Complex Jacobi matrices

by

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Abstract

Complex Jacobi matrices play an important role in the study of asymptotics and zero distribution of Formal Orthogonal Polynomials (FOPs). The latter are essential tools in several fields of Numerical Analysis, for instance in the context of iterative methods for solving large systems of linear equations, or in the study of Padé approximation and Jacobi continued fractions.

In this paper we present some known and some new results on FOPs in terms of spectral properties of the underlying (infinite) Jacobi matrix, with a special emphasis to unbounded recurrence coefficients. Here we recover several classical results for real Jacobi matrices. The inverse problem of characterizing properties of the Jacobi operator in terms of FOPs and other solutions of a given three term recurrence is also investigated. This enables us to give results on the approximation of the resolvent by inverses of finite sections, with applications to the convergence of Padé approximants.

Key words: Difference operator, Complex Jacobi matrix, Formal orthogonal polynomials, Resolvent convergence, Convergence of J-fractions, Padé approximation.
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1 Introduction

We denote by ℓ^2 the Hilbert space of complex quadratic summable sequences, with the usual scalar product $(u,v) = \sum \overline{u_j} v_j$, and by $(e_n)_{n\geq 0}$ its usual orthonormal basis. Furthermore, for a linear operator T in ℓ^2, we denote by $\mathcal{D}(T)$, $\mathcal{R}(T)$, $\mathcal{N}(T)$, and $\sigma(T)$, its domain of definition, its range, its kernel, and its spectrum, respectively.

Given complex numbers a_n, b_n, $n \geq 0$, with $a_n \neq 0$ for all n, we associate the infinite tridiagonal *complex Jacobi matrix*

$$\mathcal{A} = \begin{pmatrix} b_0 & a_0 & 0 & \cdots & \cdots \\ a_0 & b_1 & a_1 & 0 & \\ 0 & a_1 & b_2 & a_2 & \ddots \\ \vdots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{1.1}$$

In the *symmetric case* $b_n, a_n \in \mathbb{R}$ for all n one recovers the classical Jacobi matrix. Denoting by $\mathcal{C}_0 \subset \ell^2$ the linear space of finite linear combinations of the basis elements $e_0, e_1, \ldots$, we may identify via the usual matrix product a complex Jacobi matrix $\mathcal{A}$ with an operator acting on

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$\mathcal{C}_0$. Its closure A is called the corresponding second order difference operator or Jacobi operator (see Section 2.1 for a more detailed discussion).

Second (or higher) order difference operators have received much attention in the last years, partly motivated by applications to non–linear discrete dynamical systems (see [6, 19, 20, 35] and the references therein). Also, Jacobi matrices are known to be a very useful tool in the study of (formal) orthogonal polynomials ((F)OPs), which again have applications in numerous fields of Numerical Analysis. To give an example, (formal) orthogonal polynomials have been used very successfully in Numerical Linear Algebra for describing both algorithmic aspects and convergence behavior of iterative methods like Conjugate Gradients, GMRES, Lanczos, QMR, and many others. Another example is given by the study of convergence of continued fractions and Padé approximants. Indeed, also the study of higher order difference operators is of interest in all these applications, let us mention the Bogoyavlenskii discrete dynamical system [7], Ruhe's block version of the Lanczos method in Numerical Linear Algebra, or the problem of Hermite-Padé and Matrix Padé approximation (for the latter see, e.g., the surveys [4, 5]). In the present paper we will restrict ourselves to the less involved case of three diagonals.

To start with, a linear functional c acting on the space of polynomials with complex coefficients is called regular iff $\det(c(x^{j+k}))_{j,k=0,\dots,n} \neq 0$ for all $n \geq 0$. Given a regular c (with $c(1) = 1$), there exists a sequence $(q_n)_{n \geq 0}$ of FOPs, i.e., q_n is a polynomial of degree n (unique up to a sign), and $c(q_j \cdot q_k)$ vanishes if $j \neq k$, and is equal to 1 otherwise. These polynomials are known to verify a three term recurrence of the form

$$a_n q_{n+1}(z) = (z - b_n) q_n(z) - a_{n-1} q_{n-1}(z), \quad n \geq 0, \quad q_0(z) = 1,\ q_{-1}(z) = 0,$$

where $a_n = c(z q_{n+1} q_n) \in \mathbb{C} \setminus \{0\}$, and $b_n = c(z q_n q_n) \in \mathbb{C}$. Here a_n, b_n are known to be real iff c is positive, i.e., $c(P) > 0$ for each nontrivial polynomial P taking nonnegative values on the real axis, or, equivalently, $\det(c(x^{j+k}))_{j,k=0,\dots,n} > 0$ for all $n \geq 0$. Conversely, the Shohat–Favard Theorem says that any $(q_n(z))_{n \geq 0}$ verifying a three-term recurrence relation of the above form is a sequence of formal orthogonal polynomials with respect to some regular linear functional c. As shown in Remark 2.3 below, this linear functional can be given in terms of the Jacobi operator A defined above, namely $c(P) = (e_0, P(A) e_0)$ for each polynomial P. In the real case one also knows that there is orthogonality with respect to some positive Borel measure μ supported on the real axis, i.e., $c(P) = \int P(x)\, d\mu(x)$.

Notice that q_n is (up to normalisation) the characteristic polynomial of the finite submatrix $\mathcal{A}_n$ of order n of $\mathcal{A}$. Also, the second order difference equation

$$z \cdot y_n = a_n y_{n+1} + b_n y_n + a_{n-1} y_{n-1}, \quad n \geq 0 \tag{1.2}$$

($a_{-1} := 1$) may be formally rewritten as spectral equation $(z\mathcal{I} - \mathcal{A}) \cdot y = 0$. This gives somehow the idea that spectral properties of the Jacobi operator should be determined by the spectral or asymptotic properties of FOPs, and vice versa. Indeed, in the real case the link is very much known: if A is self-adjoint, then there is just one measure of orthogonality (obtained by the spectral theorem applied to A), with support being equal to the spectrum $\sigma(A)$ of A. Also, zeros of OPs lie all in the convex hull of $\sigma(A)$, are interlacing, and every point in $\sigma(A)$ is attracting zeros. Furthermore, in case of bounded A one may describe the asymptotic behavior of OPs on and outside $\sigma(A)$. Surprisingly, for formal orthogonal polynomials these questions have been investigated only recently in terms of the operator A, probably due to the fact that here things may change quite a bit (see for instance Example 3.2 below).

To our knowledge, the first detailed account on (a class of) complex Jacobi matrices was given by Wall in his treatise [56] on continued fractions. He dealed with the problem of convergence of Jacobi continued fractions (J-fractions)

$$\frac{1}{\lceil z-b_0}\Big\rfloor + \frac{-a_0^2}{\lceil z-b_1}\Big\rfloor + \frac{-a_1^2}{\lceil z-b_2}\Big\rfloor + \frac{-a_2^2}{\lceil z-b_3}\Big\rfloor + \dots \tag{1.3}$$

having at infinity the (possibly formal) expansion $f(z) = \sum_j c(x^j) z^{-j-1} = \sum_j (e_0, A^j e_0) z^{-j-1}$. Their nth convergent may be rewritten as $p_n(z)/q_n(z)$, where $(p_n(z))_{n\geq -1}$, $(q_n(z))_{n\geq -1}$ are particular solutions of (1.2) with initializations

$$q_0(z) = 1, \quad q_{-1}(z) = 0, \quad p_0(z) = 0, \quad p_{-1}(z) = -1, \tag{1.4}$$

i.e., q_n are the FOPs mentioned above. Also, p_n/q_n is just the nth Padé approximant (at infinity) of the perfect series f. Notice that, in case of a bounded operator A, f is Laurent expansion at infinity of the so-called *Weyl function* [20]

$$\phi(z) := (e_0, (zI-A)^{-1} e_0), \quad z \in \Omega(A),$$

where here and in the sequel $\Omega(A) = \mathbb{C} \setminus \sigma(A)$ denotes the resolvent set, i.e., the set of all $z \in \mathbb{C}$ such that $\mathcal{N}(zI-A) = \{0\}$ and $\mathcal{R}(zI-A) = \ell^2$ (and thus the resolvent $(zI-A)^{-1}$ is bounded).

