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# Explicit inverse of a tridiagonal $(p, r)$ -Toeplitz matrix

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## Abstract

We have named tridiagonal  $(p, r)$ -Toeplitz matrix to those tridiagonal matrices in which each diagonal is a quasi-periodic sequence,  $d(p + j) = rd(j)$ , so with period  $p \in \mathbb{N}$  but multiplied by a real number  $r$ . We present here the necessary and sufficient conditions for the invertibility of this kind of matrices and explicitly compute their inverse. The techniques we use are related with the solution of boundary value problems associated to second order linear difference equations. These boundary value problems can be expressed throughout the *discrete Schrödinger operator* and their solutions can be computed using recent advances in the study of linear difference equations with quasi-periodic coefficients. The conditions that ensure the uniqueness solution of the boundary value problem lead us to the invertibility conditions for the matrix, whereas the solutions of the boundary value problems provides the entries of the inverse matrix.

*Keywords:* tridiagonal matrices, quasi-periodic sequences, second order linear difference equations, boundary value problems, discrete Schrödinger operator

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## 1. Preliminaries

Tridiagonal matrices are commonly named Jacobi matrices, and the computation of its inverse is in relation with discrete Schrödinger operators on a finite path. If we consider  $n \in \mathbb{N} \setminus \{0\}$ , the set  $\mathcal{M}_n(\mathbb{R})$  of matrices with order  $n$  and real coefficients, and the sequences  $\{a(k)\}_{k=0}^n, \{b(k)\}_{k=0}^{n+1}, \{c(k)\}_{k=0}^n \subset \mathbb{R}$ , a Jacobi matrix  $J(a, b, c) \in \mathcal{M}_{n+2}(\mathbb{R})$  has the following structure:

$$J(a, b, c) = \begin{bmatrix} b(0) & -a(0) & 0 & \cdots & 0 & 0 \\ -c(0) & b(1) & -a(1) & \cdots & 0 & 0 \\ 0 & -c(1) & b(2) & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & b(n) & -a(n) \\ 0 & 0 & 0 & \cdots & -c(n) & b(n+1) \end{bmatrix} \quad (1)$$

As in [1], we have chosen to write down the coefficients outside the main diagonal with negative sign. This is only a convenience convention, motivated by the mentioned relationship between Jacobi matrices

and Schrödinger operators on a path, that we will use to analyze the invertibility of the Jacobi matrix. We must make also some assumptions about the coefficients of the matrix to avoid trivial situations or problems reducible to a minor order. We will require  $a(k) \neq 0$  and  $c(k) \neq 0$ ,  $k = 0, \dots, n$ , so in other case  $J(a, b, c)$  is reducible and the inversion problem leads to the invertibility of a matrix of lower order. Moreover, the values of the coefficients  $a$  and  $c$  on  $n + 1$  have no influence in the analysis of the matrix, so, without loss of generality, we can impose  $a(n + 1) = c(n)$  and  $c(n + 1) = a(n)$ . In the sequel, we also assume that  $0^0 = 1$  and the usual convention that empty sums and empty products are defined as 0 and 1 respectively.

The matrix  $J(a, b, c)$  is invertible iff for each  $f \in \mathbb{R}^{n+2}$  there exists  $u \in \mathbb{R}^{n+2}$  such that  $J(a, b, c)u = f$  so, such that

$$\begin{cases} b(0)u(0) - a(0)u(1) = f(0), \\ -a(k)u(k + 1) + b(k)u(k) - c(k - 1)u(k - 1) = f(k), & k = 1, \dots, n, \\ -c(n)u(n) + b(n + 1)u(n + 1) = f(n + 1). \end{cases} \quad (2)$$

We can recognize in previous identities the structure of a boundary value problem associated to a second order linear difference equation with coefficients  $a, b, c$  and data  $f$  or, equivalently, a Schrödinger operator  $\mathcal{L}_q$  on the directed path  $I = \{0, \dots, n + 1\}$  with conductance  $\gamma(k, k + 1) = a(k)$  and  $\gamma(k + 1, k) = c(k)$ , and potential  $q(k) = b(k) - a(k) - c(k - 1)$ ,  $k = 1, \dots, n$ .

Let  $\mathcal{C}(I)$  be the vector space of real functions whose domain is the set  $I$ , which has boundary  $\delta(I) = \{0, n + 1\}$  and hence  $\overset{\circ}{I} = \{1, \dots, n\}$ . Given  $f \in \mathcal{C}(I)$ , the equation  $\mathcal{L}_q(u)(k) = f(k)$ ,  $k \in I$  is the Schrödinger equation on  $I$  with data  $f$ , whereas the equation  $\mathcal{L}_q(u)(k) = 0$ ,  $k \in I$ , is the corresponding homogeneous Schrödinger equation on  $I$ . When  $u \in \mathcal{C}(I)$  satisfies one of the above identities,  $u$  is named a solution of the corresponding equation. Using this functional notation, Equations (2) are equivalent to the Sturm–Liouville value problem

$$\mathcal{L}_q(u) = f \text{ on } \overset{\circ}{I}, \quad \mathcal{L}_q(u)(0) = f(0) \text{ and } \mathcal{L}_q(u)(n + 1) = f(n + 1). \quad (3)$$

Therefore,  $J(a, b, c)$  is invertible iff  $\mathcal{L}_q$  is invertible. In terms of the boundary value problem, the invertibility conditions for  $J(a, b, c)$  are exactly the same conditions to ensure that the boundary value problem is *regular*, that is with a unique solution, and the computation of its inverse can be reduced to the calculus of this solution. Implicitly or explicitly, to determine the solutions for initial or final value problems is the strategy followed to achieve the inversion of tridiagonal matrices, see i.e. [2, 3, 4, 5, 6, 7, 8, 9], but either it is not analyzed the general case, or the explicit expressions of these solutions are not obtained, or the expressions obtained are excessively cumbersome.

Given two solutions  $u, v \in \mathcal{C}(I)$  of the homogeneous Schrödinger equation, their *wronskian* or *casoratian*,

see [10], is  $w[u, v] \in \mathcal{C}(I)$  defined as

$$w[u, v](k) = \det \begin{bmatrix} u(k) & v(k) \\ u(k+1) & v(k+1) \end{bmatrix} = u(k)v(k+1) - v(k)u(k+1), \quad 0 \leq k \leq n,$$

and as  $w[u, v](n+1) = w[u, v](n)$ . The wronskian is a skew-symmetric bilinear form and either  $w[u, v] = 0$  or  $w[u, v] \neq 0$  for any  $k \in \overset{\circ}{I} \cup \{0\}$ . Moreover,  $u$  and  $v$  are linearly independent iff their wronskian is non null

25 and then  $\{u, v\}$  form a basis of solutions of the homogeneous Schrödinger equation on  $I$ .

It will be very useful to introduce the *companion function* defined as

$$\rho(k) = \prod_{s=0}^{k-1} \frac{a(s)}{c(s)}, \quad k = 0, \dots, n+1.$$

Reminding the assumption  $a(k), c(k) \neq 0$ ,  $0 \leq k \leq n$ , it is easy to prove that  $\rho(k)a(k) = \rho(k+1)c(k)$ . Moreover, the companion function verifies the following meaningful result.

**Proposition 1.1.** *Given  $u, v$  two solutions of the homogeneous Schrödinger equation on  $I$ , then*

$$a(k)w[u, v](k) = c(k-1)w[u, v](k-1) \quad \text{for any } k \in \overset{\circ}{I}.$$

Therefore, the function  $\rho a w[u, v]$  is constant in  $I$  and is zero iff  $u$  and  $v$  are linearly dependent.

The *Green's function* of the homogeneous Schrödinger equation on  $I$  is the function  $g \in \mathcal{C}(I \times I)$ , defined  
30 for any  $s \in I$  as  $g(\cdot, s)$ , the unique solution of the initial value problem with conditions  $g(s, s) = 0$  and  $g(s+1, s) = -\frac{1}{a(s)}$ , when  $0 \leq s \leq n$ , and as the unique solution of the initial value problem with conditions  $g(n+1, n+1) = 0$  and  $g(n, n+1) = \frac{1}{a(n+1)}$  when  $s = n+1$ .

