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JACOBI MATRICES AND BOUNDARY VALUE PROBLEMS IN DISTANCE-REGULAR GRAPHS*

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Abstract. Regular boundary value problems on a distance-regular graph associated with Schrödinger operators are analyzed. These problems include the cases in which the boundary has one or two vertices. In each case, the Green matrices are given in terms of two families of orthogonal polynomials, one of them corresponding with the distance polynomials of the distance-regular graphs.

Key words. Jacobi Matrices, Distance-regular Graphs, Boundary Value Problems.

AMS subject classifications. 15A15, 15F10.

1. Introduction. In this work we analyze linear boundary value problems on a finite distance-regular graph associated with Schrödinger operators with non-constant potential. The key idea is to take into account that each distance-regular graph can be seen as the covering of a weighted path. Then, we obtain the Green matrix associated with each regular boundary problem in terms of two families of orthogonal polynomials, one of them given by the so-called distance polynomials that are closely related with the intersection array of the graph. In spite of its relevance the Green function on a path have been obtained only for some boundary conditions, mainly for Dirichlet conditions or more generally for the so-called Sturm–Liouville boundary conditions, see [5, 7]. Recently, some of the authors have obtained the Green function on a path for general boundary value problems related to Schrödinger operator with constant conductances and potential, [3].

Our treatment of the boundary value problems in distance-regular graphs is analogous to the treatment of boundary value problems associated with ordinary differential equations, [6, Chapters 7,11,12]. The boundary value problems here considered are of two types that correspond to the cases in which the boundary has either two or one vertices. In each case, it is essential to describe the solutions of the Schröndinger equation on the interior nodes of the path. We show that it is possible to obtain explicitly such solutions in terms of the chosen orthogonal polynomials. As an immediate consequence of this property, we can easily characterize those boundary value

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problems that are regular.

2. Definitions and notation. A network $\Gamma = (V, E, c)$ is composed of a set of elements V called vertices, a set of pairs of vertices E called edges, and a symmetric map $c : V \times V \to [0, \infty)$ named the conductance, associated to the edges. The order of the network is $n + 1$, the number of its vertices. The Laplacian matrix of the network Γ is the matrix $\mathcal{L} \in \mathcal{M}_{n+1\times n+1}$ whose elements are $(\mathcal{L})_{ij} = -c(i, j)$ for $i \neq j$, $(\mathcal{L})_{ii} = \sum_{j=0}^{n} c(i, j)$ and 0 otherwise, for any $0 \leq i, j \leq n$. The Schrödinger matrix $\mathcal{L}_Q$ on Γ with potential Q is a perturbation of the Laplacian matrix defined as $\mathcal{L}_Q = \mathcal{L} + Q$, where $Q = \operatorname{diag}(q_0, \ldots, q_n)$, $q_i \in \mathbb{R}$. Through the paper, $\vec{u}$ stands for the tuple $\vec{u} = (u_0, \ldots, u_n) \in \mathbb{R}^{n+1}$.

Given $F \subset V$, the Schrödinger equation on F with data $\vec{f}$ is the equation

$$(\mathcal{L}_Q \vec{u}^T)_i = \vec{f}_i^T, \quad i \in F, \quad \vec{u}, \vec{f} \in \mathbb{R}^{n+1}, \tag{2.1}$$

and the equation $(\mathcal{L}_Q \vec{u}^T)_i = 0$, $i \in F$, $\vec{u} \in \mathbb{R}^{n+1}$ is called the corresponding homogeneous Schrödinger equation on F.

Furthermore, the boundary of F, $\delta(F)$, is the set of vertices of $V \setminus F$ connected to a vertex in F. A linear boundary condition $\vec{\mathcal{B}}$ on $\delta(F)$ is the equation $\vec{\mathcal{B}}\vec{u}^T = g$, where $\vec{\mathcal{B}}$, $\vec{u} \in \mathbb{R}^{n+1}$, $g \in \mathbb{R}$. A two-side boundary value problem on F consists of finding the vector $\vec{u} \in \mathbb{R}^{n+1}$ satisfying the Schrödinger equation and two linear boundary conditions $\vec{\mathcal{B}}_1, \vec{\mathcal{B}}_2 \in \mathbb{R}^{n+1}$ on $\delta(F)$, i.e., $\mathcal{L}_Q \vec{u}^T = \vec{f}$, $\vec{\mathcal{B}}_1 \vec{u}^T = g_1$, $\vec{\mathcal{B}}_2 \vec{u}^T = g_2$, for a given $\vec{f} \in \mathbb{R}^{n+1}$, g_1, $g_2 \in \mathbb{R}$.

Some authors have studied boundary value problems in a path P_{n+1}, considering as $F = \{1, \ldots, n-1\}$, with conductances $c(i, i+1) = c(i+1, i)$, and $c(i, j) = 0$ otherwise, for any $0 \leq i, j \leq n$. In this case, a vector $\vec{u} \in \mathbb{R}^{n+1}$ is a solution of the Schrödinger equation with data $\vec{f} \in \mathbb{R}^{n+1}$ on F, if and only if it satisfies

$$c(i, i+1)(u_i - u_{i+1}) + c(i, i-1)(u_i - u_{i-1}) + q_i u_i = f_i, \quad 1 \leq i \leq n-1. \tag{2.2}$$