The aim of the present paper is threefold: we try to give a somehow complete account on connections between FOPs, complex J-fractions and complex Jacobi matrices presented in the last five years. Starting point is perhaps a paper of Aptekarev, Kaliaguine and Van Assche [6], but we also report about recent work by Barrios, López Lagomasino, Martínez-Finkelshtein, Torrano, Smirnova Castro, Simon, Magnus, Stahl, Baratchart, Ambroladze, Kaliaguine, and the present author. A special attention in our study is given to unbounded complex Jacobi matrices, where similar uniqueness problems occur as for the classical moment problem. Secondly, we present some new results concerning ratio-normality of FOPs and compact perturbations of complex Jacobi matrices. In addition, we show that many recent results on convergence of complex J-fractions in terms of Jacobi operators [12, 13, 14, 15, 17, 19] are in fact results on the approximation of the resolvent of complex Jacobi operators. Finally, we mention several open problems in this field of research. A main (at least partially) open question is however omitted: do these results have a counterpart for higher order difference operators?

The paper is organized as follows: Some preliminaries and spectral properties of Jacobi operators in terms of solutions of (1.2) are presented in Section 2. In Subsection 2.1 we report about the problem of associating a unique operator to (1.1), and introduce the notion of *proper* Jacobi matrices. Beside some preliminary observations, we recall in Subsection 2.2 Wall's definition of determinated Jacobi matrices and relate it to proper ones. Also, some sufficient conditions for determinacy are discussed [56, 14, 42]. Known characterizations [6, 18] of elements z of the resolvent set in terms of the asymptotic behavior of solutions of (1.2) are described in Subsection 2.3. Here we also show in Theorem 2.11 that for indeterminate complex Jacobi operators we have a similar behavior as for not self-adjoint Jacobi operators (where the corresponding moment problem does not have a unique solution). In Subsection 2.4 we highlight the significance of the Weyl function and of functions of the second kind. Their representation as Cauchy transforms is investigated in Subsection 2.5, where we also study the case of totally positive moment sequences leading to non-real compact Jacobi matrices.

In Section 3 we describe results on the asymptotic behavior of FOPs in the resolvent set. nth root asymptotics for bounded complex Jacobi matrices obtained in [6, 17, 19] are presented in

Subsection 3.1. In Subsection 3.2 we deal with the problem of localizing zeros of FOPs, thereby generalizing some results from [17]. We show that, roughly, under some additional hypotheses there are only "few" zeros in compact subsets of the resolvent set. An important tool is the study of ratios of two succeeding monic FOPs. An inverse open problem concerning zero-free regions is presented in Subsection 3.3. In Subsection 3.4 we characterize compact perturbations of complex Jacobi matrices in terms of the ratios mentioned above. Strong asymptotics for trace class perturbations are the subject of Subsection 3.5. In the final Section 4, we investigate the problem of convergence of Padé approximants (or J-fractions) and more generally of (weak, strong or norm) resolvent convergence. A version of the Kantorovitch Theorem for complex Jacobi matrices is given in Subsection 4.1, together with a discussion of its assumptions. We describe in Subsection 4.2 consequences for the approximation of the Weyl function, and finally illustrate in Subsection 4.3 some of our findings by discussing (asymptotically) periodic complex Jacobi matrices.

2 The Jacobi operator

2.1 Infinite matrices and operators

Given an infinite matrix $\mathcal{A} = (a_{j,k})_{j,k\geq 0}$ of complex numbers, can we define correctly a (closed and perhaps densely defined) operator by matrix calculus by identifying elements of ℓ^2 with infinite column vectors? Of course, since Hilbert and its collaborators, an answer to this question is known, see, e.g., [2]. In this section we briefly summarize the most important facts. Here we will restrict ourselves to matrices $\mathcal{A}$ with rows and columns being elements of ℓ^2, an assumption which is obviously true for banded matrices such as our complex Jacobi matrices.

By assumption, the formal product $\mathcal{A} \cdot y$ is defined for any $y \in \ell^2$. Thus as a natural candidate of an operator associated to $\mathcal{A}$ we could consider the so–called *maximal operator* (see [28, Example III.2.3]) $[\mathcal{A}]_{\max}$ with

$$\mathcal{D}([\mathcal{A}]_{\max}) = \{y \in \ell^2 : \mathcal{A} \cdot y \in \ell^2\} \tag{2.1}$$

and $[\mathcal{A}]_{\max} y := \mathcal{A} \cdot y \in \ell^2$. However, there are other operators having interesting properties which may be associated to $\mathcal{A}$. For instance, since the columns of $\mathcal{A}$ are elements of ℓ^2, we may define a linear operator on $\mathcal{C}_0$ (also denoted by $\mathcal{A}$) by setting

$$\mathcal{A} e_k = (a_{j,k})_{j\geq 0}, \quad k = 0, 1, 2, ...$$

Notice that $[\mathcal{A}]_{\max}$ is an extension[2] of $\mathcal{A}$.

A minimum requirement in the spectral theory of linear operators is that the operator in question is closed [28, Section III.5.2]. In general, our operator $\mathcal{A}$ is not closed, but closable [28, Section III.5.3], i.e., for any sequence $(y^{(n)})_{n\geq 0}$ with $(y^{(n)}, \mathcal{A} y^{(n)}) \to (0, v)$ we have $v = 0$. To see this, notice that

$$(e_j, v) = \lim_{n\to\infty} \sum_{k=0}^{\infty} a_{j,k} y_n^{(k)} = \lim_{n\to\infty} (v_j, y^{(k)})$$

[2]Given two operators T, S in ℓ^2, we say that S is an extension of T (and write $T \subset S$) if $\mathcal{D}(T) \subset \mathcal{D}(S)$, and $Ty = Sy$ for all $y \in \mathcal{D}(T)$.

where $v_j = (\overline{a_{j,k}})_{k\geq 0} \in \ell^2$ by assumption on the rows of $\mathcal{A}$. Thus we may consider the *closure* $[\mathcal{A}]_{\min}$ of $\mathcal{A}$, i.e., the smallest closed extension of $\mathcal{A}$. Notice that

$$\mathcal{D}([\mathcal{A}]_{\min}) = \{y \in \ell^2 : \exists \quad \begin{array}{l} (y^{(n)})_{n\geq 0} \subset \mathcal{C}_0 \ \text{ converging to } y, \text{ and} \\ (\mathcal{A}y_n)_{n\geq 0} \subset \ell^2 \ \text{ converging (to } [\mathcal{A}]_{\min} y)\}. \end{array} \tag{2.2}$$

We have the following links between the operators $[\mathcal{A}]_{\min}$, $[\mathcal{A}]_{\max}$, and their adjoints.

Lemma 2.1 *Let* $\mathcal{A}^H := (\overline{a_{j,k}})_{k=0,1,\ldots}^{j=0,1,\ldots}$. *Then*

$$([\mathcal{A}]_{\min})^* = [\mathcal{A}^H]_{\max}, \quad ([\mathcal{A}]_{\max})^* = [\mathcal{A}^H]_{\min}.$$

In particular, the maximal operator $[\mathcal{A}]_{\max}$ *is a closed extension of* $[\mathcal{A}]_{\min}$.

Proof: In order to show the first equality, we write shorter $A = [\mathcal{A}]_{\min}$. By definition of the adjoint [28, Section III.5.5]), $\mathcal{D}(A^*)$ equals the set of all $y \in \ell^2$ such that there exists a $y^* \in \ell^2$ with

$$(y, Ax) = (y^*, x) \ \text{ for all } \ x \in \mathcal{D}(A),$$

and $y^* = A^* y$. According to the characterization of $\mathcal{D}(A)$ given above and the continuity of the scalar product, it is sufficient to require that $(y, Ax) = (y^*, x)$ holds for all $x \in \mathcal{C}_0$, or, equivalently,

$$y_j^* = (e_j, y^*) = (Ae_j, y) \ \text{ for all } \ j \geq 0.$$

Since (Ae_j, y) coincides with the jth component of the formal product $\mathcal{A}^H y$, we obtain $A^* = [\mathcal{A}^H]_{\max}$ by the definition (2.1) of $\mathcal{D}([\mathcal{A}^H]_{\max})$.