**Lemma 1.2.** *If  $u, v \in \mathcal{C}(I)$  are two linearly independent solutions of the homogeneous Schrödinger equation on  $\overset{\circ}{I}$ , then*

$$g(k, s) = \frac{1}{a(s)w[u, v](s)} [v(s)u(k) - u(s)v(k)], \quad k, s \in I.$$

Hence,  $g(s, s+1) = \frac{1}{c(s)}$ , for any  $s \in \overset{\circ}{I} \cup \{0\}$ .

**Proposition 1.3.** *Given a function  $f \in \mathcal{C}(I)$  and  $m \in \overset{\circ}{I} \cup \{0\}$ , the function  $y \in \mathcal{C}(I)$  such that*

$$y(k) = \sum_{s=\min\{k, m\}+1}^{\max\{k, m\}} g(k, s)f(s), \quad \text{for } k \in I,$$

is the unique solution of the problem  $\mathcal{L}_q(y) = f$  on  $\overset{\circ}{I}$ , with initial conditions  $y(m) = y(m+1) = 0$ .

35 PROOF. Obviously  $y(m+1) = g(m+1, m+1)f(m+1) = 0$  and  $y(m) = 0$ . Indeed, we just have to prove that  $\mathcal{L}_q(y)(k) = f(k)$ , for any  $1 \leq k \leq n$

$$\begin{aligned}
\mathcal{L}_q(y)(k) &= a(k)[y(k) - y(k+1)] + c(k-1)[y(k) - y(k-1)] + q(k)y(k) \\
&= a(k) \left[ \sum_{\min\{k,m\}+1}^{\max\{k,m\}} g(k,s)f(s) - \sum_{\min\{k+1,m\}+1}^{\max\{k+1,m\}} g(k+1,s)f(s) \right] \\
&\quad + c(k-1) \left[ \sum_{\min\{k,m\}+1}^{\max\{k,m\}} g(k,s)f(s) - \sum_{\min\{k-1,m\}+1}^{\max\{k-1,m\}} g(k-1,s)f(s) \right] \\
&\quad + q(k) \sum_{\min\{k,m\}+1}^{\max\{k,m\}} g(k,s)f(s) \\
&= -a(k)g(k+1, k+1)f(k+1) + c(k-1)g(k-1, k)f(k) = f(k).
\end{aligned}$$

## 2. Regular boundary value problems

According to Equations (3) and defining the pair of conditions  $(\mathbf{c}_1, \mathbf{c}_2)$  as  $\mathbf{c}_1(u) = \mathcal{L}_q(u)(0) = b(0)u(0) - a(0)u(1)$  and  $\mathbf{c}_2(u) = \mathcal{L}_q(u)(n+1) = -c(n)u(n) + b(n+1)u(n+1)$ , we consider the Sturm–Liouville boundary value problem  $(\mathcal{L}_q, \mathbf{c}_1, \mathbf{c}_2)$  and for any  $f \in \mathcal{C}(\mathbb{I})$ , we should determine if there exists  $u \in \mathcal{C}(\mathbb{I})$  such that

$$\mathcal{L}_q(u) = f \text{ on } \overset{\circ}{\mathbb{I}}, \quad \mathbf{c}_1(u) = f(0) \text{ and } \mathbf{c}_2(u) = f(n+1).$$

The boundary value problem  $(\mathcal{L}_q, \mathbf{c}_1, \mathbf{c}_2)$  is called homogeneous when  $f = 0$ .

40 We are only interested in *regular problems*; that is, in those boundary value problems with a unique solution. In this case, for the resolution of the boundary value problem we determine the so-called *resolvent kernel*. The process of determining the resolvent kernel always depends on an appropriate choice of solutions of the corresponding homogeneous Schrödinger equation. The approach we make here is slightly different and more general than that followed in [11], since in that reference the *Green's kernel of boundary value problems* is determined, but associated to equations with constant coefficients

**Definition 2.1.** We called Wronskian of the pair of boundary conditions  $(\mathbf{c}_1, \mathbf{c}_2)$  to the function  $W: \mathcal{C}(\mathbb{I}) \times \mathcal{C}(\mathbb{I}) \rightarrow \mathbb{R}$  defined as

$$W[u, v] = \det \begin{bmatrix} \mathbf{c}_1(u) & \mathbf{c}_1(v) \\ \mathbf{c}_2(u) & \mathbf{c}_2(v) \end{bmatrix} = \mathbf{c}_1(u)\mathbf{c}_2(v) - \mathbf{c}_1(v)\mathbf{c}_2(u), \quad u, v \in \mathcal{C}(\mathbb{I}).$$

Clearly,  $W$  is a skew-symmetric bilinear form and, hence, if  $\phi = a_1u + b_1v$  and  $\psi = a_2u + b_2v$ , then

$$W[\phi, \psi] = W[u, v] \det \begin{bmatrix} a_1 & b_1 \\ a_2 & b_2 \end{bmatrix}. \quad (4)$$

**Proposition 2.2.** *If  $g: I \times I \rightarrow \mathbb{R}$  is the Green's function of the homogeneous Schrödinger equation  $\mathcal{L}_q(u) = 0$  on  $\overset{\circ}{I}$ , then the function  $D: I \rightarrow \mathbb{R}$  defined as  $D(n+1) = D(n)$  and*

$$D(s) = \frac{a(0)a(s)}{\rho(s+1)} W[g(\cdot, s), g(\cdot, s+1)], \quad s = 0, \dots, n,$$

<sup>45</sup> *is constant.*

PROOF. If we defined  $u = g(\cdot, 0)$  and  $v = g(\cdot, 1)$ , then  $w[u, v](0) = a(0)^{-1}c(0)^{-1}$  and, moreover, Proposition 1.1 and Lemma 1.2 establish that

$$g(\cdot, s) = \frac{1}{a(s)w[u, v](s)} [v(s)u - u(s)v] = c(0)\rho(s) [v(s)u - u(s)v], \quad s = 0, \dots, n+1.$$

Applying now Identity (4), we obtain

$$\begin{aligned} W[g(\cdot, s), g(\cdot, s+1)] &= c(0)^2 \rho(s+1) \rho(s) w[u, v](s) W[u, v] \\ &= a(0)c(0)^2 \rho(s+1) a(s)^{-1} w[u, v](0) W[u, v] \\ &= c(0)\rho(s+1) a(s)^{-1} W[u, v], \quad s = 0, \dots, n, \end{aligned}$$

and then, it is satisfied

$$D(s) = a(0)c(0)W[u, v] = D(0),$$

since  $\rho(1) = a(0)c(0)^{-1}$ . □

**Definition 2.3.** *We called Determinant of the boundary value problem  $(\mathcal{L}_q, \mathbf{c}_1, \mathbf{c}_2)$  to the value*

$$D_{a,b,c} = a(n)\rho(n)D(0) = a(n)\rho(n)a(0)c(0)W[g(\cdot, 0), g(\cdot, 1)]$$

**Definition 2.4.** *The boundary value problem  $(\mathcal{L}_q, \mathbf{c}_1, \mathbf{c}_2)$  is called regular if the solution of the corresponding homogeneous problem is unique, and so the trivial one.*

**Proposition 2.5.** *The following assertions are equivalent:*

- <sup>50</sup> (i) *The boundary value problem  $(\mathcal{L}_q, \mathbf{c}_1, \mathbf{c}_2)$  is regular.*  
(ii) *For any  $f \in \mathcal{C}(I)$  the corresponding boundary value problem has a unique solution.*  
(iii)  *$D_{a,b,c} \neq 0$ .*