Therefore, $\mathcal{L}_Q$ is a Jacobi matrix with nonpositive off–diagonal entries. By using the usual techniques for solving second order difference equations (see for instance [1]), given two solutions $\vec{u}$, $\vec{v} \in \mathbb{R}^{n+1}$ of the homogeneous Schrödinger equation on F, their associated Wronskian is $w[\vec{u}, \vec{v}](i) = u_i v_{i+1} - v_i u_{i+1}$, $0 \leq i \leq n-1$. Two solutions $\vec{u}$, $\vec{v} \in \mathbb{R}^{n+1}$ are linearly independent if and only if their Wronskian is not null. Moreover, it is known that the product $c(i, i+1) w[\vec{u}, \vec{v}](i) = c(0, 1) w[\vec{u}, \vec{v}](0)$ is constant since $\mathcal{L}_Q$ is a symmetric matrix. The Green matrix $\mathcal{G}_H \in \mathcal{M}_{n+1\times n+1}$ of the homogeneous Schrödinger equation on F is defined as follows: Given $\vec{u}$ and $\vec{v}$ two linearly independent solutions of the homogeneous Schrödinger equation, we consider

$$(\mathcal{G}_H)_{ij} = \frac{1}{c(j, j+1) w[\vec{u}, \vec{v}](j)} [u_i v_j - u_j v_i], \quad 0 \leq i, j \leq n.$$

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The above expression does not depend on the chosen linearly independent solutions $\vec{u}$ and $\vec{v}$, and its relation with initial value problems is given in the following results.

LEMMA 2.1. *The Green matrix $\mathcal{G}_H$ satisfies that for a fixed $j \in F$ the vector $\vec{y} \in \mathbb{R}^{n+1}$ such that $(\vec{y})_i = (\mathcal{G}_H)_{ij}$, for any $0 \le i \le n$, is the unique solution of the homogeneous Schrödinger equation on F satisfying also $(\mathcal{G}_H)_{jj} = 0$ and $(\mathcal{G}_H)_{j+1,j} = -1/c(j, j+1)$.*

Proof. First we prove that for a fixed j, $(\vec{y})_i = (\mathcal{G}_H)_{ij}$ satisfies the homogeneous Schrödinger equation for any $0 \le i \le n$:

$$c(i,i+1)((\mathcal{G}_H)_{ij} - (\mathcal{G}_H)_{i+1j}) + c(i,i-1)((\mathcal{G}_H)_{ij} - (\mathcal{G}_H)_{i-1j}) + q(i)(\mathcal{G}_H)_{ij} = 0$$

$$\iff \frac{1}{c(j,j+1)w[\vec{u},\vec{v}](j)} \cdot \Big[c(i,i+1)\Big((u_iv_j - u_jv_i) - (u_{i+1}v_j - u_jv_{i+1})\Big) +$$

$$+c(i,i-1)\Big((u_iv_j - u_jv_i) - (u_{i-1}v_j - u_jv_{i-1})\Big) + q(i)(u_iv_j - u_jv_i)\Big] =$$

$$= \frac{1}{c(j,j+1)w[\vec{u},\vec{v}](j)} \cdot \Big[\Big(c(i,i+1)(u_i - u_{i+1}) + c(i,i-1)(u_i - u_{i-1}) + q(i)u_i\Big)v_j +$$

$$+\Big(c(i,i+1)(v_i - v_{i+1}) + c(i,i-1)(v_i - v_{i-1}) + q(i)v_i\Big)u_j\Big] = 0.$$

Besides, it is straightforward that $(\mathcal{G}_H)_{jj} = 0$ and

$$(\mathcal{G}_H)_{j+1,j} = \frac{1}{c(j,j+1)w[\vec{u},\vec{v}](j)}[u_{j+1}v_j - u_jv_{j+1}] = -\frac{1}{c(j,j+1)}.$$

□

PROPOSITION 2.2. *Given $\vec{f} \in \mathbb{R}^{n+1}$, the vector $\vec{y} \in \mathbb{R}^{n+1}$ such that*

$$(\vec{y})_0 = 0, \quad (\vec{y})_i = \sum_{j=1}^{i} (\mathcal{G}_H)_{ij} f_j, \quad \text{for} \quad 1 \le i \le n,$$

is the unique solution of the problem $\mathcal{L}_Q \vec{y}^T = \vec{f}^T$, with conditions $(\vec{y})_0 = 0$, $(\vec{y})_1 = 0$.

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

$$(\mathcal{L}_Q\vec{y})_k = c(k,k+1)[(\vec{y})_k - (\vec{y})_{k+1}] + c(k,k-1)[(\vec{y})_k - (\vec{y})_{k-1}] + q(k)(\vec{y})_k$$

$$= c(k,k+1)\Big[\sum_{j=1}^{k}(\mathcal{G}_H)_{kj}f_j - \sum_{j=1}^{k+1}(\mathcal{G}_H)_{k+1j}f_j\Big] +$$

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$$c(k,k-1)\Big[\sum_{j=1}^{k}(\mathcal{G}_H)_{kj}f_j-\sum_{j=1}^{k-1}(\mathcal{G}_H)_{k-1j}f_j\Big]+q(k)\sum_{j=1}^{k}(\mathcal{G}_H)_{kj}f_j=$$

$$\sum_{j=1}^{k-1}\big[c(k,k+1)((\mathcal{G}_H)_{kj}-(\mathcal{G}_H)_{k+1j})+c(k,k-1)((\mathcal{G}_H)_{kj}-(\mathcal{G}_H)_{k-1j})+q(k)(\mathcal{G}_H)_{kj}\big]f_j+$$

$$\big[c(k,k+1)((\mathcal{G}_H)_{kk}-(\mathcal{G}_H)_{k+1k})+c(k,k-1)(\mathcal{G}_H)_{kk}+q(k)(\mathcal{G}_H)_{kk}\big]f_k$$

$$-c(k,k+1)((\mathcal{G}_H)_{k+1k+1}=c(k,k+1)[-(\mathcal{G}_H)_{k+1k}]f_k=f_k$$

Finally $(\vec{y})_0=\sum_{j=1}^{1}(\mathcal{G}_H)_{0j}f_j=(\mathcal{G}_H)_{00}f_0=0$. □

3. Jacobi matrices in distance-regular graphs. In a previous work [2], the authors define the Schrödinger matrix associated to a family of orthogonal polynomials in a weighted path of $n+2$ vertices, P_{n+2}, which is a Jacobi matrix, and study BVP associated to it. In this work we extend the problem to distance-regular graphs.