The second identity of Lemma 2.1 follows from the fact that $A^{**} = A$ by [28, Theorem III.5.29]. Finally, we obtain the last claim by observing that $[\mathcal{A}]_{\max}$ is an extension of $\mathcal{A}$, and $[\mathcal{A}]_{\max}$ is closed (since an adjoint of a densely defined operator is closed [28, Theorem III.5.29]). □

Definition 2.2 *The infinite matrix* $\mathcal{A}$ *with rows and columns in* ℓ^2 *is called* proper *if the operators* $[\mathcal{A}]_{\max}$ *and* $[\mathcal{A}]_{\min}$ *coincide.*

Notice that any operator B defined by matrix product (i.e., $By = \mathcal{A} \cdot y$ for $y \in \mathcal{D}(B)$) necessarily is a restriction of $[\mathcal{A}]_{\max}$ by (2.1). From Lemma 2.1 we obtain the equivalent description $\mathcal{A}^H \subset B^*$. If in addition $\mathcal{C}_0 \subset \mathcal{D}(B)$, then $\mathcal{A} \subset B \subset [\mathcal{A}]_{\max}$. We may conclude that any closed operator B defined by matrix product and $\mathcal{C}_0 \subset \mathcal{D}(B)$ satisfies $[\mathcal{A}]_{min} \subset B \subset [\mathcal{A}]_{\max}$, and such an operator B is unique if and only if $\mathcal{A}$ is proper. [3]

Let us have a look at the special case of hermitian matrices $\mathcal{A}$, i.e., $\mathcal{A} = \mathcal{A}^H$. Here Lemma 2.1 tells us that $A := [\mathcal{A}]_{\min}$ has the adjoint $A^* = [\mathcal{A}]_{\max}$ (see also [49, p.90] or [28, Example V.3.13]), which is an extension of A. Hence A is symmetric, and we obtain the following equivalencies: A is self-adjoint (i.e., $A = A^*$) if and only if $\mathcal{A}$ is proper if and only if there exists a unique symmetric closed extension of $\mathcal{A}$. (compare with [28, Problem III.5.25]).

[3] Some authors consider other extensions of $\mathcal{A}$ which are not defined by matrix product, or which are defined by Hilbert space extensions.

Remark 2.3 The notion of proper Jacobi matrices may be motivated by considering the following problem: given a regular functional c acting on the space of polynomials, can we describe its action by a densely defined closed operator B, namely $c(P) = (f, P(B)g)$ and, more generally,

$$c(P \cdot Q) = (Q(B)^* f, P(B)g) \quad \text{for all polynomials } P, Q \tag{2.3}$$

with suitable $f, g \in \ell^2$?

Let us first show that any closed operator B with $\mathcal{A}_{\min} \subset B \subset \mathcal{A}_{\max}$ satisfies (2.3) with $f = g = e_0$. Obviously, it is sufficient to show the relation

$$e_j = q_j(B)e_0 = q_j(B)^* e_0, \quad j \geq 0.$$

Indeed, $e_0 = q_0(B)e_0$ by (1.4), and by recurrence using (1.2) we obtain

$$a_j q_{j+1}(B)e_0 = Bq_j(B) - b_j q_j(B)e_0 - a_{j-1}q_{j-1}(B)e_0 = Be_j - b_j - a_{j-1}e_{j-1} = a_j e_{j+1},$$

the last equality following from $\mathcal{A} \subset B$. Since $a_j \neq 0$, the relation $e_{j+1} = q_{j+1}(B)e_0$ follows. In a similar way the other identity is shown using the relation $\mathcal{A}^H \subset B^*$.

Let us now show that this are essentially all operators. Notice first that B is only properly characterized by (2.3) if f is a cyclic element of B (i.e., $f \in \mathcal{D}(B^k)$ for all k, and $\text{span}\{B^j f : j \geq 0\}$ is dense in ℓ^2), and g is a cyclic element of B^*. In this case, using the orthogonality relations of the FOPs q_j, we may conclude that $(f_n)_{n\geq 0}$ and $(g_n)_{n\geq 0}$, defined by $f_n = q_n(B)f$ and $g_n = q_n(B)^* g$, is a complete normalized biorthogonal system. The expansion coefficients of Bf_k (and $B^* g_j$, respectively) with respect to the system $(f_n)_{n\geq 0}$ (and $(g_n)_{n\geq 0}$, respectively) are given by

$$(g_j, Bf_k) = \overline{(f_k, B^* g_j)} = c(zq_jq_k) = (e_j, \mathcal{A}e_k) = \begin{cases} a_{\min(j,k)} & \text{if } j = k+1 \text{ or } k = j+1, \\ b_j & \text{if } j = k, \\ 0 & \text{else.} \end{cases}$$

In other words, up to the representation of ℓ^2 and its dual with help of these different bases, we have $\mathcal{A} \subset B$ and $\mathcal{A}^H \subset B^*$, and thus $\mathcal{A}_{\min} \subset B \subset \mathcal{A}_{\max}$. We may conclude in particular that an operator as in (2.3) is unique (up to basis transformations) if and only if $\mathcal{A}$ is proper. □

For an infinite matrix $\mathcal{A}$, define the quantity

$$||\mathcal{A}|| := \sup_{u,v \in \mathcal{C}_0} |\frac{(u, \mathcal{A}v)}{(u, v)}| = \sup_{n \geq 0} ||\mathcal{A}_n||,$$

where on the right-hand side $\mathcal{A}_n$ denotes the principal submatrix of order n of $\mathcal{A}$. Clearly, $||\mathcal{A}||$ is the operator norm of $\mathcal{A}$, and $[\mathcal{A}]_{\min}$ is bounded (with $||[\mathcal{A}]_{\min}|| = ||\mathcal{A}||$) iff $||\mathcal{A}|| < \infty$. One easily checks that in this case $\mathcal{D}([\mathcal{A}]_{\min}) = \ell^2$. Conversely, if $\mathcal{D}([\mathcal{A}]_{\min}) = \ell^2$, then $\mathcal{A}$ is bounded by the closed graph theorem [28, Theorem III.5.20]. Finally, we recall the well-known estimate [28, Example III.2.3]

$$||\mathcal{A}||^2 \leq [\sup_j \sum_{k=0}^{\infty} |a_{j,k}|] \cdot [\sup_k \sum_{j=0}^{\infty} |a_{j,k}|]. \tag{2.4}$$

Using this formula one easily verifies the well-known fact that banded matrices $\mathcal{A}$ are bounded iff their entries are uniformly bounded.

We may conclude that a bounded matrix $\mathcal{A}$ is proper, and thus we may associate a unique close operator $A = [\mathcal{A}]_{\min}$ whose action is described via matrix calculus. However, these properties do not remain necessarily true for unbounded matrices.

2.2 Spectral properties of Jacobi operators

In what follows $\mathcal{A}$ will be the complex Jacobi matrix of (1.1) with entries $a_n, b_n \in \mathbb{C}$, $a_n \neq 0$, We refer to its closure $A = [\mathcal{A}]_{\min}$ as the corresponding *difference operator* or *Jacobi operator*, and denote by $A^\# = [\mathcal{A}]_{\max}$ the maximal closed extension of A defined by matrix product. Since $\mathcal{A}^H$ is obtained from $\mathcal{A}$ by taking the complex conjugate of each entry, we may conclude from Lemma 2.1 that $A^\# = \Pi A^* \Pi$, where Π denotes the complex conjugation operator defined by $\Pi(y_j)_{j\geq 0} = (\overline{y_j})_{j \geq 0}$.

The aim of this section is to summarize some basic properties of the operators A, $A^\#$ in terms of solutions $q(z) := (q_n(z))_{n\geq 0}$ and $p(z) := (p_n(z))_{n \geq 0}$ of the recurrence (1.2), (1.4).

We will require the projection operators Π_j defined by

$$\Pi_j(y_0, y_1, y_2, ...) = (y_0, y_1, ..., y_{j-1}, 0, 0, ...) \in \mathcal{C}_0, \quad j \geq 0.$$

Clearly, $\Pi_j y \to y$ for $j \to \infty$ for any $y \in \ell^2$. Also, one easily checks that, for any sequence $y = (y_n)_{n \geq 0}$, $\Pi_j y \in \mathcal{D}(A)$, with

$$A(\Pi_j y) = \Pi_j(\mathcal{A} \cdot y) + a_{j-1} \cdot (\underbrace{0, ..., 0}_{j-1}, -y_j, y_{j-1}, 0, 0, ...). \tag{2.5}$$

Using (2.4) one easily verifies that A is bounded if and only if the entries of $\mathcal{A}$ are uniformly bounded, more precisely,

$$\sup_{n\geq 0} \sqrt{|a_{n-1}|^2 + |b_n|^2 + |a_n|^2} \leq ||A|| \leq \sup_{n \geq 0}(|a_{n-1}| + |b_n| + |a_n|) \tag{2.6}$$

(where we tacitly put $a_{-1} = 0$). Also, notice that $\mathcal{A}$ is hermitian if and only if it is real.