PROOF. If  $z_1 = g(\cdot, 0)$  and  $z_2 = g(\cdot, 1)$ , then  $\{z_1, z_2\}$  form a basis of solutions of the homogeneous Schrödinger equation  $\mathcal{L}_q(u) = 0$  on  $\overset{\circ}{I}$ . If we consider a particular solution  $y$  of the Schrödinger equation with data  $f$  for any  $f \in \mathcal{C}(I)$ , the function  $u = \alpha z_1 + \beta z_2 + y$  where  $\alpha, \beta \in \mathbb{R}$ , is a solution of the boundary value problem

$$\mathcal{L}_q(u) = f \text{ on } \overset{\circ}{I}, \quad \mathbf{c}_1(u) = f(0) \text{ and } \mathbf{c}_2(u) = f(n+1),$$

iff  $\alpha$  and  $\beta$  are solutions of the linear system

$$\begin{bmatrix} \mathbf{c}_1(z_1) & \mathbf{c}_1(z_2) \\ \mathbf{c}_2(z_1) & \mathbf{c}_2(z_2) \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} f(0) - \mathbf{c}_1(y) \\ f(n+1) - \mathbf{c}_2(y) \end{bmatrix}.$$

When  $f$  goes over  $\mathcal{C}(\mathbf{I})$ , then the right term of the previous system goes over all  $\mathbb{R}^2$ . Therefore, the system has a solution for any  $f \in \mathcal{C}(\mathbf{I})$  iff the trivial solution is the unique solution of the corresponding homogeneous system ; that is, iff the coefficient matrix is non-singular, so the system has a unique solution. As the homogeneous system associated with the previous one determines the solutions of the homogeneous boundary value problem, the problem is regular if the homogeneous system has as its unique solution the trivial one. Therefore, (i) and (ii) are equivalent and, in addition, the coefficient matrix is non-singular and it implies that its determinant is different from 0. Hence, (i) and (iii) are equivalent.  $\square$

**Definition 2.6.** Let  $(\mathcal{L}_q, \mathbf{c}_1, \mathbf{c}_2)$  be a regular boundary value problem. We call Resolvent kernel of the boundary value problem to  $R_{a,b,c}: \mathbf{I} \times \mathbf{I} \rightarrow \mathbb{R}$  characterized by

$$\begin{aligned} \mathcal{L}_q(R_{a,b,c}(\cdot, s)) &= \varepsilon_s \text{ on } \overset{\circ}{\mathbf{I}}, \\ \mathbf{c}_1(R_{a,b,c}(\cdot, s)) &= \varepsilon_s(0), \quad \mathbf{c}_2(R_{a,b,c}(\cdot, s)) = \varepsilon_s(n+1), \quad s \in \mathbf{I}. \end{aligned}$$

We call Green's kernel of the boundary value problem to  $G_{a,b,c}: \mathbf{I} \times \mathbf{I} \rightarrow \mathbb{R}$  characterized by  $G_{a,b,c}(\cdot, s) = 0$  if  $s \in \delta(\mathbf{I})$  and by

$$\mathcal{L}_q(G_{a,b,c}(\cdot, s)) = \varepsilon_s \text{ on } \overset{\circ}{\mathbf{I}}, \quad \mathbf{c}_1(G_{a,b,c}(\cdot, s)) = \mathbf{c}_2(G_{a,b,c}(\cdot, s)) = 0, \quad s \in \overset{\circ}{\mathbf{I}}.$$

We call Poisson's kernel of the boundary value problem to  $P_{a,b,c}: \mathbf{I} \times \mathbf{I} \rightarrow \mathbb{R}$  characterized by  $P_{a,b,c}(\cdot, s) = 0$  if  $s \in \overset{\circ}{\mathbf{I}}$  and by

$$\begin{aligned} \mathcal{L}_q(P_{a,b,c}(\cdot, s)) &= 0 \text{ on } \overset{\circ}{\mathbf{I}}, \\ \mathbf{c}_1(P_{a,b,c}(\cdot, s)) &= \varepsilon_s(0), \quad \mathbf{c}_2(P_{a,b,c}(\cdot, s)) = \varepsilon_s(n+1), \quad s \in \delta(\mathbf{I}). \end{aligned}$$

Note that if the boundary value problem is regular, then there is a unique Resolvent kernel, a unique Green's kernel and a unique Poisson's kernel, which are determined by fixing its second variable and finding the unique solution of the given boundary problems. The importance of these kernels is shown in the following result.

**Proposition 2.7.** If the boundary value problem  $(\mathcal{L}_q, \mathbf{c}_1, \mathbf{c}_2)$  is regular and  $G_{a,b,c}$ ,  $P_{a,b,c}$  and  $R_{a,b,c}$  are the Green's, Poisson's and Resolvent kernel, respectively, then

$$R_{a,b,c} = G_{a,b,c} + P_{a,b,c}.$$

Moreover, for any  $f \in \mathcal{C}(\mathbf{I})$  the function

$$v(k) = \sum_{s \in \overset{\circ}{\mathbf{I}}} G_{a,b,c}(k, s) f(s) = \sum_{s=1}^n G_{a,b,c}(k, s) f(s), \quad k \in \mathbf{I},$$

is the unique solution of the semi-homogeneous boundary problem

$$\mathcal{L}_q(v) = f \text{ on } \overset{\circ}{\mathbb{I}}, \quad \mathbf{c}_1(v) = \mathbf{c}_2(v) = 0,$$

the function

$$z(k) = \sum_{s \in \delta(\mathbb{I})} P_{a,b,c}(k, s) f(s) = P_{a,b,c}(k, 0) f(0) + P_{a,b,c}(k, n+1) f(n+1), \quad k \in \mathbb{I},$$

is the unique solution of the boundary value problem

$$\mathcal{L}_q(z) = 0 \text{ on } \overset{\circ}{\mathbb{I}}, \quad \mathbf{c}_1(z) = f(0), \quad \mathbf{c}_2(z) = f(n+1)$$

and, therefore, the function  $u = v + z$ , that is, that determined by the expression

$$u(k) = \sum_{s \in \mathbb{I}} R_{a,b,c}(k, s) f(s), \quad k \in \mathbb{I},$$

is the unique solution of the boundary value problem with data  $f$ , i.e.

$$\mathcal{L}_q(u) = f \text{ on } \overset{\circ}{\mathbb{I}}, \quad \mathbf{c}_1(u) = f(0), \quad \mathbf{c}_2(u) = f(n+1).$$

**Definition 2.8.** Consider  $\nu, \mu \in \mathcal{C}(\mathbb{I})$  the unique solutions of the homogeneous Schrödinger equation on  $\overset{\circ}{\mathbb{I}}$  determined by the conditions

$$\nu(0) = a(0), \quad \nu(1) = b(0), \quad \mu(n) = -b(n+1), \quad \mu(n+1) = -c(n).$$

We call fundamental solutions of the homogeneous Schrödinger equation on  $\overset{\circ}{\mathbb{I}}$ , related to the boundary conditions  $\mathbf{c}_1$  and  $\mathbf{c}_2$  or, simply, fundamental solutions to the functions

$$\phi_{a,b,c} = a(n)\rho(n)\nu \quad \text{and} \quad \psi_{a,b,c} = a(0)\mu.$$

The reason to choose these definitions for the fundamental solutions is shown in the following result.

**Proposition 2.9.** If  $\phi_{a,b,c}$  and  $\psi_{a,b,c}$  are the fundamental solutions of the homogeneous Schrödinger equation on  $\overset{\circ}{\mathbb{I}}$ , related to the boundary conditions  $\mathbf{c}_1$  and  $\mathbf{c}_2$ , then

$$\mathbf{c}_1(\phi_{a,b,c}) = \mathbf{c}_2(\psi_{a,b,c}) = 0, \quad -\mathbf{c}_1(\psi_{a,b,c}) = \mathbf{c}_2(\phi_{a,b,c}) = D_{a,b,c}$$

and, moreover,

$$W[\phi_{a,b,c}, \psi_{a,b,c}] = (D_{a,b,c})^2 \quad \text{and} \quad w[\phi_{a,b,c}, \psi_{a,b,c}](0) = a(n)\rho(n)D_{a,b,c}.$$

65 PROOF. Consider  $\{u, v\}$  the basis of solutions of the homogeneous Schrödinger equation that satisfy  $u(0) = 1$ ,  $u(1) = 0$ ,  $v(0) = 0$  and  $v(1) = 1$ ; that is,  $u = c(0)g(\cdot, 1)$  and  $v = -a(0)g(\cdot, 0)$ . Moreover,  $w[u, v](0) = 1$ .