Consider a distance-regular graph $\Gamma=(V,E)$ of order n and degree δ. Let $\Gamma_i(u)$ denote the set of vertices of Γ that are at distance i from u, then $k_i=|\Gamma_i(u)|$ and it holds $k_ic_i=k_{i-1}b_{i-1}$, for any $0\le i\le d$. The intersection matrix of Γ is the non-symmetric Jacobi matrix

$$i(\Gamma)=\begin{pmatrix} a_0 & b_0 & \dots & 0 & 0\\ c_1 & a_1 & \dots & 0 & 0\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ 0 & 0 & \dots & a_{d-1} & b_{d-1}\\ 0 & 0 & \dots & c_d & a_d \end{pmatrix},$$

where $a_i+b_i+c_i=\delta$, $0\le i\le d$, $a_0=0$, $c_1=1$, $b_0=\delta$. For a given $0\le i\le d$, let A_i be the i-distance matrix of the graph, that is, the matrix whose elements $a^i_{uv}=1$ if the vertices u, v are at distance i. Note that $A_0=I$ and $A_1=A$ is the adjacency matrix of the graph. Now recall (see [4]) that in a distance-regular graph these matrices are polynomial, that is, $A_i=p_i(A)$. These polynomials are called the distance polynomials and are a family of orthogonal polynomials, as they satisfy the following recurrence relation

$$p_i(x)=\left(\frac{x}{c_i}-\frac{a_{i-1}}{c_i}\right)p_{i-1}(x)-\frac{b_{i-2}}{c_i}p_{i-2}(x),\quad 1\le i\le d, \tag{3.1}$$

where $p_{-1}(x)=0$, $p_0(x)=1$ and $p_1(x)=x$.

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Moreover, any distance-regular graph Γ can be seen as the covering of a weighted path P_{d+1}, with conductances $c(i,i-1)=b_i$, $c(i,i)=a_i$ and $c(i,i+1)=c_i$, for any $0\le i\le d-1$, and 0 otherwise, (see [5]). Therefore, considering a vertex $u\in V(\Gamma)$ and the set of vertices of the graph at maximum distance from u, that is $\Gamma_d(u)$, let F' be the rest of the vertices of the graph. To solve a BVP in the boundary $\delta(F')$ of the distance-regular graph is equivalent to solve it in the boundary of the set $F=\{1,\dots,d-1\}\subset V(P_{d+1})=\{0,\dots,d\}$. Observe that the adjacency matrix of the path is just $i(\Gamma)$, however is not a symmetric matrix. In order to obtain the Schrödinger matrix associated to P_{d+1} (which must be symmetric), we pre-multiply $i(\Gamma)$ on the left side by a diagonal matrix $H=\mathrm{diag}(k_0^{-1},\dots,k_d^{-1})$. We point out that this technique is also possible for Jacobi matrices, because the difference equations associated to them are second order difference equations. The weighted path associated to this symmetric matrix is the one having as conductances $c(i,i+1)=c_{i+1}/k_i$, for any $0\le i\le d-1$.

Therefore, for any $x\in\mathbb{R}$ we define the Schrödinger matrix $\mathcal{L}_Q(x)$ associated to a distance-regular graph, with potential $Q(x)=\mathrm{diag}(q_0(x),\dots,q_d(x))$ as the matrix

$$\mathcal{L}_Q(x)=\begin{pmatrix} (x-a_0)/k_0 & -b_0/k_1 & 0 & \dots & 0\\ -c_1/k_0 & (x-a_1)/k_1 & -b_1/k_2 & \dots & 0\\ 0 & -c_2/k_1 & (x-a_2)/k_2 & \dots & 0\\ \vdots & \vdots & \vdots & \ddots & \vdots\\ 0 & 0 & \dots & & (x-a_d)/k_d \end{pmatrix}, \tag{3.2}$$

where $q_i(x)=\frac{x-a_i}{k_i}-\frac{c_{i+1}}{k_i}-\frac{c_i}{k_{i-1}}$ is the potential of each vertex, for any $0\le i\le d-1$. Observe that the matrix is symmetric, since $b_{i-1}/k_i=c_i/k_{i-1}$, for $1\le i\le d-1$.

Now consider the following two families of orthogonal polynomials: the distance polynomials $\{p_n\}_{n=-1}^d$ and $\{r_n\}_{n=-1}^d$, with $r_0(x)=1$, $r_1(x)=r_{-1}(x)=ax+b$. By choosing as $b_{-1}=1$, $a=1/2$ and $b=0$ in the family $\{r_n\}_{n=-1}^d$, we also consider $x\neq 0$, we get the following result.

