)$ is an eigenvalue and u is an associated eigenfunction, then $\mathcal{L}_q(u) = 0$ on F. Therefore, if λ is a double eigenvalue of (15), then any solution of the homogeneous Schrödinger equation, $\mathcal{L}_q(v) = 0$ on F, verifies $av(n)+bv(n+1) = 0$. As $v(k) = \bar{b}U_{n-k-1}(q) - \bar{a}U_{n-k}(q)$ verifies that $av(n)+bv(n+1) = -(|a|^2+|b|^2) < 0$, any eigenvalue must be simple.

On the other hand, if u is an eigenfunction there exist $A, B \in \mathbb{C}$ such that $u(k) = AU_{n-k-1}(q) + BU_{n-k}(q)$ and $aB - bA = 0$. Therefore, u is a multiple of $aU_{n-k-1}(q) + bU_{n-k}(q)$. Observe that $\mathcal{L}_q(u)(0) = 0$, since $bV_{n+1}(q) + aV_n(q) = 0$. $\square$

5. THE POISSON EQUATION

In this section we study the Poisson equation associated with the Schrödinger operator on the finite path $\mathcal{P}_{n+2}$. The *Poisson equation on V* consists in finding $u \in \mathcal{C}(V)$ such that $\mathcal{L}_q(u) = f$ on V for any $f \in \mathcal{C}(V)$ and it is called *regular* if the corresponding homogeneous problem $\mathcal{L}_q(u) = 0$ on V has the null function as its unique solution or, in an equivalent manner, if $\mathcal{L}_q(u) = f$ has a unique solution for any data f. In addition, $P(z) = 2(q-1)U_{n+1}(z)$ is called *the Poisson polynomial.*

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

$$\mathcal{L}_q(G_q(\cdot, s)) = \varepsilon_s \quad \text{on } V, \qquad \text{for any } s \in V. \tag{19}$$

Newly, the analysis of the Poisson equation can be easily derived from the study of two–side boundary value problems since the Poisson equation can be seen as the following two–side Sturm–Liouville problem

$$\mathcal{L}_q(u) = f, \quad \text{on} \quad F, \qquad \mathcal{B}_1(u) = f(0) \quad \text{and} \quad \mathcal{B}_2(u) = f(n+1), \tag{20}$$

where $\mathcal{B}_1(u) = (2q-1)u(0) - u(1)$ and $\mathcal{B}_2(u) = -u(n) + (2q-1)u(n+1)$.

Lemma 5.1. *Given $f \in \mathcal{C}(V)$ the function $u \in \mathcal{C}(V)$ satisfies that $\mathcal{L}_q(u) = f$ iff the function*

$$v = u - \varepsilon_0 - \Big(2q - 1 - f(0)\Big)\varepsilon_1 - \Big(2q - 1 - f(n+1)\Big)\varepsilon_n - \varepsilon_{n+1}$$

satisfies that

$$\mathcal{L}_q(v) = f + \varepsilon_1 + \Big(2q-1-f(0)\Big)(\varepsilon_2 - 2q\varepsilon_1) + \Big(2q-1-f(n+1)\Big)(\varepsilon_{n-1} - 2q\varepsilon_n) + \varepsilon_n$$

on F and $(2q-1)v(0) - v(1) = v(n) - (2q-1)v(n+1) = 0$.

Observe that the boundary polynomial determined for the above Sturm-Liouville problem is given by

$$\begin{aligned} P(z) &= (2q-1)^2 U_n(z) - 2(2q-1)U_{n-1}(z) + U_{n-2}(z) \\ &= (4q^2 - 4q + 1)U_n(z) + (2-4q)U_{n-1}(z) - U_n(z) + 2qU_{n-1}(z) \\ &= (4q^2 - 4q)U_n(z) + (2-2q)U_{n-1}(z) = 2(q-1)U_{n+1}(z); \end{aligned}$$

that is, the Poisson polynomial.

Proposition 5.2. *The Poisson equation is regular iff $q \neq \cos\left(\dfrac{k\pi}{n+2}\right)$, for any $k = 0, \dots, n+1$ and then its Green's function is given by*

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

Proof. If $\widehat{G}_q$ denotes the Green's function of the above Sturm–Liouville problem, then from Corollary 3.11 we get that

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

The result follows applying the same reasoning as in the above section and Lemma 5.1.

Proposition 5.3. *If* $q_j = \cos\left(\dfrac{k\pi}{n+2}\right)$, $j = 0, \ldots, n$, *then the eigenvalues of the Poisson eigenvalue problem*

$$\mathcal{L}u = \lambda u, \quad \text{on } V$$

are $\lambda_j = 2 - 2q_j$, $j = 0, \ldots, n+1$. *Moreover, all of them are simple and* $V_k(q_j)$ *is a non–null eigenfunction associated with* λ_j.

Proof. The expression for the eigenvalues is a straightforward consequence of Proposition 5.2. Moreover, if $\lambda = 2(1-q)$ is an eigenvalue and u is an associated eigenfunction, then $\mathcal{L}_q(u) = 0$ on F. Therefore, if λ is a double eigenvalue of (15), then any solution of the homogeneous Schrödinger equation, $\mathcal{L}_q(v) = 0$ on F, verifies $(2q-1)v(0) - v(1) = 0$. As $v(k) = U_{k-1}(q)$ verifies that $(2q-1)v(0) - v(1) = -1$, any eigenvalue must be simple.

On the other hand, if u is an eigenfunction there exist $A, B \in \mathbb{C}$ such that $u(k) = AU_{k-1}(q) + BU_{k-2}(q)$ and $A = B(1-2q)$. Therefore, u is a multiple of $V_k(q)$. Observe that $\mathcal{L}_q(u)(n+1) = 0$, since $2(q-1)U_{n+1}(q) = 0$. □

Notice that taking into account that $V_k(1) = 1$, the above proposition when $j = 0$ gives the well–known result: 0 is an eigenvalue of the Poisson equation whose corresponding eigenfunctions are constant.

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