If we prove that

$$\phi_{a,b,c} = a(n)\rho(n)(\mathbf{c}_1(u)v - \mathbf{c}_1(v)u) \quad \text{and} \quad \psi_{a,b,c} = a(n)\rho(n)(\mathbf{c}_2(u)v - \mathbf{c}_2(v)u),$$

then, clearly,  $\mathbf{c}_1(\phi_{a,b,c}) = \mathbf{c}_2(\psi_{a,b,c}) = 0$ . Besides,  $-\mathbf{c}_1(\psi_{a,b,c}) = \mathbf{c}_2(\phi_{a,b,c})$  and

$$\mathbf{c}_2(\phi_{a,b,c}) = a(n)\rho(n)W[u, v] = a(n)\rho(n)a(0)c(0)W[g(\cdot, 0), g(\cdot, 1)] = D_{a,b,c}.$$

Moreover,

$$w[\phi_{a,b,c}, \psi_{a,b,c}](0) = a(n)^2\rho(n)^2W[u, v]w[u, v](0) = a(n)\rho(n)D_{a,b,c}.$$

To verify the previous equalities  $\phi_{a,b,c} = a(n)\rho(n)(\mathbf{c}_1(u)v - \mathbf{c}_1(v)u)$  and  $\psi_{a,b,c} = a(n)\rho(n)(\mathbf{c}_2(u)v - \mathbf{c}_2(v)u)$  let us first observe that

$$\mathbf{c}_1(u)v - \mathbf{c}_1(v)u = b(0)v - a(0)u = z.$$

Since  $z$  is a solution of the homogeneous Schrödinger equation on  $\overset{\circ}{\mathbb{I}}$  with initial conditions  $z(0) = a(0)$ ,  $z(1) = b(0)$ , then  $z = \nu$  and  $\phi_{a,b,c} = a(n)\rho(n)\nu$  as expected.

On the other hand,  $\mathbf{c}_2(u)v - \mathbf{c}_2(v)u = w$ , where

$$w = -c(n)(u(n)v - v(n)u) + b(n+1)(u(n+1)v - v(n+1)u),$$

75 is the solution of the homogeneous Schrödinger equation on  $\overset{\circ}{\mathbb{I}}$  that verifies  $w(n) = -b(n+1)w[u, v](n)$  and  $w(n+1) = -c(n)w[u, v](n)$ , which implies that  $w = w[u, v](n)\mu$  and  $\psi_{a,b,c} = a(n)\rho(n)w[u, v](n)\mu = a(0)\mu$  as expected.  $\square$

**Corollary 2.10.** *The boundary value problem  $(\mathcal{L}_q, \mathbf{c}_1, \mathbf{c}_2)$  is regular iff the fundamental solutions are a basis of solutions of the homogeneous Schrödinger equation on  $\overset{\circ}{\mathbb{I}}$ .*

### 75 3. Resolvent kernel for the Sturm–Liouville boundary value problem

The next step is to obtain the Poisson's and the Green's kernels, and hence the Resolvent kernel, for a regular boundary value problem with Sturm-Liouville conditions as functions of the fundamental solutions.

**Theorem 3.1.** *If the Sturm–Liouville boundary value problem  $(\mathcal{L}_q, \mathbf{c}_1, \mathbf{c}_2)$  is regular, the Poisson's kernel is given by the identities*

$$P_{a,b,c}(k, 0) = \frac{-a(0)\psi_{a,b,c}(k)}{w[\phi_{a,b,c}, \psi_{a,b,c}](n)} \quad \text{and} \quad P_{a,b,c}(k, n+1) = \frac{a(0)\phi_{a,b,c}(k)}{w[\phi_{a,b,c}, \psi_{a,b,c}](n)},$$

for any  $k = 0, \dots, n+1$ , whereas the Green's kernel is given by

$$G_{a,b,c}(k, s) = -\frac{\rho(s)\phi_{a,b,c}(\min\{k, s\})\psi_{a,b,c}(\max\{k, s\})}{a(0)w[\phi_{a,b,c}, \psi_{a,b,c}](0)},$$

for any  $s = 1, \dots, n$  and  $k = 0, \dots, n+1$ .

PROOF. Taking into account  $a(s)\rho(s)w[\phi_{a,b,c}, \psi_{a,b,c}](s) = a(0)w[\phi_{a,b,c}, \psi_{a,b,c}](0)$ , from Lemma 1.2 the Green's function of the Schrödinger equation on  $\overset{\circ}{\mathbb{I}}$  for any  $k, s = 0, \dots, n+1$  is given by the identity

$$g(k, s) = \frac{\rho(s)}{a(0)w[\phi_{a,b,c}, \psi_{a,b,c}](0)} [\psi_{a,b,c}(s)\phi_{a,b,c}(k) - \phi_{a,b,c}(s)\psi_{a,b,c}(k)].$$

If  $f \in \mathcal{C}(\mathbb{I})$ , the set of solutions of the Schrödinger equation  $\mathcal{L}_q(u) = f$  on  $\overset{\circ}{\mathbb{I}}$  is given by the identity

$$u = \alpha\phi_{a,b,c} + \beta\psi_{a,b,c} + y, \quad \alpha, \beta \in \mathbb{R}.$$

where if  $g_0 = -(a(0)w[\phi_{a,b,c}, \psi_{a,b,c}](0))^{-1}$ , according to Proposition 1.3

$$y(k) = g_0\psi_{a,b,c}(k) \sum_{s=1}^k \phi_{a,b,c}(s)\rho(s)f(s)ds - g_0\phi_{a,b,c}(k) \sum_{s=1}^k \psi_{a,b,c}(s)\rho(s)f(s)ds.$$

Using the properties of the fundamental solutions described in Proposition 2.9, it follows that  $\mathbf{c}_1(u) = f(0)$  and  $\mathbf{c}_2(u) = f(n+1)$  iff

$$\alpha = \frac{1}{D_{a,b,c}} [f(n+1) - \mathbf{c}_2(y)] \quad \text{and} \quad \beta = \frac{1}{D_{a,b,c}} [\mathbf{c}_1(y) - f(0)].$$

To determine the Green's and Poisson's kernels, we must to substitute the function  $f$  in the previous identities by  $\varepsilon_s$ ,  $s = 0, \dots, n+1$ . Also, note that as  $w[\phi_{a,b,c}, \psi_{a,b,c}](0) = a(n)\rho(n)D_{a,b,c}$ , then  $w[\phi_{a,b,c}, \psi_{a,b,c}](n) = a(0)D_{a,b,c}$ .

If we consider  $f = \varepsilon_0$ , then  $y = 0$ , hence  $\mathbf{c}_1(y) = \mathbf{c}_2(y) = 0$  and, therefore  $\alpha = 0$  and  $\beta = -\frac{1}{D_{a,b,c}}$ . Definitely, we obtain

$$P_{a,b,c}(k, 0) = -\frac{1}{D_{a,b,c}}\psi_{a,b,c}(k).$$

If we consider  $f = \varepsilon_{n+1}$ , then  $y = 0$ , hence  $\mathbf{c}_1(y) = \mathbf{c}_2(y) = 0$  and, therefore  $\beta = 0$  and  $\alpha = \frac{1}{D_{a,b,c}}$ . Definitely, we obtain

$$P_{a,b,c}(k, n+1) = \frac{1}{D_{a,b,c}}\phi_{a,b,c}(k).$$

If we consider  $f = \varepsilon_s$ ,  $s = 1, \dots, n$ , then  $\alpha = -\frac{\mathbf{c}_2(y)}{D_{a,b,c}}$ ,  $\beta = \frac{\mathbf{c}_1(y)}{D_{a,b,c}}$ , whereas

$$y(k) = \begin{cases} 0, & k \leq s, \\ g_0\rho(s) [\psi_{a,b,c}(k)\phi_{a,b,c}(s) - \phi_{a,b,c}(k)\psi_{a,b,c}(s)], & k \geq s, \end{cases}$$

or, equivalently,

$$y(k) = -g_0\rho(s)\phi_{a,b,c}(k)\psi_{a,b,c}(s) + g_0\rho(s) \begin{cases} \phi_{a,b,c}(k)\psi_{a,b,c}(s), & k \leq s, \\ \psi_{a,b,c}(k)\phi_{a,b,c}(s), & k \geq s, \end{cases}$$

that is,

$$y(k) = g_0\rho(s) [\phi_{a,b,c}(\min\{k, s\})\psi_{a,b,c}(\max\{k, s\}) - \phi_{a,b,c}(k)\psi_{a,b,c}(s)].$$