Some further elementary observations are summarized in

Lemma 2.4 **(a)** *For $z \in \mathbb{C}$ there holds*

$$0 \leq \dim \mathcal{N}(zI - A) \leq \dim \mathcal{N}(zI - A^\#) \leq 1,$$

with $\mathcal{N}(zI - A^\#) = \ell^2 \cap \{\lambda \cdot q(z) : \lambda \in \mathbb{C}\}$.

(b) *For $n \geq 0$ and $z \in \mathbb{C}$ we have $e_n - q_n(z) e_0 \in \mathcal{R}(zI - A)$.*

(c) *For $z \in \mathbb{C}$ there holds $\{y \in \mathcal{D}(A^\#) : (zI - A^\#)y = e_0\} = \ell^2 \cap \{\gamma \cdot q(z) - p(z) : \gamma \in \mathbb{C}\}$.*

(d) *For all $z \in \mathbb{C}$ we have $\mathcal{D}(zI - A^\#) = \mathcal{D}(A^\#) = \Pi \mathcal{D}(A^*)$, $\mathcal{N}(zI - A^\#) = \Pi \mathcal{N}((zI - A)^*)$, and $\mathcal{R}(zI - A^\#) = \Pi \mathcal{R}((zI - A)^*)$.*

Proof: **(a)** Since $A \subset A^\#$, we only have to show the last assertion. By (2.1), $y = (y_n)_{n \geq 0} \in \mathcal{N}(zI - A^\#)$ if and only if $y \in \ell^2$, and we have $(z\mathcal{I} - \mathcal{A}) \cdot y = 0$. The latter identity may be rewritten as

$$-a_n y_{n+1} + (z - b_n) y_n - a_{n-1} y_{n-1} = 0, \quad n \geq 0, \quad y_{-1} = 0.$$

Comparing with (1.2), (1.4), we see that $(z\mathcal{I} - \mathcal{A}) \cdot y = 0$ iff $y = y_0 \cdot q(z)$, leading to the above description of $\mathcal{N}(zI - A^{\#})$.
(b) Notice that (1.2), (1.4) may be rewritten as

$$(z\mathcal{I} - \mathcal{A}) \cdot q(z) = 0, \quad (z\mathcal{I} - \mathcal{A}) \cdot p(z) = -e_0.$$

Combining this with (2.5), we obtain

$$(zI - A)\Pi_{n+1}p(z) = -e_0 + a_n \cdot (\underbrace{0, .., 0}_{n}, p_{n+1}(z), -p_n(z), 0, 0, ...), \tag{2.7}$$

$$(zI - A)\Pi_{n+1}q(z) = a_n \cdot (\underbrace{0, .., 0}_{n}, q_{n+1}(z), -q_n(z), 0, 0, ...). \tag{2.8}$$

Also, one easily verifies by recurrence using (1.2) that

$$a_n \cdot (q_n(z) \cdot p_{n+1}(z) - q_{n+1}(z) \cdot p_n(z)) = 1, \quad n \geq -1, \quad z \in \mathbb{C}. \tag{2.9}$$

Thus we have found an element of $\mathcal{C}_0 \subset \mathcal{D}(A)$ verifying

$$\begin{aligned}&(zI - A)\Pi_{n+1}[q_n(z)p(z) - p_n(z)q(z)] \\ &= -q_n(z)e_0 + a_n a_n \cdot (\underbrace{0, .., 0}_{n}, q_n(z)p_{n+1}(z) - p_n(z)q_{n+1}(z), 0, 0, ...) = e_n - q_n(z)e_0.\end{aligned}$$

(c) Since $(zI - \mathcal{A}) \cdot (\gamma \cdot q(z) - p(z)) = e_0$ for all γ, a proof for this assertion follows the same lines as the one of part (a). We omit the details.
(d) This part is an immediate consequence of the fact that

$$(zI - A)^* = \overline{z}I - A^* = \overline{z}I - \Pi A^{\#}\Pi = \Pi(zI - A^{\#})\Pi.$$

□

For a closed densely defined linear operator T in ℓ^2, the integer $\dim \mathcal{N}(T)$ usually is referred to as the *nullity* of T, and $\mathcal{N}(zI-T)$ coincides with the geometric multiplicity of the "eigenvalue" z (if larger than zero). One also defines the *deficiency* of T as the codimension in ℓ^2 of $\mathcal{R}(T)$. Provided that $\mathcal{R}(T)$ is closed, it follows from [28, Theorem IV.5.13 and Lemma III.1.40] that the deficiency of T coincides with $\dim \mathcal{N}(T^*)$, and that also $\mathcal{R}(T^*)$ is closed. Taking into account Lemma 2.4(a),(d), we may conclude that both deficiency and nullity are bounded by one for our operators $zI - A$ and $zI - A^{\#}$ provided one of them has closed range. Consequently, we obtain for the essential spectrum [28, Chapter IV.5.6]

$$\sigma_{ess}(A) = \sigma_{ess}(A^{\#}) = \{z \in \mathbb{C} : \mathcal{R}(zI - A) \text{ is not closed }\}. \tag{2.10}$$

Recall that this (closed) part of the spectrum of A (or $A^{\#}$) remains invariant under compact perturbations [28, Theorem IV.5.35]. Let us relate Definition 2.2 to the notion of determinacy as introduced by Wall.

Definition 2.5 (see [56, Definition 22.1])
The complex Jacobi matrix $\mathcal{A}$ is called determinate *if at least one of the sequences $p(0)$ or $q(0)$ is not an element of ℓ^2.*

According to [56, Theorem 22.1], $\mathcal{A}$ is indeterminate if $p(z)$ and $q(z)$ are elements of ℓ^2 for one $z \in \mathbb{C}$, and in this case they are elements of ℓ^2 for all $z \in \mathbb{C}$. It is also known (see [1, pp.138-141] or [35, p.76]) that a real Jacobi matrix is proper (i.e., self-adjoint) if and only if it is determinate. In the general case we have the following

Theorem 2.6 (compare with [18, Proposition 3.2])
(a) A determinate complex Jacobi matrix $\mathcal{A}$ with $\sigma_{ess}(A) \neq \mathbb{C}$ is proper.
(b) A proper complex Jacobi matrix $\mathcal{A}$ is determinate.
(c) If $\Omega(A) \neq \emptyset$ then $\mathcal{A}$ is proper.

Proof: Part (a) has been established in [18, Proposition 3.2], the proof is mainly based on Lemma 2.4(d) and the fact that in the case $z \notin \sigma_{ess}(A)$ the set $\mathcal{R}(zI - A)$ (and $\mathcal{R}((zI - A)^*)$, respectively) coincides with the orthogonal complement of $\mathcal{N}((zI - A)^*)$ (and of $\mathcal{N}(zI - A)$, respectively).

In order to show part (b), suppose that $\mathcal{A}$ is not determinate. Then $\dim \mathcal{N}(zI - A^\#) = 1$ and $\mathcal{C}_0 \subset \mathcal{R}(zI - A^\#)$ for all $z \in \mathbb{C}$ according to Lemma 2.4(a),(b),(c), and thus $\mathcal{C}_0 \subset \mathcal{R}((zI - A)^*)$ by Lemma 2.4(d). Taking into account that $\mathcal{N}(zI - A)$ is just the orthogonal complement $\mathcal{R}((zI - A)^*)^\perp$ of $\mathcal{R}((zI - A)^*)$, we may conclude that $\dim \mathcal{N}(zI - A) = 0$, showing that $A \neq A^\#$.