Lemma 3.1. *The vectors $\vec{p}=(p_0(x),\dots,p_d(x))$, $\vec{r}=(r_0(x),\dots,r_d(x))\in\mathbb{R}^{d+1}$ form a basis of the solution space of the homogenous Schrödinger equation if and only if $x\neq 0$. Their Wronskian is $w[\vec{p},\vec{r}](n)=x/2$, for any $0\le n\le d-1$. The Green matrix $\mathcal{G}_H$ of the homogenous Schrödinger equation is determined by*

$$(\mathcal{G}_H)_{ij}=\frac{2}{x}[p_i(x)r_j(x)-p_j(x)r_i(x)],\quad 0\le i,j\le d,\quad x\in\mathbb{R}. \tag{3.3}$$

Thus, the general solution $\vec{y}$ of the Schrödinger equation on F with data $\vec{f}\in\mathbb{R}^{d+1}$ is given for any $0\le i\le d$ by

$$(\vec{y})_i=\alpha p_i(x)+\beta r_i(x)+\sum_{k=1}^{i}(\mathcal{G}_H)_{ij}f_j,\quad \alpha,\beta\in\mathbb{R}.$$

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Proof. It is straightforward to check that $\vec{p}$ and $\vec{r}$ verify the homogeneous Schrödinger equation $\mathcal{L}_Q\vec{u}^T = \vec{0}$ as both verify the recurrence relation (3.1). Their Wronskian can be computed also by applying the same recurrence relation to the polynomials $p_{n+1}(x)$ and $r_{n+1}(x)$ as

$$c(n,n+1)w[\vec{p},\vec{r}](n) = \begin{vmatrix} p_n(x) & r_n(x) \\ p_{n+1}(x) & r_{n+1}(x) \end{vmatrix} = \frac{c_{n+1}}{k_n}[p_n(x)r_{n+1}(x) - p_{n+1}(x)r_n(x)] =$$
$$\cdots = \frac{c_1}{k_0}w[\vec{p},\vec{r}](0) = p_1(x) - r_1(x) = \frac{x}{2}.$$

Thus $\vec{p}$ and $\vec{r}$ are two independent solutions if and only if $x \neq 0$, and the general solution of the homogeneous Schrödinger equation is given by $\vec{y}_h = \alpha\vec{p} + \beta\vec{r}$, with α, $\beta \in \mathbb{R}$. Besides we have to find a particular solution of the Schr̈odinger equation. Consider the particular solution obtained in Proposition (2.2) $(\vec{y}_p)_k = \sum_{j=1}^{k}(\mathcal{G}_H)_{kj}f_j$, for any $1 \leq k \leq d$, $(\vec{y}_p)_0 = 0$, then, the general solution of the Schrödinger equation on F will be given by $\vec{y} = \vec{y}_h + \vec{y}_p$ and the result holds.
□

4. Green matrix of two side boundary value problems. In this section we study problems with two side boundary conditions. Recall that a two side boundary value problem on F consists in finding $\vec{u} \in \mathbb{R}^{d+1}$ such that

$$\mathcal{L}_Q\vec{u}^T = \vec{f}^T \quad \text{on } F, \quad \vec{\mathcal{B}}_1\vec{u}^T = g_1, \quad \vec{\mathcal{B}}_2\vec{u}^T = g_2, \tag{4.1}$$

for given $\vec{f} \in \mathbb{R}^{d+1}$ and $g_1, g_2 \in \mathbb{R}$, where the boundary conditions $\vec{\mathcal{B}}_1$ and $\vec{\mathcal{B}}_2$ are linearly independent, i.e., the rank of the following matrix is 2

$$\begin{pmatrix} \vec{\mathcal{B}}_1 \\ \vec{\mathcal{B}}_2 \end{pmatrix} = \begin{pmatrix} m_{10} & m_{11} & 0 & \dots & 0 & m_{1d-1} & m_{1d} \\ m_{20} & m_{21} & 0 & \dots & 0 & m_{2d-1} & m_{2d} \end{pmatrix}.$$

Let μ_{ij} be the determinant of each 2×2 submatrix, $\mu_{ij} = m_{1i}m_{2j} - m_{2i}m_{1j}$ for all $i, j \in B = \{0, 1, d-1, d\}$ and 0 otherwise. Besides $\mu_{ii} = 0$ and $\mu_{ij} = -\mu_{ji}$ for any $i, j \in B$. On the other hand consider the following associated BVP

$$\mathcal{L}_Q\vec{u}^T = \vec{0} \quad \text{on } F, \quad \vec{\mathcal{B}}_1\vec{u}^T = g_1, \quad \vec{\mathcal{B}}_2\vec{u}^T = g_2, \tag{4.2}$$

$$\mathcal{L}_Q\vec{u}^T = \vec{f}^T \quad \text{on } F, \quad \vec{\mathcal{B}}_1\vec{u}^T = 0, \quad \vec{\mathcal{B}}_2\vec{u}^T = 0, \tag{4.3}$$

$$\mathcal{L}_Q\vec{u}^T = \vec{0} \quad \text{on } F, \quad \vec{\mathcal{B}}_1\vec{u}^T = 0, \quad \vec{\mathcal{B}}_2\vec{u}^T = 0. \tag{4.4}$$

The last problem (4.4) is called the homogeneous BVP. The BVP (4.1) is regular if and only if the homogeneous BVP (4.4) has the null vector as its unique solution.

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It follows by standard arguments that the BVP (4.1) is regular if and only if for each $\vec{f} \in \mathbb{R}^{d+1}$ has a unique solution. Moreover the homogeneous BVP problem (4.4) has a unique solution $\vec{y} = \alpha\vec{v}_1 + \beta\vec{v}_2$, where $\vec{v}_1$, $\vec{v}_2$ are two independent solutions of the homogeneous Schrödinger equation, if and only if the coefficient matrix of the following linear system is nonsingular

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

Therefore the homogeneous BVP problem (4.4) is regular if and only if the determinant of this matrix, that is, the boundary polynomial $P_{\mathcal{B}}(x) = \mathcal{B}_1\vec{v}_1 \cdot \mathcal{B}_2\vec{v}_2 - \mathcal{B}_2\vec{v}_1 \cdot \mathcal{B}_1\vec{v}_2$ is not null, and hence, it also holds that the BVP (4.1) is regular.