On the other hand, we also obtain

$$\begin{aligned}\mathbf{c}_1(y) &= g_0\rho(s) \left[ \mathbf{c}_1(\phi_{a,b,c}(k))\psi_{a,b,c}(s) - \mathbf{c}_1(\phi_{a,b,c}(k))\psi_{a,b,c}(s) \right] = 0, \\ \mathbf{c}_2(y) &= g_0\rho(s) \left[ \phi_{a,b,c}(s)\mathbf{c}_2(\psi_{a,b,c}(k)) - \mathbf{c}_2(\phi_{a,b,c}(k))\psi_{a,b,c}(s) \right] \\ &= -g_0\rho(s)D_{a,b,c}\psi_{a,b,c}(s),\end{aligned}$$

which implies

$$\begin{aligned}G_{a,b,c}(k, s) &= g_0\rho(s) \left[ \phi_{a,b,c}(\min\{k, s\})\psi_{a,b,c}(\max\{k, s\}) - \phi_{a,b,c}(k)\psi_{a,b,c}(s) \right] \\ &\quad + g_0\rho(s)\phi_{a,b,c}(k)\psi_{a,b,c}(s) \\ &= g_0\rho(s)\phi_{a,b,c}(\min\{k, s\})\psi_{a,b,c}(\max\{k, s\}).\end{aligned}\quad \square$$

**Corollary 3.2.** *The Sturm–Liouville boundary value problem  $(\mathcal{L}_q, \mathbf{c}_1, \mathbf{c}_2)$  is regular iff  $b(0)\psi_{a,b,c}(0) \neq a(0)\psi_{a,b,c}(1)$  or, equivalently, iff  $c(n)\phi_{a,b,c}(n) \neq b(n+1)\phi_{a,b,c}(n+1)$  and its resolvent kernel is determined by*

$$R_{a,b,c}(k, s) = \frac{\rho(s)\phi_{a,b,c}(\min\{k, s\})\psi_{a,b,c}(\max\{k, s\})}{a(0)a(n)\rho(n)[c(n)\phi_{a,b,c}(n) - b(n+1)\phi_{a,b,c}(n+1)]},$$

for any  $k, s = 0, \dots, n+1$ .

PROOF. The regularity condition is obtained taking into account  $D_{a,b,c} = (a(n)\rho(n))^{-1}w[\phi_{a,b,c}, \psi_{a,b,c}](0)$  or  $D_{a,b,c} = a(0)^{-1}w[\phi_{a,b,c}, \psi_{a,b,c}](n)$ , so  $D_{a,b,c} = a(0)\psi_{a,b,c}(1) - b(0)\psi_{a,b,c}(0) = -c(n)\phi_{a,b,c}(n) + b(n+1)\phi_{a,b,c}(n+1)$ .

On the other hand, since

$$a(0)w[\phi_{a,b,c}, \psi_{a,b,c}](0) = a(n)\rho(n)w[\phi_{a,b,c}, \psi_{a,b,c}](n) = a(0)a(n)\rho(n)D_{a,b,c},$$

the identity given for  $R_{a,b,c}$  corresponds to that obtained for the Green's kernel in Theorem 3.1. As  $R_{a,b,c} = G_{a,b,c} + P_{a,b,c}$ , the equality holds for any  $k = 0, \dots, n+1$ , when  $s = 1, \dots, n$ .

Finally, if we consider  $A_0, A_{n+1} \in \mathcal{C}(\mathbb{I})$  the functions obtained allowing  $s = 0$  and  $s = n+1$  in the Green's kernel expression, we obtain

$$A_0(k) = -\frac{\phi_{a,b,c}(0)\psi_{a,b,c}(k)}{a(0)w[\phi_{a,b,c}, \psi_{a,b,c}](0)} = -\frac{a(n)\rho(n)a(0)\psi_{a,b,c}(k)}{a(0)w[\phi_{a,b,c}, \psi_{a,b,c}](0)} = P_{a,b,c}(k, 0)$$

and

$$\begin{aligned}A_{n+1}(k) &= -\frac{\rho(n+1)\phi_{a,b,c}(k)\psi_{a,b,c}(n+1)}{a(0)w[\phi_{a,b,c}, \psi_{a,b,c}](0)} = \frac{\rho(n+1)a(0)c(n)\phi_{a,b,c}(k)}{a(0)w[\phi_{a,b,c}, \psi_{a,b,c}](0)} \\ &= P_{a,b,c}(k, n+1),\end{aligned}$$

where it has been considered  $a(n)\rho(n) = c(n)\rho(n+1)$  in the last identity.  $\square$

Let us remind that the boundary conditions associated to the Jacobi matrix were  $\mathbf{c}_1(u) = \mathcal{L}_q(u)(0)$  and  $\mathbf{c}_2(u) = \mathcal{L}_q(u)(n+1)$ , so the boundary value problem  $(\mathcal{L}_q, \mathbf{c}_1, \mathbf{c}_2)$  associated to the inversion of that matrix is the Poisson equation  $\mathcal{L}_q(u) = f$  on  $\mathbb{I}$ . Applying now Corollary 3.2 to this equation using the basis

$$\Phi_{a,b,c} = (a(n)\rho(n))^{-1}\phi_{a,b,c} \quad \text{and} \quad \Psi_{a,b,c} = a(0)^{-1}\psi_{a,b,c}, \quad (5)$$

90 we obtain the fundamental result for the inversion of Jacobi matrices.

**Theorem 3.3.** *Consider  $\Phi_{a,b,c}$  and  $\Psi_{a,b,c}$  the unique solutions of the homogeneous Schrödinger equation on  $\overset{\circ}{\mathbb{I}}$  that verify*

$$\Phi_{a,b,c}(0) = a(0), \quad \Phi_{a,b,c}(1) = b(0), \quad \Psi_{a,b,c}(n) = -b(n+1), \quad \Psi_{a,b,c}(n+1) = -c(n).$$

Then,

$$a(0)\left(b(0)\Psi_{a,b,c}(0) - a(0)\Psi_{a,b,c}(1)\right) = a(n)\rho(n)\left(c(n)\Phi_{a,b,c}(n) - b(n+1)\Phi_{a,b,c}(n+1)\right),$$

the Schrödinger operator  $\mathcal{L}_q$  is invertible iff  $b(0)\Psi_{a,b,c}(0) \neq a(0)\Psi_{a,b,c}(1)$  and, moreover, given  $f \in \mathcal{C}(\mathbb{I})$ ,

$$(\mathcal{L}_q)^{-1}(f)(k) = \sum_{s \in \mathbb{I}} \frac{\Phi_{a,b,c}(\min\{k, s\})\Psi_{a,b,c}(\max\{k, s\})}{a(0)\left[b(0)\Psi_{a,b,c}(0) - a(0)\Psi_{a,b,c}(1)\right]} \rho(s)f(s),$$

for any  $k = 0, \dots, n+1$ .

#### 4. The inverse of a tridiagonal $(p, r)$ -Toeplitz matrix

A *Toeplitz matrix* is a square matrix with constant diagonals. Therefore, a tridiagonal matrix (or Jacobi matrix) which is also a Toeplitz matrix has the three main diagonals constant and the rest are null.