Part (c) was also mentioned in [18, Proposition 3.2]: Let $z \in \Omega(A)$. Then $\mathcal{R}(zI - A) = \ell^2$ by definition of the resolvent set. Hence $\mathcal{N}((zI - A)^*) = \{0\}$, implying that $\mathcal{N}(zI - A^\#) = \{0\}$ by Lemma 2.4(d). From Lemma 2.4(a) we may conclude that $(q_n(z))_{n \geq 0} \notin \ell^2$, and hence $\mathcal{A}$ is determined. Finally, since $\mathbb{C} \setminus \sigma_{ess}(A) \supset \Omega(A)$ is non-empty, it follows from Theorem 2.6(a) that $\mathcal{A}$ is proper. □

The *numerical range* (or *field of values*) [28, Section V.3.2] of a linear operator T in ℓ^2 is defined by

$$\Theta(T) = \{(y, Ty) : y \in \mathcal{D}(T), ||y|| = 1\}$$

By a theorem of Hausdorff, $\Theta(T)$ and its closure $\Gamma(T)$ are convex. Also, $\sigma_{ess}(A) \subset \Gamma(A)$ by [28, Theorem V.3.2]. Hence, for complex Jacobi matrices with $\sigma_{ess}(A) \neq \mathbb{C}$ or $\Gamma(A) \neq \mathbb{C}$, the notions of determinacy and properness are equivalent. This includes the case of real Jacobi matrices since here $\Gamma(A) \subset \mathbb{R}$. Notice that $\Gamma(A) \neq \mathbb{C}$ implies that $\Gamma(A)$ is included in some half-plane of $\mathbb{C}$. The case of the lower half plane $\{Im(z) \leq 0\}$ was considered by Wall [56, Definition 16.1] who called the corresponding J-faction *positive definite* and gave characterizations of such complex Jacobi matrices in terms of chain sequences [56, Theorem 16.2]. In this context we should also mention that $\Gamma(A)$ is compact if and only if A is bounded; indeed, one knows [25, Eqn.(1.6)] that $\sup\{|z| : z \in \Gamma(A)\} \in [||A||/2, ||A||]$.

It is not known whether there exists a determinate complex Jacobi matrix which is not proper. Since many of the results presented below are valid either for proper or for indetermi-nated Jacobi matrices, a clarification of this problem seems to be desirable.

Results related to Theorem 2.6 have been discussed by several authors: Barrios, López, Martínez and Torrano [14, Lemma 3] showed that a complex Jacobi matrix $\mathcal{A} = \mathcal{A}' + \mathcal{A}''$ with $\mathcal{A}'$ self-adjoint and $\mathcal{A}''$ bounded is determinate. More generally, Smirnova Castro [42, Theorem 2] proved that a bounded perturbation of a real Jacobi matrix $\mathcal{A}$ is determined[4] if and only if $\mathcal{A}$ is determined. It is an interesting open problem to characterize determinacy or properness in terms of the real and the imaginary part of a Jacobi matrix.

Let us here have a look at some sufficient condition which will be used later.

Example 2.7 *It is known [56, Theorem 25.1] that $\mathcal{A}$ is determinate provided that*

$$\sum_{n=0}^{\infty} \frac{1}{|a_n|} = +\infty.$$

We claim that then $\mathcal{A}$ is also proper. To see this, let $y \in \mathcal{D}(A^{\#})$. Choose integers $n_0 < n_1 < \dots$ with

$$\alpha_\ell := \sum_{j=n_\ell}^{n_{\ell+1}-1} \frac{1}{|a_{j-1}|} \geq 1, \quad \ell \geq 0,$$

and put

$$y^{(\ell)} = \frac{1}{\alpha_\ell} \sum_{j=n_\ell}^{n_{\ell+1}-1} \frac{1}{|a_{j-1}|} \Pi_j y \in \mathcal{C}_0.$$

Since $n_\ell \to \infty$ and $\Pi_j y \to y$, one obtains $y^{(\ell)} \to y$. Furthermore, according to (2.5),

$$\begin{aligned} ||Ay^{(\ell)} - A^{\#}y|| &\leq \frac{1}{\alpha_\ell} \sum_{j=n_\ell}^{n_{\ell+1}-1} \frac{||\Pi_j A^{\#} y - A^{\#} y||}{|a_{j-1}|} + \frac{1}{\alpha_\ell} || \sum_{j=n_\ell}^{n_{\ell+1}-1} \frac{A\Pi_j y - \Pi_j A^{\#} y}{|a_{j-1}|} || \\ &\leq ||\Pi_{n_\ell} A^{\#} y - A^{\#} y|| + \frac{1}{\alpha_\ell} || \sum_{j=n_\ell}^{n_{\ell+1}-1} (\underbrace{0, \dots, 0}_{j-1}, |y_j|, |y_{j-1}|, 0, 0, \dots) || \\ &\leq ||\Pi_{n_\ell} A^{\#} y - A^{\#} y|| + \frac{2}{\alpha_\ell} ||\Pi_{n_\ell} y - y||, \end{aligned}$$

and the right-hand side clearly tends to 0 for $\ell \to \infty$. Thus $y \in \mathcal{D}(A)$ by (2.2).

Combining Example 2.7 with the techniques of [17, Example 5.2], one may construct for any closed set $E \subset \mathbb{C}$ a proper difference operator A satisfying $\sigma_{ess}(A) = E$. In particular [17, Example 5.2], notice that (in contrast to the real case) the resolvent set may consist of several connected components.

To conclude this part, let us recall from [18] a further characterization of the essential spectrum in terms of *associated* Jacobi matrices. We denote by $\mathcal{A}^{(k)}$ the "shifted" (complex) Jacobi matrix obtained by replacing (a_j, b_j) in $\mathcal{A}$ by (a_{j+k}, b_{j+k}), $j \geq 0$. As in [28, Chapter IV.6.1] one shows that the operators corresponding to $\mathcal{A} = \mathcal{A}^{(0)}$, and to $\mathcal{A}^{(k)}$, respectively, have the same essential spectrum for any $k \geq 0$. In our case we have the following stronger assertion.

Theorem 2.8 (see [18, Proposition 3.4])
Suppose that $\mathcal{A}$ is determinate. Then $\sigma_{ess}(A) = \sigma(A^{(k)}) \cap \sigma(A^{(k+1)})$ for any $k \geq 0$. More precisely, for any $z \in \mathbb{C} \setminus \sigma_{ess}(A)$ there exists a non-trivial ℓ^2-solution $(s_n(z))_{n \geq -1}$ of (1.2), with

$$\Omega(A^{(k)}) = \{z \in \mathbb{C} \setminus \sigma_{ess}(A) : s_{k-1}(z) \neq 0\}, \quad k \geq 0. \tag{2.11}$$

[4] Of course, by (2.1), (2.2), a proper Jacobi matrix $\mathcal{A}$ remains proper after adding some bounded perturbation.

If the entries of the difference of two (complex) Jacobi matrices tend to zero along diagonals, then the difference of the corresponding difference operators is known to be *compact* [2]. We can now give a different characterization of the essential spectrum, namely

$$\sigma_{ess}(A) = \bigcap \{\sigma(A') : A' \text{ is a difference operator and } A - A' \text{ is compact}\}. \tag{2.12}$$

Here the inclusion $\subset$ is true even in a more general setting [28, Theorem IV.5.35]. In order to see the other inclusion, notice that for the particular solution of Theorem 2.8 there necessarily holds $|s_{-1}(z)| + |s_0(z)| \neq 0$. Therefore, by Theorem 2.8, the essential spectrum is already obtained by taking the intersection with respect to all difference operators found by varying the entry a_0 of $\mathcal{A}$, i.e., by rank 1 perturbations.

2.3 Characterization of the spectrum

In this subsection we are concerned with the problem of characterizing the spectrum of a difference operator in terms of solutions of the recurrence relation (1.2). This connection can be exploited in several ways: on the one hand side one sometimes knows the asymptotic behavior of solutions of (1.2) (as for instance in the case of (asymptotically) periodic recurrence coefficients, compare [12, 13, 19, 24, 32]), and it is possible to determine the shape of the spectrum. On the other hand, we will see in Section 3 that we obtain nth root asymptotics for FOPs and functions of the second kind on the resolvent set.

A description of the resolvent operator (or more precisely of a (formal) "right reciprocal") in terms of the solutions $p(z)$, $q(z)$ of the recurrence (1.2) has been given already by Wall [56, Sections 59-61]. Starting with a paper of Aptekarev, Kaliaguine and Van Assche [6], the problem of characterizing the spectrum has received much attention in the last years, see [13, 14, 18, 19] for Jacobi matrices and the survey papers [4, 5] and the references therein for higher order difference operators. A typical example of characterizing the spectrum in terms of only one solution of (1.2) is the following.