Now by using Lemma 3.1, we consider two independent solutions of the homogeneous Schrödinger equation, $\vec{p} = (p_0(x), \dots, p_d(x))$ and $\vec{r} = (r_0(x), \dots, r_d(x))$, and compute the boundary polynomial in this case

$$P_{\mathcal{B}}(x) = \mathcal{B}_1\vec{p} \cdot \mathcal{B}_2\vec{r} - \mathcal{B}_2\vec{p} \cdot \mathcal{B}_1\vec{r} = \sum_{i,j \in B} \mu_{ij} p_i(x) r_j(x) = \frac{x}{2} \sum_{\substack{i<j \\ i,j \in B}} \mu_{ij} (\mathcal{G}_H)_{ij}.$$

Furthermore the unique solution for problem (4.1) can be obtained as the sum of two solutions $\vec{u} = \vec{u}_1 + \vec{u}_2$, the respective unique solutions of both problems (4.2) and (4.3). Nevertheless, the following lemma shows that any general BVP (4.1) is equivalent to a semi-homogenous one of type (4.3).

LEMMA 4.1. *Let $\vec{\mathcal{B}}_1$, $\vec{\mathcal{B}}_2$ be two linear boundary conditions and let $\vec{u}_p \in \mathbb{R}^{d+1}$ such that $\vec{\mathcal{B}}_1\vec{u}_p^T = g_1$, $\vec{\mathcal{B}}_2\vec{u}_p^T = g_2$. Then $\vec{u} \in \mathbb{R}^{d+1}$ is a solution of the boundary value problem $\mathcal{L}_Q\vec{u}^T = \vec{f}$ on F, $\vec{\mathcal{B}}_1\vec{u}^T = g_1$, $\vec{\mathcal{B}}_2\vec{u}^T = g_2$ if and only if $\vec{v} = \vec{u} - \vec{u}_p$ is the solution of the boundary value problem $\mathcal{L}_Q\vec{v} = \vec{f} - \mathcal{L}_Q\vec{u}_p^T$ on F, $\vec{\mathcal{B}}_1\vec{v}^T = 0$, $\vec{\mathcal{B}}_2\vec{v}^T = 0$.*

Therefore, just by considering the vector $\vec{u}_p = \alpha\vec{\varepsilon}_0 - \beta\vec{\varepsilon}_1 - \gamma\vec{\varepsilon}_{d-1} - \delta\vec{\varepsilon}_d$ where $\vec{\varepsilon}_i$ is the i-th characteristic vector, $\alpha, \beta, \gamma, \delta \in \mathbb{R}$, the boundary value problem (4.1) can be restricted to the semi-homogeneous boundary problem (4.3) with

$$\begin{aligned} \mathcal{L}_Q\vec{v}^T = \vec{f} &+ \left(-\beta\frac{(x-a_1)}{k_1} + \alpha\frac{c_1}{k_0}\right)\vec{\varepsilon}_1 + \beta\frac{c_2}{k_1}\beta\vec{\varepsilon}_2 + \gamma\frac{b_{d-2}}{k_{d-1}}\beta\vec{\varepsilon}_{d-2} \\ &+ \left(-\gamma\frac{(x-a_{d-1})}{k_{d-1}} + \delta\frac{b_{d-1}}{k_d}\right)\vec{\varepsilon}_{d-1}, \end{aligned}$$

on F and boundary conditions $\vec{\mathcal{B}}_1\vec{v}^T = \vec{\mathcal{B}}_2\vec{v}^T = 0$. Thus, we focus on solving regular BPV of type (4.3).

The solution of any regular BVP (4.3) can be obtained by considering its resolvent

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kernel, *i.e.*, the matrix $\mathcal{G}_Q(x) \in \mathcal{M}_{V\times F}$ such that fixing a column $s \in F$

$$\sum_{k=0}^{d} \mathcal{L}_Q \cdot (\mathcal{G}_Q(x))_{\cdot s} = \vec{\epsilon_s}, \quad \vec{\mathcal{B}_1} \cdot (\mathcal{G}_Q(x))_{\cdot s} = \vec{\mathcal{B}_2} \cdot (\mathcal{G}_Q(x))_{\cdot s} = 0.$$

This matrix is named the *Green matrix* for Problem (4.1). Notice that for any $\vec{f} \in \mathbb{R}^{d+1}$ the unique solution of the problem (4.3) is given by $\vec{u}_k = \sum_{s=1}^{d-1}(\mathcal{G}_Q(x))_{ks} \cdot \vec{f}_s$, for any $k \in V$.