**Definition 4.1.** *Consider  $p \in \mathbb{N} \setminus \{0\}$  and  $r \in \mathbb{R} \setminus \{0\}$ . The Jacobi matrix  $\mathbf{J}(a, b, c)$ , where  $a, b, c \in \mathcal{C}(\mathbb{I})$ ,  $a(k) \neq 0$  and  $c(k) \neq 0$  for any  $k = 0, \dots, n$ ,  $a(n+1) = c(n)$  and  $c(n+1) = a(n)$ , is a  $(p, r)$ -Toeplitz matrix if there exists  $m \in \mathbb{N} \setminus \{0\}$  such that  $n+2 = mp$ , and  $a, b$  and  $c$  are quasi-periodic coefficients; that is*

$$a(p+j) = ra(j), \quad b(p+j) = rb(j) \quad \text{and} \quad c(p+j) = rc(j), \quad j = 0, \dots, (m-1)p.$$

95 If  $r = 1$ , the Jacobi  $(p, 1)$ -Toeplitz matrices are the ones so-called *tridiagonal  $p$ -Toeplitz matrices*, see for instance [3], whose coefficients are periodic with period  $p$ . When  $p = 1$  too, the Jacobi  $(1, 1)$ -Toeplitz matrices are the matrices referenced at the beginning of this section, the *tridiagonal and Toeplitz matrices*. Note also that Jacobi  $(1, r)$ -Toeplitz matrices are those whose diagonals are *geometrical sequences with ratio  $r$* .

100 Since a Jacobi  $(p, r)$ -Toeplitz matrix is in fact a Jacobi matrix, to determine its inverse,  $\mathbf{J}^{-1} = \mathbf{R} = (r_{ks})$ , is equivalent to obtain the inverse of the Schrödinger operator on a path described in Theorem 3.3. Our goal is to compute explicitly the functions  $\Phi_{a,b,c}$  and  $\Psi_{a,b,c}$ .

The first result correspond to the easiest case, the Jacobi (1,1)-Toeplitz matrices. In this case, the Schrödinger operator corresponds to a second order linear difference equation with constant coefficients, so its solution can be expressed in terms of Chebyshev polynomials. The expression obtained coincides with that published by Fonseca and Petronilho in [2, Corollary 4.1] and [3, Equation 4.26]. The explicit expression of the inverse of these matrices appeared before in [12, Example 1.3], but in terms of the roots of the characteristic polynomial of the difference equation.

**Proposition 4.2.** *If  $\alpha\gamma \neq 0$ , the Jacobi (1,1)-Toeplitz matrix of order  $n + 2$*

$$J(\alpha, \beta, \gamma) = \begin{bmatrix} \beta & -\alpha & 0 & \cdots & 0 & 0 \\ -\gamma & \beta & -\alpha & \cdots & 0 & 0 \\ 0 & -\gamma & \beta & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \beta & -\alpha \\ 0 & 0 & 0 & \cdots & -\gamma & \beta \end{bmatrix}$$

is invertible iff

$$\beta \neq 2\sqrt{\alpha\gamma} \cos\left(\frac{k\pi}{n+3}\right), \quad k = 1, \dots, n+2,$$

and then, the entries of the inverse of  $J(\alpha, \beta, \gamma)$  are explicitly given by

$$r_{ks} = \frac{1}{U_{n+2}(q)} \begin{cases} \alpha^{s-k} (\sqrt{\alpha\gamma})^{k-s-1} U_k(q) U_{n-s+1}(q), & \text{if } 0 \leq k \leq s \leq n+1, \\ \gamma^{k-s} (\sqrt{\alpha\gamma})^{s-k-1} U_s(q) U_{n-k+1}(q), & \text{if } 0 \leq s \leq k \leq n+1, \end{cases}$$

where  $q = \frac{\beta}{2\sqrt{\alpha\gamma}}$ .

Moreover,

$$\det R = (-1)^n \alpha \gamma^{-(n+1)^2} (\sqrt{\alpha\gamma})^{(n+4)(n+1)} U_{n+2}\left(\frac{\beta}{2\sqrt{\alpha\gamma}}\right)^{n+1}.$$

PROOF. The first part is consequence of Theorem 3.3 taking into account that the functions  $\Phi_{a,b,c}$  and  $\Psi_{a,b,c}$  are the solutions of a second order linear homogeneous difference equation with constant coefficients, hence can be expressed as a linear combination of Chebyshev polynomials of second kind. Applying [13, Theorem 2.4] and imposing

$$\Phi_{a,b,c}(0) = \alpha, \quad \Phi_{a,b,c}(1) = \beta, \quad \Psi_{a,b,c}(n) = -\beta, \quad \Psi_{a,b,c}(n+1) = -\gamma,$$

then

$$\begin{aligned}
\Phi_{a,b,c}(k) &= \beta(\sqrt{\alpha^{-1}\gamma})^{k-1}U_{k-1}(q) - \alpha(\sqrt{\alpha^{-1}\gamma})^kU_{k-2}(q) \\
&= \alpha(\sqrt{\alpha^{-1}\gamma})^k[2qU_{k-1}(q) - U_{k-2}(q)] = \alpha^{1-k}(\sqrt{\alpha\gamma})^kU_k(q), \\
\Psi_{a,b,c}(k) &= \gamma(\sqrt{\alpha^{-1}\gamma})^{k-n-1}U_{n-k-1}(q) - \beta(\sqrt{\alpha^{-1}\gamma})^{k-n}U_{n-k}(q) \\
&= \gamma(\sqrt{\alpha^{-1}\gamma})^{k-n-1}[U_{n-k-1}(q) - 2qU_{n-k}(q)] \\
&= -\gamma^{k-n}(\sqrt{\alpha\gamma})^{n-k+1}U_{n-k+1}(q),
\end{aligned}$$

110 for any  $k = 0, \dots, n+1$ .

On the other hand,

$$\begin{aligned}
\beta\Psi_{a,b,c}(0) - \alpha\Psi_{a,b,c}(1) &= -\beta\gamma^{-n}(\sqrt{\alpha\gamma})^{n+1}U_{n+1}(q) + \alpha\gamma^{1-n}(\sqrt{\alpha\gamma})^nU_n(q) \\
&= \alpha\gamma^{1-n}(\sqrt{\alpha\gamma})^n[U_n(q) - 2qU_{n+1}(q)] \\
&= -\alpha\gamma^{1-n}(\sqrt{\alpha\gamma})^nU_{n+2}(q),
\end{aligned}$$

so  $\beta\Psi_{a,b,c}(0) \neq \alpha\Psi_{a,b,c}(1)$  iff  $q$  is not a zero of the polynomial  $U_{n+2}(x)$ ; that is, iff  $q \neq \cos\left(\frac{k\pi}{n+3}\right)$ ,  $k = 1, \dots, n+2$ , see [14]. In that case  $J(\alpha, \beta, \gamma)$  is invertible and then

$$r_{ks} = -\frac{\Phi_{a,b,c}(\min\{k, s\})\Psi_{a,b,c}(\max\{k, s\})}{\alpha^{2-s}\gamma^{s-n+1}(\sqrt{\alpha\gamma})^nU_{n+2}(q)}.$$

□

**Corollary 4.3.** *If  $\alpha \neq 0$ , the symmetric Jacobi  $(1, 1)$ -Toeplitz matrix of order  $n+2$*

$$J(\alpha, \beta) = \begin{bmatrix} \beta & -\alpha & 0 & \cdots & 0 & 0 \\ -\alpha & \beta & -\alpha & \cdots & 0 & 0 \\ 0 & -\alpha & \beta & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \beta & -\alpha \\ 0 & 0 & 0 & \cdots & -\alpha & \beta \end{bmatrix}$$

is invertible iff

$$\beta \neq 2\alpha \cos\left(\frac{k\pi}{n+3}\right), \quad k = 1, \dots, n+2,$$

and then, the entries of the inverse of  $J(\alpha, \beta)$  are explicitly given by

$$r_{ks} = \frac{U_{\min\{k,s\}}\left(\frac{\beta}{2\alpha}\right)U_{n-\max\{k,s\}+1}\left(\frac{\beta}{2\alpha}\right)}{\alpha U_{n+2}\left(\frac{\beta}{2\alpha}\right)}, \quad k, s = 0, \dots, n+1.$$

The expression for the inverse of a symmetric Jacobi and Toeplitz matrix is well-known, see for instance [2, Corollary 4.2] and the references of this article.

At the general case, the Jacobi  $(p, r)$ -Toeplitz matrix, the Schrödinger equation has quasi-periodic coefficients, so we can apply the results presented in [13], a previous work of the authors devoted to the study of these kind of equations. We reproduce here its main result, [13, Theorem 3.3], and some of the developments in [13, Section 4], for the sake of completeness.