Theorem 2.9 (see [18, Theorem 2.3])
Let A be bounded. Then $z \in \Omega(A)$ if and only if

$$\sup_{n\geq 0} \frac{\sum_{j=0}^{n} |q_j(z)|^2}{|a_n|^2[|q_n(z)|^2 + |q_{n+1}(z)|^2]} < \infty. \tag{2.13}$$

Indeed, using (2.8) we obtain for $z \in \Omega(A)$ and $n \geq 0$

$$\frac{1}{||zI - A||^2} \leq \frac{\sum_{j=0}^{n} |q_j(z)|^2}{|a_n|^2[|q_n(z)|^2 + |q_{n+1}(z)|^2]} = \frac{||\Pi_{n+1} q(z)||^2}{||(zI - A)\Pi_{n+1} q(z)||^2} \leq ||(zI - A)^{-1}||^2, \tag{2.14}$$

showing that (2.13) holds. The other implication is more involved, here one applies the characterization of Theorem 2.12 below. Notice that we may reformulate Theorem 2.9 as follows: we have $z \in \sigma(A)$ if and only if the sequence $(\Pi_n q(z)/||\Pi_n q(z)||)_{n\geq 0}$ contains a subsequence of approximate eigenvectors.

In view of (2.13), (2.14), we can give another formulation of Theorem 2.9: we have $z \in \Omega(A)$ if and only if the sequence of numerators in (2.13), and denominators in (2.13), respectively, have the same asymptotic behavior. It becomes clear from the following considerations (and can also be checked directly) that then both sequences will grow exponentially. It seems that, even for the classical case of real bounded Jacobi matrices, this result has only been found recently [18]. As mentioned before, here the spectrum of A coincides with the support of the measure of orthogonality μ of $(q_n)_{n\geq 0}$.

Some further consequences of relation (2.13) concerning the distribution of zeros of FOPs will be discussed in Section 3.

In order to describe other characterisations of the spectrum, we will fix $z \in \mathbb{C}$, and denote by $\mathcal{R}(\gamma)$, $\gamma \in \mathbb{C}$, the infinite matrix with elements

$$\mathcal{R}(\gamma)_{j,k} = \begin{cases} q_j(z) \cdot \{\gamma \cdot q_k(z) - p_k(z)\} & \text{if } 0 \leq j \leq k, \\ \{q_j(z) \cdot \gamma - p_j(z)\} \cdot q_k(z) & \text{if } 0 \leq k \leq j, \end{cases}$$

$j, k = 0, 1, 2, \ldots$. These matrices are just the (formal) "right reciprocals" mentioned by Wall [56, Theorem 60.2]. In the next statement we characterize the resolvent set of possibly unbounded difference operators in terms of two solutions of (1.2). A special case of this assertion may be found in [56, Theorem 61.2].

Theorem 2.10 *We have $z \in \Omega(A)$ if and only if $\mathcal{A}$ is proper, and there exists a $\gamma \in \mathbb{C}$ such that $\mathcal{R}(\gamma)$ is bounded. In this case, γ is unique, and the resolvent is given by $(zI - A)^{-1} = [\mathcal{R}(\gamma)]_{\min}$, in particular $\gamma = (e_0, (zI - A)^{-1} e_0)$.*

Proof: Let $z \in \Omega(A)$, and denote by $\mathcal{R} = (\mathcal{R}_{j,k})_{j,k=0,1,\ldots}$ the (bounded) infinite matrix corresponding to the resolvent operator $(zI - A)^{-1}$. It follows from Theorem 2.6(c) that $\mathcal{A}$ is proper. Thus the first implication follows by showing that $\mathcal{R} = \mathcal{R}(\gamma)$ for $\gamma = (e_0, (zI - A)^{-1} e_0)$. Since $\mathcal{R}((zI - A)^{-1}) = \mathcal{D}(zI - A)$, we obtain

$$(zI - A)[\mathcal{R} \cdot e_0] = (zI - A)[(zI - A)^{-1} e_0] = e_0.$$

From Lemma 2.4(c) we get the form of the first column of $\mathcal{R}$, namely $\mathcal{R}_{j,0} = \gamma q_j(z) - p_j(z) = \mathcal{R}(\gamma)_{j,0}$ for some $\gamma \in \mathbb{C}$. Here the identity $\gamma = (e_0, (zI - A)^{-1} e_0)$ is obtained by comparing the values for the index $j = 0$. The form of the other columns of $\mathcal{R}$ is obtained from Lemma 2.4(b) and its proof. Indeed, we have for $j \geq 1$, $k \geq 0$

$$\mathcal{R}_{j,k} - q_k(z)\mathcal{R}_{j,0} = \Big(e_j, (zI - A)^{-1}[e_k - q_k(z) e_0]\Big) = \Big(e_j, \Pi_{k+1}[q_k(z)p(z) - p_k(z)q(z)]\Big),$$

and thus $\mathcal{R}_{j,k} = \mathcal{R}(\gamma)_{j,k}$.

Conversely, suppose that $\mathcal{R}(\gamma)$ is bounded, and denote by R its closure. By some elementary calculations using (1.2) and (2.9) one verifies that

$$\mathcal{R}(\gamma) \cdot (z e_j - \mathcal{A} e_j) = e_j, \quad j \geq 0,$$

and thus $R(zI - A)y = y$ for all $y \in \mathcal{C}_0$ by linearity. Recalling (2.2), we may conclude that

$$\inf_{y \in \mathcal{D}(A)} \frac{||(zI - A)y||}{||y||} = \inf_{y \in \mathcal{C}_0} \frac{||(zI - A)y||}{||y||} = \inf_{y \in \mathcal{C}_0} \frac{||(zI - A)y||}{||R(zI - A)y||} \geq \frac{1}{||R||} > 0.$$

Consequently, $\mathcal{N}(zI - A) = \{0\}$, and from [28, Theorem IV.5.2] if follows that $\mathcal{R}(zI - A)$ is closed. In order to establish our claim $z \in \Omega(A)$, it remains to show that $\mathcal{R}(zI - A)$ is dense in ℓ^2. Since $\mathcal{R}(\gamma)$ is bounded, its first column $y(\gamma)$ is an element of ℓ^2. Using Lemma 2.4(c) we may conclude that $e_0 \in \mathcal{R}(zI - A^\#)$, and thus $e_0 \in \mathcal{R}(zI - A)$ since $\mathcal{A}$ is proper. Combining this with Lemma 2.4(b), we find that $\mathcal{C}_0 \subset \mathcal{R}(zI - A)$, and hence $\mathcal{R}(zI - A) = \ell^2$.

For establishing the second sentence of Theorem 2.10, we still need to show that the γ of the preceding part of the proof necessarily coincides with $(e_0, (zI - A)^{-1} e_0)$. By construction of $y(\gamma)$ we have $(zI - A^\#) y(\gamma) = (zI - A) y(\gamma) = e_0$, and thus $\gamma = (e_0, y(\gamma)) = (e_0, (zI - A)^{-1} e_0)$. □

For the sake of completeness, let us also describe the case of operators A which are not proper. Here we have either the trivial case $\sigma_{ess}(A) = \mathbb{C}$, or otherwise $\mathcal{A}$ is indeterminate by Theorem 2.6(a). In the latter case, we find exactly the same phenomena as for real Jacobi matrices (see, e.g., [1, 35] or [41, Theorem 2.6]).

Theorem 2.11 *Suppose that $\mathcal{A}$ is indeterminate. Then the following assertions hold:*
(a) $\sigma_{ess}(A) = \emptyset$ *and* $\sigma(A) = \sigma(A^\#) = \mathbb{C}$.
(b) $A^\#$ *is a two-dimensional extension of A. Furthermore, all other operators $A_{[\eta]}$ with $A \subset A_{[\eta]} \subset A^\#$ are one-dimensional extensions of A, they may be parametrized by $\eta \in \mathbb{C} \cup \{\infty\}$ via*

$$\mathcal{D}(A_{[\eta]}) = \{y + \lambda \cdot \frac{\eta \cdot q(0) - p(0)}{1 + |\eta|} : y \in \mathcal{D}(A), \lambda \in \mathbb{C}\}.$$

(c) *We have $\sigma_{ess}(A_{[\eta]}) = \emptyset$, and $A_{[\eta]}^* = \Pi A_{[\eta]} \Pi$ for all η. Furthermore, there exist entire functions $a_1, a_2, a_3, a_4 : \mathbb{C} \to \mathbb{C}$ with $a_1 a_4 - a_2 a_3 = 1$ such that*

$$\sigma(A_{[\eta]}) = \{z \in \mathbb{C} : \phi_{[\eta]}(z) = \infty\}, \quad \text{where} \quad \phi_{[\eta]}(z) := \frac{a_1(z) - a_2(z)\eta}{a_3(z) - a_4(z)\eta}.$$

Finally, the resolvent of $A_{[\eta]}$ at $z \in \Omega(A)$ is given by the closure of $\mathcal{R}(\phi_{[\eta]}(z))$, which is a compact operator of Schmidt class.