THEOREM 4.2. *The BVP (4.1) is regular if and only if*

$$P_{\mathcal{B}}(x) = \frac{x}{2} \sum_{\substack{i<j \\ i,j\in\{1,\dots,d-1\}}} \mu_{ij}(\mathcal{G}_H(x))_{ij} \neq 0$$

The Green matrix of the BVP problem (4.1), for any $s \in F$, $k \in V$, is the matrix whose ks-element, $(\mathcal{G}_Q(x))_{ks}$, is given by

$$\frac{x}{2P_{\mathcal{B}}(x)} \left[\frac{k_{d-1}}{c_d}\mu_{d-1d}(\mathcal{G}_H(x))_{sk} + \sum_{i=0}^{1}(\mathcal{G}_H(x))_{ik}\left(\sum_{j=d-1}^{d}\mu_{ij}(\mathcal{G}_H(x))_{sj}\right)\right] + \begin{cases} 0 & k \le s, \\ (\mathcal{G}_H(x))_{ks} & k \ge s. \end{cases}$$

Proof. The unique solution of the problem (4.3) can be expressed as the sum of the general solution of the homogenous Schrödinger equation plus a particular solution of the problem (4.3): $\vec{u} = \vec{u}_h + \vec{u}_p$. The general solution of the homogeneous Schrödinger equation $\vec{u}_h$ is given by Lemma 3.1 and we can also consider as $\vec{u}_p$ the one computed there, that is, $\vec{u}_p = \mathcal{G}_H(x)\vec{f}$. Then $\vec{u} = a\vec{p} + b\vec{r} + \mathcal{G}_H(x)\vec{f}$, and we just have to impose the boundary conditions $\vec{\mathcal{B}_1}\vec{u} = 0$, $\vec{\mathcal{B}_2}\vec{u} = 0$ to obtain the value of the parameters a, $b \in \mathbb{R}$ of the unique solution of problem (4.3). Observe also from the Lemma that for a fixed column $s \in F$, $k \in V$, the Green matrix $\mathcal{G}_Q(x)$ of the boundary value problem (4.3) is given by

$$(\mathcal{G}_Q(x))_{ks} = a(s)p_k(x) + b(s)r_k(x) + \begin{cases} 0 & \text{if} \quad k < s, \\ (\mathcal{G}_H(x))_{ks} & \text{if} \quad k \ge s. \end{cases}$$

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

$$\begin{pmatrix} \vec{\mathcal{B}_1}\vec{p}^T & \vec{\mathcal{B}_1}\vec{r}^T \\ \vec{\mathcal{B}_2}\vec{p}^T & \vec{\mathcal{B}_2}\vec{r}^T \end{pmatrix} \begin{pmatrix} a(s) \\ b(s) \end{pmatrix} = -\begin{pmatrix} \vec{\mathcal{B}_1}(\mathcal{G}_H(x))_{\cdot s} \\ \vec{\mathcal{B}_2}(\mathcal{G}_H(x))_{\cdot s} \end{pmatrix},$$

and thus

$$P_{\mathcal{B}}(x)a(s) = \vec{\mathcal{B}_1}\vec{r}^T\vec{\mathcal{B}_2}(\mathcal{G}_H(x))_{\cdot s} - \vec{\mathcal{B}_2}\vec{r}^T\vec{\mathcal{B}_1}(\mathcal{G}_H(x))_{\cdot s},$$
$$P_{\mathcal{B}}(x)b(s) = \vec{\mathcal{B}_1}\vec{r}^T\vec{\mathcal{B}_2}(\mathcal{G}_H(x))_{\cdot s} - \vec{\mathcal{B}_2}\vec{r}^T\vec{\mathcal{B}_1}(\mathcal{G}_H(x))_{\cdot s}.$$

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From Proposition 2.2 we have that for $i = 1, 2$

$$\vec{\mathcal{B}}_i \mathcal{G}_H(x)_{\cdot s} = m_{id-1}(\mathcal{G}_H(x))_{d-1s} + m_{id}(\mathcal{G}_H(x))_{ds}.$$

And thus

$$P_{\mathcal{B}}(x)a(s) = \sum_{i=0}^{1}\sum_{j=d-1}^{d} \mu_{ij} r_i(x)(\mathcal{G}_H(x))_{js} - \mu_{d-1d}(\mathcal{G}_H(x))_{d-1d} r_s(x),$$

$$P_{\mathcal{B}}(x)b(s) = -\sum_{i=0}^{1}\sum_{j=d-1}^{d} \mu_{ij} p_i(x)(\mathcal{G}_H(x))_{js} + \mu_{d-1d}(\mathcal{G}_H(x))_{d-1d} p_s(x).$$

Finally we obtain $P_{\mathcal{B}}(x)[a(s)p_k(x) + b(s)r_k(x)] =$

$$\frac{x}{2}\left[\mu_{d-1d}(\mathcal{G}_H(x))_{d-1d}(\mathcal{G}_H(x))_{sk} + \sum_{i=0}^{1}(\mathcal{G}_H(x))_{ik}\left(\sum_{j=d-1}^{d}\mu_{ij}(\mathcal{G}_H(x))_{sj}\right)\right].$$

□

Finally, we would like to point out that the solution for problem (4.2) can be also expressed in terms of the homogeneous problem Green matrix $\mathcal{G}_H(x)$. A vector $\vec{u}_1 \in \mathbb{R}^{d+1}$ is a solution of problem (4.2) if and only if $\vec{u}_1 = \alpha\vec{u} + \beta\vec{v}$, where $\alpha, \beta \in \mathbb{R}$ and $\{\vec{u}, \vec{v}\}$ is a basis of solutions of the homogeneous equation on F, satisfies

$$\vec{\mathcal{B}}_1 \vec{u}_1^T = 0, \quad \vec{\mathcal{B}}_2 \vec{u}_1^T = 0 \iff \begin{pmatrix} \mathcal{B}_1\vec{u}^T & \mathcal{B}_1\vec{v}^T \\ \mathcal{B}_2\vec{u}^T & \mathcal{B}_2\vec{v}^T \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} g_1 \\ g_2 \end{pmatrix}.$$