The main result in [13] establishes that (irreducible) second order difference equations with quasi-periodic coefficients are basically equivalent to a Chebyshev equation.

**Lemma 4.4.** ([13, Theorem 3.3]) Consider  $p \in \mathbb{N} \setminus \{0\}$ ,  $r \in \mathbb{R} \setminus \{0\}$ ,  $a, b, c \in \mathcal{C}(\mathbb{Z})$ ,  $a(k) \neq 0, c(k) \neq 0, k \in \mathbb{Z}$  and  $\theta = \sqrt{r\rho(p)}$ . There exists  $q_{p,r}(a, b, c) \in \mathbb{C}$  such that  $u \in \mathcal{C}(\mathbb{Z})$  is a solution of the equation  $\mathcal{L}_q(u) = 0$  iff for any  $m \in \mathbb{Z}$ ,  $\theta^k u(kp + m)$  is a solution of the Chebyshev equation

$$v(k+1) - 2q_{p,r}(a, b, c)v(k) + v(k-1) = 0, \quad k \in \mathbb{Z}.$$

The next result recovered from [13] corresponds to the explicit computation of the parameter  $q_{p,r}(a, b, c)$ , so-called *Floquet function*. We need to introduce before some notations and concepts presented too in the mentioned paper.

A *binary multi-index of order  $p$*  is a  $p$ -tuple  $\alpha = (\alpha_0, \dots, \alpha_{p-1}) \in \{0, 1\}^p$  and its length is defined as  $|\alpha| = \sum_{j=0}^{p-1} \alpha_j \leq p$ . So  $|\alpha| = m$  iff exactly  $m$  components of  $\alpha$  are equal to 1 and exactly  $p - m$  components of  $\alpha$  are equal to 0. The only multi-index of order  $p$  which length equals  $p$  is  $\pi_p = (1, \dots, 1)$ . If  $\alpha \in \{0, 1\}^p$  and  $|\alpha| = m \geq 1$ , we consider  $0 \leq i_1 < \dots < i_m \leq p - 1$  such that  $\alpha_{i_1} = \dots = \alpha_{i_m} = 1$ . Given  $p \in \mathbb{N} \setminus \{0\}$ , we define the following subsets of the set of binary multi-indexes of order  $p$ :

- (i)  $\Lambda_p^0 = \{\alpha : |\alpha| = 0\} = \{(0, \dots, 0)\}$  for  $p \geq 1$ ,
- (ii)  $\Lambda_p^1 = \{\alpha : |\alpha| = 1\}$ , for  $p \geq 2$ ,
- (iii)  $\Lambda_p^m = \{\alpha : |\alpha| = m, i_{j+1} - i_j \geq 2, 1 \leq j \leq m - 1 \text{ and } i_m \leq p - 2 \text{ if } i_1 = 0\}$  for  $p \geq 4$  and  $m = 2, \dots, \lfloor \frac{p}{2} \rfloor$ .

In addition, if  $p \geq 2$ ,  $m = 1, \dots, \lfloor \frac{p}{2} \rfloor$  and  $\alpha \in \Lambda_p^m$ , let  $0 \leq i_1 < \dots < i_m \leq p - 1$  be the indexes such that  $\alpha_{i_1} = \dots = \alpha_{i_m} = 1$ . Then, we define the multi-index  $\bar{\alpha}$  of order  $p$  as

$$\bar{\alpha}_{i_j} = \bar{\alpha}_{i_{j+1}} = 0, \quad j = 1, \dots, m, \quad \text{and} \quad \bar{\alpha}_i = 1 \quad \text{otherwise,}$$

where if  $i_m = p - 1$ , then  $\bar{\alpha}_p = \bar{\alpha}_0 = 0$ . Moreover, if  $\alpha \in \Lambda_p^0$ ; that is if  $\alpha = (0, \dots, 0)$ , then we define  $\bar{\alpha} = \pi_p$ . It is clear that, in any case,  $|\bar{\alpha}| = p - 2m$ .

Given  $\alpha \in \{0, 1\}^p$  and a function  $a \in \mathcal{C}(\mathbb{Z})$ , we consider the value  $a^\alpha = \prod_{j=0}^{p-1} a(j)^{\alpha_j}$ . Finally, we are ready to show the closed formula for the Floquet function  $q_{p,r}(a, b, c)$ .

**Lemma 4.5.** ([13, Theorem 4.4]) Given  $p \in \mathbb{N}^*$  and  $r \in \mathbb{R}^*$  then for any  $a, c \in \ell(\mathbb{R}^*; p, r)$  and  $b \in \ell(\mathbb{R}; p, r)$ , we have that

$$q_{p,r}(a, b, c) = \frac{1}{2} \sqrt{\frac{r}{a^{\pi_p} c^{\pi_p}}} \sum_{j=0}^{\lfloor \frac{p}{2} \rfloor} (-1)^j \sum_{\alpha \in \Lambda_p^j} r^{-\alpha_{p-1}} a^\alpha b^{\bar{\alpha}} c^\alpha.$$

The entries  $a, c \in \mathcal{C}(\mathbb{I})$  of the Jacobi  $(p, r)$ -Toeplitz matrix are quasi-periodic with period  $p$ , then  $a^{\pi p} c^{\pi p} = \rho(p)^{-1} \prod_{j=0}^{p-1} a(j)^2$ . Reminding  $\theta = \sqrt{r\rho(p)}$ , the Floquet function has the expression

$$q_{p,r} = \frac{\theta}{2 \prod_{j=0}^{p-1} |a(j)|} \sum_{j=0}^{\lfloor \frac{p}{2} \rfloor} (-1)^j \sum_{\alpha \in \Lambda_p^j} r^{-\alpha_{p-1}} a^\alpha b^{\bar{\alpha}} c^\alpha. \quad (6)$$

We also need some results introduced in [15], a work of the authors devoted to the study of general second order difference equations. In particular, in Section 7 of this article it has been proved that the solution of that kind of equations can be expressed as a linear combination of the functions  $P_k(x, y)$  called *k-th Chebyshev functions* and defined for any  $k \in \mathbb{N} \setminus \{0\}$  and for any  $x, y \in \mathcal{C}(\mathbb{Z})$  as

$$P_k(x, y) = \sum_{m=0}^{\lfloor \frac{k}{2} \rfloor} (-1)^m \sum_{\alpha \in \ell_k^m} x^{\bar{\alpha}} y^\alpha, \quad (7)$$

135 where  $\alpha = (\alpha_1, \dots, \alpha_p)$  is again a binary multi-index where we denote by  $i_1, \dots, i_m$  the indices such that  $1 \leq i_1 < \dots < i_m \leq p$  and  $\alpha_{i_j} = 1, j = 1, \dots, m$ . But now this  $\alpha$  is an element of the set  $\ell_p$  defined as

(i)  $\ell_p^0 = \{\alpha : |\alpha| = 0\} = \{(0, \dots, 0)\}$ , for  $p \in \mathbb{N} \setminus \{0\}$ ,

(ii)  $\ell_p^1 = \{\alpha : \alpha_p = 0 \text{ and } |\alpha| = 1\}$ , for  $p \geq 2$ ,

(iii)  $\ell_p^m = \{\alpha : \alpha_p = 0, |\alpha| = m \text{ and } i_{j+1} - i_j \geq 2, j = 1, \dots, m-1\}$ , for  $p \geq 4$  and  $m = 2, \dots, \lfloor \frac{p}{2} \rfloor$ .