Proof: For $z \in \mathbb{C}$, consider the infinite matrix $\mathcal{S}(z)$ with entries

$$\mathcal{S}(z)_{j,k} = \begin{cases} q_k(z) p_j(z) - q_j(z) p_k(z) & \text{if } 0 \le j \le k, \\ 0 & \text{if } 0 \le k \le j. \end{cases}$$

Since $\mathcal{A}$ is indeterminate, we get $\sum_{j,k} |\mathcal{S}(z)_{j,k}|^2 < \infty$. In particular, the closure $S(z)$ of $\mathcal{S}(z)$ is bounded, and more precisely a compact operator of Schmidt class [28, Section V.2.4]. By some elementary calculations using (1.2) and (2.9) one verifies that $\mathcal{S}(z) \cdot (z e_j - \mathcal{A} e_j) = e_j$ for $j \ge 0$. As in the last part of the proof of Theorem 2.10 it follows that $S(z)$ is a left inverse of $zI - A$, and it follows that $\mathcal{R}(zI - A)$ is closed and $\mathcal{N}(zI - A) = \{0\}$. Since by assumption $\mathcal{N}(zI - A^\#) = \text{span}(q(z))$, we obtain

$$\mathcal{R}(zI - A^\#) = \mathcal{N}(zI - A)^\perp = \ell^2, \quad \mathcal{R}(zI - A) = \Pi \mathcal{N}(zI - A^\#)^\perp = \text{span}(\Pi q(z))^\perp, \quad z \in \mathbb{C}.$$

Using (2.10), we may conclude that part (a) holds.

For a proof of (b), let $y \in \mathcal{D}(A^\#)$. Since $A^\# p(0) = -e_0$ by Lemma 2.4(c), we have

$$A^\#(y + (\Pi q(0), A^\# y) \cdot p(0)) \in \operatorname{span}(\Pi q(0))^\perp = \mathcal{R}(A).$$

Consequently, there exists a $y' \in \mathcal{D}(A)$ with $0 = A^\#(y + (\Pi q(0), A^\# y) \cdot p(0)) - Ay' = A^\#(y + (\Pi q(0), A^\# y) \cdot p(0) - y')$, showing that $y + (\Pi q(0), A^\# y) \cdot p(0) - y'$ is a multiple of $q(0)$. Hence $A^\#$ is a two-dimensional extension of A. Since any other extension either has a nontrivial kernel ($\eta = \infty$) or otherwise the image ℓ^2 ($\eta \neq \infty$), the second part of the assertion follows.

It remains to show part (c). Following [56, Section 23], we define the entire functions

$$a_1(z) = z \sum_{j=0}^{\infty} p_j(0) p_j(z), \quad a_2(z) = 1 + z \sum_{j=0}^{\infty} q_j(0) p_j(z),$$
$$a_3(z) = -1 + z \sum_{j=0}^{\infty} p_j(0) q_j(z), \quad a_4(z) = z \sum_{j=0}^{\infty} q_j(0) q_j(z).$$

It is shown in [56, Theorem 23.1] that indeed $a_1(z)a_4(z) - a_2(z)a_3(z) = 1$ for all $z \in \mathbb{C}$. Let $z \in \mathbb{C}$. We claim that, for a suitable unique $\gamma \in \mathbb{C} \cup \{\infty\}$ (depending on η, z),

$$\Pi \frac{\gamma q(z) - p(z)}{1 + |\gamma|} \in \mathcal{D}((zI - A_{[\eta]})^*), \quad \text{with} \quad (zI - A_{[\eta]})^* \Pi \frac{\gamma q(z) - p(z)}{1 + |\gamma|} = \frac{e_0}{1 + |\gamma|}. \tag{2.15}$$

Indeed, for any $y \in \mathcal{D}(A)$ and $\lambda \in \mathbb{C}$

$$\begin{aligned}
&\Big(\frac{e_0}{1+|\gamma|}, y + \lambda \frac{\eta \cdot q(0) - p(0)}{1 + |\eta|}\Big) - \Big(\Pi \frac{\gamma q(z) - p(z)}{1+|\gamma|}, (zI - A_{[\eta]})(y + \lambda \frac{\eta \cdot q(0) - p(0)}{1+|\eta|})\Big) = \\
&\frac{(e_0, y) + \lambda\eta/(1+|\eta|)}{1+|\gamma|} - \Big((zI - A)^* \Pi \frac{\gamma q(z) - p(z)}{1+|\gamma|}, y\Big) - \Big(\Pi \frac{\gamma q(z) - p(z)}{1+|\gamma|}, \frac{\lambda(\eta z q(0) - z p(0) + e_0)}{1+|\eta|}\Big) \\
&= \frac{\lambda}{(1+|\eta|)(1+|\gamma|)} \Big[\eta - \gamma - z\Big(\Pi(\gamma q(z) - p(z)), \eta q(0) - p(0)\Big)\Big] \\
&= \frac{\lambda}{(1+|\eta|)(1+|\gamma|)} \Big[-[a_1(z) - a_2(z)\eta] + \gamma[a_3(z) - a_4(z)\eta]\Big],
\end{aligned}$$

and the term on the right-hand side equals zero for $\gamma = \phi_{[\eta]}(z)$. Thus (2.15) holds.

We are now prepared to show part (c). First, notice that also $zI - A_{[\eta]}$ is a one-dimensional extension of $zI - A$ for all $z \in \mathbb{C}$. Therefore, $\mathcal{R}(zI - A_{[\eta]})$ equals either ℓ^2 or $\mathcal{R}(zI - A)$, and hence is closed for all $z \in \mathbb{C}$. Consequently, $\sigma_{ess}(A_{[\eta]}) = \emptyset$. Secondly, $A \subset A_{[\eta]} \subset A^\#$ implies that $\Pi A \Pi = (A^\#)^* \subset A_{[\eta]}^* \subset \Pi A^\# \Pi = A^*$, and hence $A_{[\eta]}^*$ is a one-dimensional extension of $\Pi A \Pi$. Noticing that $\phi_{[\eta]}(0) = \eta$, we may conclude from (2.15) for $z = 0$ that $\Pi(\eta q(0) - p(0))/(1 + |\eta|) \in \mathcal{D}(A_{[\eta]}^*)$. Since the one-dimensional extensions of $\Pi A \Pi$ have been parametrized in part (b), it follows that $A_{[\eta]}^* = \Pi A_{[\eta]} \Pi$ for all η. Taking into account that $\mathcal{R}(zI - A_{[\eta]})$ is closed, we may conclude that $\mathcal{N}(zI - A_{[\eta]}) = \emptyset$ iff $\mathcal{R}(zI - A_{[\eta]}) = \ell^2$, which by (2.15) is equivalent to $\phi_{[\eta]}(z) \neq \infty$. In the latter case, applying [28, Theorem IV.5.2] we find that $z \in \Omega(A_{[\eta]})$, and thus $\sigma(A_{[\eta]})$ has the form claimed in the assertion.