The parameters α and β can be computed just by solving the above linear system, obtaining that

$$\alpha = \frac{1}{P_{\mathcal{B}}(x)}[\vec{\mathcal{B}}_2\vec{v}^T g_1 - \vec{\mathcal{B}}_1\vec{v}^T g_2], \quad \beta = \frac{1}{P_{\mathcal{B}}(x)}[\vec{\mathcal{B}}_1\vec{u}^T g_2 - \vec{\mathcal{B}}_2\vec{u}^T g_1],$$

and therefore, the solution $\vec{u}_1 = \alpha\vec{u} + \beta\vec{v}$ of problem (4.2) is given by

$$(\vec{u}_1)_k = \frac{x}{2P_{\mathcal{B}}(x)}\left[\sum_{i\in\{0,1,d-1,d\}}(\mathcal{G}_H(x))_{ik}(m_{1i}g_2 - m_{2i}g_1)\right]. \tag{4.5}$$

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

The pair of boundary conditions $(\vec{\mathcal{B}}_1, \vec{\mathcal{B}}_2)$ is called *unilateral* if either $m_{1,j} = m_{2,j} = 0$, for any $j \in \{d-1, d\}$ (initial value problem) or $m_{1,i} = m_{2,i} = 0$, for any

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$i \in \{0,1\}$ (final value problem). Therefore for the initial value problem we have that only $\mu_{01} \neq 0$ and $P_{\mathcal{B}}(x) = \frac{x}{2}\mu_{01}(\mathcal{G}_H)_{01} = -\mu_{01}$, and for the final value problem only $\mu_{d-1,d} \neq 0$ and $P_{\mathcal{B}}(x) = \frac{x}{2}\mu_{d-1d}(\mathcal{G}_H)_{d-1d} = \frac{x}{2}\frac{k_{d-1}}{c_d}\mu_{d-1d}$. Observe that in both cases since the boundary conditions are linearly independent, both unilateral boundary problems are regular. Therefore, any unilateral pair is equivalent to either (u_0, u_1) for initial value problems, or (u_{d-1}, u_d) for final value problems.

Corollary 5.1. *The Green matrix for the initial value problem is given by*

$$(\mathcal{G}_Q(x))_{ks} = \begin{cases} 0 & k \leq s, \\ (\mathcal{G}_H)_{ks} & k \geq s. \end{cases}$$

Whereas the Green matrix for the final value problem is

$$(\mathcal{G}_Q(x))_{ks} = \frac{2}{xP_{\mathcal{B}}(x)}\frac{k_{d-1}}{c_d}\mu_{d-1d}(\mathcal{G}_H)_{sk} + \begin{cases} (\mathcal{G}_H)_{ks} & k \leq s, \\ 0 & k \geq s, \end{cases}$$

for any $s \in F$, $k \in V$.

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

$$\vec{\mathcal{B}_1}\vec{u} = au_0 + bu_1 \quad \text{and} \quad \vec{\mathcal{B}_2}\vec{u} = cu_{d-1} + du_d, \tag{5.1}$$

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

Corollary 5.2. *Given $a,b,c,d \in \mathbb{R}$ such that $(|a|+|b|)(|c|+|d|) > 0$ and the Sturm-Liouville boundary conditions, then*

$$P_B(x) = \frac{x}{2}\Big[\big(a + bp_1(x)\big)\big(cr_{d-1}(x) + dr_d(x)\big) - \big(a + br_1(x)\big)\big(cp_{d-1}(x) + dp_d(x)\big)\Big],$$

and the Green matrix for the Sturm-Liouville BVP is for any $0 \leq k \leq s \leq d-1$ and $1 \leq s$; whereas

$$\begin{aligned}(\mathcal{G}_Q(x))_{ks} = \tfrac{2}{xP_{\mathcal{B}}(x)} \quad & \Big[\big(a + bp_1(x)\big)r_k(x) - \big(a + br_1(x)\big)p_k(x)\Big] \\ \cdot \quad & \Big[\big(dr_d(x) + cr_{d-1}(x)\big)p_s(x) - \big(dp_d(x) + cp_{d-1}(x)\big)r_s(x)\Big],\end{aligned}$$

for any $d \geq k \geq s \geq 1$ and $s \leq d-1$. As a consequence, the boundary polynomial for the Dirichlet problem is

$$P_B(x) = \frac{1}{2}xad\Big[(1 + p_1(x)r_d(x)) - (1 + r_1(x)p_d(x))\Big],$$

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and hence it is regular if and only if $r_d(x) \neq p_d(x)$, and the Green's matrix is given by

$$\mathcal{G}_Q(x)_{ks} = \begin{cases} \dfrac{\Big(p_k(x)-r_k(x)\Big)\Big(r_d(x)p_s(x)-p_d(x)r_s(x)\Big)}{p_1(x)\Big(r_d(x)-p_d(x)\Big)}, & k \leq s \\[2ex] \dfrac{\Big(p_s(x)-r_s(x)\Big)\Big(r_d(x)p_k(x)-p_d(x)r_k(x)\Big)}{p_1(x)\Big(r_d(x)-p_d(x)\Big)}, & k \geq s. \end{cases}$$