And  $\bar{\alpha}$  is the binary multi-index of the same order as  $\alpha$  defined by

$$\bar{\alpha}_{i_j} = \bar{\alpha}_{i_{j+1}} = 0, \quad j = 1, \dots, m, \quad \text{and} \quad \bar{\alpha}_i = 1 \quad \text{otherwise.}$$

Therefore, the basis of solutions  $\{\Phi_{a,b,c}(k), \Psi_{a,b,c}(n+1-k)\}$  of the homogenous Schrödinger equation  $\mathcal{L}_q(u) = 0$  on  $\mathbb{I}$  can be obtained by the formulas

$$\Phi_{a,b,c}(k) = \left( \prod_{j=1}^{k-1} a(j) \right)^{-1} \left[ b(0)P_{k-1}(b, ac) - a(0)c(0)P_{k-2}(b_1, a_1c_1) \right] \quad \text{and}$$

$$\Psi_{a,b,c}(n+1-k) = \left( \prod_{j=n+1-k}^{n-1} c(j) \right)^{-1} \left[ a(n)c(n)P_{k-2}(b_{n+1-k}, a_{n+1-k}c_{n+1-k}) - b(n+1)P_{k-1}(b_{n+1-k}, a_{n+1-k}c_{n+1-k}) \right],$$

140 where  $a, b, c \in \mathcal{C}(\mathbb{I})$  are the coefficients of the second order difference equation associated to the Schrödinger equation.

Our main result appears now as a consequence of Lemma 4.4 and the above expressions of  $\Phi_{a,b,c}(k)$  and  $\Psi_{a,b,c}(n+1-k)$ .



**Theorem 4.6.** Consider  $p, m \in \mathbb{N}^*$ , such that  $pm = n + 2$ ,  $r \in \mathbb{R} \setminus \{0\}$ ,  $J(a, b, c)$  a Jacobi  $(p, r)$ -Toeplitz matrix of order  $n + 2$ , the Floquet function  $q_{p,r}$  and the functions

$$\begin{aligned} u(k, \ell) &= \theta \Phi_{a,b,c}(p + \ell) U_{k-1}(q_{p,r}) - \Phi_{a,b,c}(\ell) U_{k-2}(q_{p,r}), \\ v(k, \ell) &= \Psi_{a,b,c}(n + 2 - 2p + \ell) U_{m-k-2}(q_{p,r}) \\ &\quad - \theta \Psi_{a,b,c}(n + 2 - p + \ell) U_{m-k-3}(q_{p,r}), \end{aligned}$$

defined for any  $k = 0, \dots, m - 1$  and for any  $\ell = 0, \dots, p - 1$ , where

$$\begin{aligned} \Phi_{a,b,c}(k) &= \left( \prod_{j=1}^{k-1} a(j) \right)^{-1} \left[ b(0) P_{k-1}(b, ac) - a(0) c(0) P_{k-2}(b_1, a_1 c_1) \right] \quad \text{and} \\ \Psi_{a,b,c}(n + 1 - k) &= \left( \prod_{j=n+1-k}^{n-1} c(j) \right)^{-1} \left[ a(n) c(n) P_{k-2}(b_{n+1-k}, a_{n+1-k} c_{n+1-k}) \right. \\ &\quad \left. - b(n + 1) P_{k-1}(b_{n+1-k}, a_{n+1-k} c_{n+1-k}) \right]. \end{aligned}$$

Then,  $J(a, b, c)$  is invertible iff

$$b(0)v(0, 0) \neq a(0)v(0, 1)$$

and, moreover, the entries of the inverse of  $J(a, b, c)$  are explicitly given by

$$r_{kp+\ell, sp+\hat{\ell}} = \frac{\rho(\hat{\ell})}{a(0)r^s \theta^{k-s} d_J} \begin{cases} u(k, \ell)v(s, \hat{\ell}), & si \ k < s, \\ u(s, \hat{\ell})v(k, \ell), & si \ k < s, \\ u(s, \min\{\ell, \hat{\ell}\})v(s, \max\{\ell, \hat{\ell}\}), & si \ k = s, \end{cases}$$

where  $d_J = b(0)v(0, 0) - a(0)v(0, 1)$ .

PROOF. Lemma 4.4 establishes that

$$\Phi_{a,b,c}(kp + \ell) = \theta^{-k} u(k, \ell) \quad \text{and} \quad \Psi_{a,b,c}(kp + \ell) = \theta^{m-k-2} v(k, \ell),$$

for any  $k = 0, \dots, m - 1$  and for any  $\ell = 0, \dots, p - 1$ . Taking into account  $\rho(kp + \ell) = \rho(p)^k \rho(\ell)$  for any  $k \in \mathbb{N}$  and for any  $\ell = 0, \dots, p - 1$  and considering the identities

$$\begin{aligned} \prod_{j=1}^{p-1+\ell} a(j) &= r^\ell \left( \prod_{j=1}^{p-1} a(j) \right) \left( \prod_{j=0}^{\ell-1} a(j) \right) \\ \prod_{j=n+1-p-\ell}^{n-1} c(j) &= r^{-\ell} \left( \prod_{j=n+1-p}^{n-1} c(j) \right) \left( \prod_{j=n+1-\ell}^n c(j) \right), \end{aligned}$$

145 to evaluate the required values of the functions  $\Phi_{a,b,c}(k)$  and  $\Psi_{a,b,c}(n + 1 - k)$ ,  $k = 0, \dots, 2p - 1$ , we just need to apply Theorem 3.3.  $\square$

The last result corresponds to applying the previous theorem to tridiagonal matrices whose diagonals are geometric sequences and, in our opinion, a new result in the literature.

**Corollary 4.7.** *If  $r \in \mathbb{R} \setminus \{0\}$ , the Jacobi  $(1, r)$ -Toeplitz matrix*

$$J(\alpha, \beta, \gamma; r) = \begin{bmatrix} \beta & -\alpha & 0 & \cdots & 0 & 0 \\ -\gamma & \beta r & -\alpha r & \cdots & 0 & 0 \\ 0 & -\gamma r & \beta r^2 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & \beta r^n & -\alpha r^n \\ 0 & 0 & 0 & \cdots & -\gamma r^n & \beta r^{n+1}. \end{bmatrix}$$

is invertible iff

$$\beta\sqrt{r} \neq 2\sqrt{\alpha\gamma} \cos\left(\frac{k\pi}{n+3}\right), \quad k = 1, \dots, n+2,$$

and then, the entries of the inverse of  $J(\alpha, \beta, \gamma; r)$  are explicitly given by

$$r_{ks} = \frac{\left(\sqrt{\frac{\alpha r}{\gamma}}\right)^{s+1-k} U_{\min\{k,s\}}\left(\frac{\beta}{2}\sqrt{\frac{r}{\alpha\gamma}}\right) U_{n+1-\max\{k,s\}}\left(\frac{\beta}{2}\sqrt{\frac{r}{\alpha\gamma}}\right)}{\alpha r^s U_{n+2}\left(\frac{\beta}{2}\sqrt{\frac{r}{\alpha\gamma}}\right)}.$$

PROOF. In this case  $\theta = \sqrt{\frac{\alpha r}{\gamma}}$  and  $q = \frac{\beta}{2}\sqrt{\frac{r}{\alpha\gamma}}$ ,

$$\begin{aligned} u(k) &= \theta\beta U_{k-1}(q) - \alpha U_{k-2}(q) = \alpha \left[ 2q U_{k-1}(q) - U_{k-2}(q) \right] = \alpha U_k(q), \\ v(k) &= -r^{n+1}\beta U_{n-k}(q) + r^n\gamma\theta U_{n-k-1}(q) \\ &= -r^n\gamma\theta \left[ 2q U_{n-k}(q) - U_{n-k-1}(q) \right] = -r^n\sqrt{\alpha\gamma r} U_{n+1-k}(q). \end{aligned}$$

Since

$$\Phi_{a,b,c}(k) = \theta^{-k}u(k) \quad \text{and} \quad \Psi_{a,b,c}(k) = \theta^{n-k}v(k),$$

it follows that

$$\begin{aligned} \beta\Psi_{a,b,c}(0) - \alpha\Psi_{a,b,c}(1) &= -r^n\alpha\theta^{n-1}\sqrt{\alpha\gamma r} \left[ 2q U_{n+1}(q) - U_n(q) \right] \\ &= -r^n\alpha\gamma\theta^n U_{n+2}(q) \end{aligned}$$

and the matrix  $J(\alpha, \beta, \gamma; r)$  is invertible iff  $U_{n+2}(q) \neq 0$  and, then,

$$r_{ks} = \frac{\theta^{s+1-k} U_{\min\{k,s\}}(q) U_{n+1-\max\{k,s\}}(q)}{\alpha r^s U_{n+2}(q)}.$$

□

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