Finally, for Neumann boundary problem, the boundary polynomial is

$$P_B(x) = \frac{x}{2}ac\Big[\big(1-p_1(x)\big)\big(r_{d-1}(x)-r_d(x)\big) - \big(1-r_1(x)\big)\big(p_{d-1}(x)-p_d(x)\big)\Big]$$

and the (k,s)-element of the Green matrix, $(\mathcal{G}_Q(x))_{ks}$, for the Neumann problem is

$$\frac{\Big[(1-r_1(x))p_k(x)-\Big(1-p_1(x)\Big)r_k(x)\Big]\Big[r_s(x)\Big(p_d(x)-p_{d-1}(x)\Big)-p_s(x)\Big(r_d(x)-r_{d-1}(x)\Big)\Big]}{p_1(x)\Big[\Big(1-r_1(x)\Big)\Big(p_d(x)-p_{d-1}(x)\Big)-\Big(1-p_1(x)\Big)\Big(r_d(x)-r_{d-1}(x)\Big)\Big]}$$

for any $0 \leq k \leq s \leq d-1$ and $1 \leq s$; whereas

$$\frac{\Big[(1-r_1(x))p_s(x)-\Big(1-p_1(x)\Big)r_s(x)\Big]\Big[r_k(x)\Big(p_d(x)-p_{d-1}(x)\Big)-p_k(x)\Big(r_d(x)-r_{d-1}(x)\Big)\Big]}{p_1(x)\Big[\Big(1-r_1(x)\Big)\Big(p_d(x)-p_{d-1}(x)\Big)-\Big(1-p_1(x)\Big)\Big(r_d(x)-r_{d-1}(x)\Big)\Big]}$$

for any $d \geq k \geq s \geq 1$ and $s \leq d-1$.

6. One side boundary problems. In the last section we analyze one side boundary value problems; i.e, the boundary conditions are located at one side of the path P_{n+2}. So if we consider the vertex subset $\widehat{F} = \{0, 1, \ldots, d-1\}$, the vector $\vec{\mathcal{B}} = (0, \ldots, 0, a, b) \in \mathbb{R}^{d+1}$ such that

$$\mathcal{B}\vec{u}^T = au_{d-1} + bu_d, \quad \text{for any } \vec{u} \in \mathbb{R}^{d+1},$$

is a *linear one side boundary condition on* $\widehat{F}$ with coefficients a, $b \in \mathbb{R}$, wherever $|a| + |b| > 0$. Moreover, an *one side boundary value problem on* $\widehat{F}$ consists in finding $\vec{u} \in \mathbb{R}^{d+1}$ such that

$$\mathcal{L}_Q\vec{u}^T = \vec{f} \text{ on } \widehat{F}, \quad \vec{\mathcal{B}}\vec{u} = g, \tag{6.1}$$

for a given $\vec{f} \in \mathbb{R}^{d+1}$ and $g \in \mathbb{R}$. The problem is called semi–homogenous when $g = 0$ and homogeneous if, in addition, $\vec{f} = \vec{0} \in \mathbb{R}^{d+1}$. Again, the one side boundary value problem is regular if the corresponding homogeneous problem has the null function as its unique solution; equivalently, (6.1) is regular if and only if for any data $\vec{f} \in \mathbb{R}^{d+1}$

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and $g \in \mathbb{R}$ it has a unique solution. In this case, the *Green function for the one side boundary value problem (6.1)* is the function $\mathcal{G}_Q(x) \in \mathcal{M}_{V\times\widehat{F}}$ characterized by

$$\mathcal{L}_Q(\mathcal{G}_Q(x))_{\cdot,s} = \varepsilon_s \ \text{ on } \widehat{F}, \quad \vec{\mathcal{B}}(\mathcal{G}_Q(x))_{\cdot,s} = 0, \quad \text{for any } s \in \widehat{F}. \tag{6.2}$$

The analysis of one side boundary value problems can be easily derived from the study of two side boundary value problems by observing that (6.1) can be re–written as a two side Sturm–Liouville problem as follows

$$\mathcal{L}_Q\vec{u}^T = \vec{f} \text{ on } F, \quad (x-a_0)u_0 - c_1u_1 = k_0f_0, \quad \vec{\mathcal{B}}\vec{u} = g. \tag{6.3}$$

Corollary 6.1. *Given the one side boundary value problem (6.1), then*

$$\begin{aligned} P_{\mathcal{B}}(x) = \ & \tfrac{x}{2}\Big[\big(x-a_0-c_1p_1(x)\big)\big(ar_{d-1}(x)+br_d(x)\big) \\ & -\big(x-a_0-c_1r_1(x)\big)\big(ap_{d-1}(x)+bp_d(x)\big)\Big], \end{aligned}$$

and the Green function is

$$\begin{aligned} \mathcal{G}_Q(x)_{ks} = \ & \frac{\Big[r_k(x)\Big(1-p_1(x)\Big)-p_k(x)\Big]}{p_1(x)\Big[\Big(p_1(x)-1\Big)\Big(br_d(x)+ar_{d-1}(x)\Big)+bp_d(x)+ap_{d-1}(x)\Big]} \\ & \times \ \Big[\Big(br_d(x)+ar_{d-1}(x)\Big)p_s(x) - \Big(bp_d(x)+ap_{d-1}(x)\Big)r_s(x)\Big] \end{aligned}$$

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

$$\begin{aligned} \mathcal{G}_Q(x)_{ks} = \ & \frac{\Big[r_s(x)\Big(1-p_1(x)\Big)-p_s(x)\Big]}{p_1(x)\Big[\Big(p_1(x)-1\Big)\Big(br_d(x)+ar_{d-1}(x)\Big)+bp_d(x)+ap_{d-1}(x)\Big]} \\ & \times \ \Big[\Big(br_d(x)+ar_{d-1}(x)\Big)p_k(x) - \Big(bp_d(x)+ap_{d-1}(x)\Big)r_k(x)\Big] \end{aligned}$$

for any $d \ge k \ge s \ge 0$ *and* $s \le d-1$.

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