Finally, in the case $\gamma = \phi_{[\eta]}(z) \neq \infty$, it follows again from (2.15) that $(e_j, (zI - A_{[\eta]})^{-1} e_0) = \phi_{[\eta]}(z) q_j(z) - p_j(z)$ for $j \geq 0$, and the characterisation $(zI - A)^{-1} = [\mathcal{R}(\phi_{[\eta]}(z))]_{\min}$ is proved as in the first part of the proof of Theorem 2.10. Since

$$\mathcal{R}(\phi_{[\eta]}(z)) = \mathcal{S}(z) + ((\phi_{[\eta]}(z) q_j(z) - p_j(z)) q_k(z))_{j,k=0,1,\ldots}$$

and $\mathcal{S}(z)$ is of Schmidt class, the same is true for $\mathcal{R}(\phi_{[\eta]}(z))$. This terminates the proof of Theorem 2.11. $\square$

Under the assumptions of Theorem 2.11, suppose in addition that $\mathcal{A}$ is real. Then the extension $A_{[\eta]}$ of A is symmetric iff $\eta \in \mathbb{R} \cup \{\infty\}$. It follows from part (b) that $A_{[\eta]}$ is self-adjoint, i.e., we obtain all self-adjoint extensions of the difference operator A in ℓ^2 (compare with [1], [41, Theorem 2.6]). Notice also that then the corresponding functions $\phi_{[\eta]}(z)$ are just the Cauchy transforms of the *extremal* [40, Theorem 2.13] or *Neumann* solutions [41] of the moment problem (which according to part (c) are discrete).

Suppose that A is bounded (and thus $\mathcal{A}$ is proper and determinate). In this case it is known [21] that there is an exponential decay rate for the entries of the resolvent of the form (2.16). Conversely, any infinite matrix with entries verifying (2.16) is bounded. We thus obtain the following result of Aptekarev, Kaliaguine and Van Assche mentioned already in the introduction.

Theorem 2.12 (compare with [6, Theorem 1])
Let A be bounded. Then $z \in \Omega(A)$ if and only if there exists a $\gamma(z) \in \mathbb{C}$ and positive constants $\beta(z)$ and $\delta(z)$ such that for all $j, k \geq 0$

$$|\mathcal{R}(\gamma(z))_{j,k}| \leq \beta(z) \cdot \delta(z)^{|k-j|}, \quad \delta(z) < 1. \tag{2.16}$$

The equivalence of Theorem 2.12 remains true for unbounded difference operators where the sequence of offdiagonal entries $(a_n)_{n \geq 0}$ is bounded (see, e.g., [23, Proposition 2.2]) or contains a sufficiently dense bounded subsequence [17, Theorem 2.1]. In these two cases, the matrix $\mathcal{A}$ is proper according to Example 2.7.

Notice that in the original statement of [6, Theorem 1] the authors impose some additional conditions on z which are not necessary. Also, the authors treat general tridiagonal matrices $\mathcal{A}$ where the entries of the superdiagonal may differ from those on the subdiagonal. Such operators can be obtained by multiplying a complex Jacobi matrix on the left by some suitable diagonal matrix and on the right by its inverse, i.e., we rescale our recurrence relation (1.2). Such recurrence relations occur for instance in the context of monic (F)OPs, whereas we have chosen the normalization of orthonormal FOPs. The following result of Kaliaguine and Beckermann shows that our normalization gives the smallest spectrum.

Theorem 2.13 ([19, Theorem 2.3])
Let $\mathcal{A}$ be a bounded complex Jacobi matrix, and consider a bounded tridiagonal matrix $\mathcal{A}' = \mathcal{D}\mathcal{A}\mathcal{D}^{-1}$ with diagonal $\mathcal{D}$. Then for the corresponding difference operators A and A' we have $\Omega(A') \subset \Omega(A)$.

As an example, take the tridiagonal Toeplitz matrix with diagonal entries $a/2, 0, 1/(2a)$. Here it is known that the spectrum is the interior and the boundary of an ellipse with foci ± 1 and half axes $|a \pm 1/a|/2$, and it is minimal (namely the interval $[-1, 1]$) for $a = 1$. Notice also that for monic FOPs one chooses the normalization $a = 1/2$.

It would be interesting to generalize Theorem 2.13 to unbounded Jacobi matrices.

2.4 The Weyl function and functions of the second kind

Following Berezanskii (see [20]), we call

$$\phi(z) := (e_0, (zI - A)^{-1}e_0), \quad z \in \Omega(A), \tag{2.17}$$

the *Weyl function* of A. Since the resolvent is analytic on $\Omega(A)$, the same is true for the Weyl function. If the operator A is bounded (or, equivalently, if the entries of $\mathcal{A}$ are uniformly bounded) then ϕ is analytic for $|z| > ||A||$. Then its Laurent series at infinity is given by

$$\phi(z) \sim \sum_{j=0}^{\infty} \frac{(A^j e_0, e_0)}{z^{j+1}}, \tag{2.18}$$

i.e., its coefficients are the moments of the linear functional c of formal orthogonality (some authors refer to the series on the right-hand side of (2.18) as the symbol of c). In the case where the numerical range of A is not the whole plane (as for instance for real Jacobi matrices), one may show (see, e.g., [56, Theorem 84.3]) that (2.18) can be interpreted as an asymptotic expansion of ϕ in some sector.

The associated *functions of the second kind* are given by

$$r_n(z) = (e_n, (zI - A)^{-1}e_0) = q_n(z)\phi(z) - p_n(z), \quad n \geq 0, \quad z \in \Omega(A),$$

where the last representation follows from Theorem 2.10 and the construction of $\mathcal{R}(\phi(z))$. Similarly, we may express the other entries as

$$(e_j, (zI - A)^{-1}e_k) = (e_k, (zI - A)^{-1}e_j) = r_k(z)q_j(z), \quad 0 \leq j \leq k, \quad z \in \Omega(A). \tag{2.19}$$

In case of a bounded operator A, we know from [17, Theorem 5.3] that the Weyl function contains already all information about isolated points of the spectrum. The proof given for this assertion only uses the representation (2.19), and thus also applies for unbounded operators.

Theorem 2.14 ([17, Theorem 5.3 and Corollary 5.6])
Let ζ be an isolated point of $\sigma(A)$. Then $\zeta \in \sigma_{ess}(A)$ if and only if ϕ has an essential singularity in ζ, and ζ is an eigenvalue of algebraic multiplicity $m < \infty$ if and only if ϕ has a pole of multiplicity m. In particular, if $\sigma(A)$ is countable, then the set of singularities of ϕ coincides with $\sigma(A)$.

A proof of the second sentence of Theorem 2.14 is based on the observation that any element of a countable set $\Sigma \subset \mathbb{C}$ is either an isolated point or a limit of isolated points of Σ. Notice that the spectrum is in particular countable and has the only accumulation point $b \in \mathbb{C}$ if $A - bI$ is compact, i.e., $a_n \to 0$ and $b_n \to b$ (see for instance Corollary 2.17 below). Here the Weyl function is analytic in $\Omega(A)$ (and in no larger set), meromorphic in $\mathbb{C} \setminus \{b\}$, and has an essential singularity at b. For a nice survey on compact Jacobi matrices we refer the reader to Van Assche [54].

Relation (2.19) allows us also to compare the growth of FOPs and of functions of the second kind. Indeed, according to (2.9) we have

$$a_n(q_{n+1}(z)r_n(z) - r_{n+1}(z)q_n(z)) = 1, \quad n \geq -1, \quad z \in \Omega(A). \tag{2.20}$$

This implies that

$$\begin{aligned} 1 &\leq |a_n| \cdot \sqrt{|q_n(z)|^2 + |q_{n+1}(z)|^2} \cdot \sqrt{|r_n(z)|^2 + |r_{n+1}(z)|^2} \\ &\leq 1 + 2|a_n| \cdot ||(zI - A)^{-1}||, \end{aligned} \tag{2.21}$$

$$\begin{aligned} 1 &\leq \sqrt{|q_n(z)|^2 + |a_n q_{n+1}(z)|^2} \cdot \sqrt{|r_n(z)|^2 + |a_n r_{n+1}(z)|^2} \\ &\leq 1 + (1 + |a_n|^2) \cdot ||(zI - A)^{-1}|| \end{aligned} \tag{2.22}$$

for all $z \in \Omega(A)$ and $n \geq 0$. Indeed, the left-hand inequalities of (2.21), (2.22) follow by applying the Cauchy–Schwarz inequality on (2.20). In order to verify the right-hand estimate in, e.g., (2.21), we notice that, by (2.20),

$$\begin{aligned} & |a_n|^2 \cdot (|q_n(z)|^2 + |q_{n+1}(z)|^2) \cdot (|r_n(z)|^2 + |r_{n+1}(z)|^2) \\ = \; & |a_n|^2 \cdot [|q_n(z) r_n(z)|^2 + |q_n(z) r_{n+1}(z)|^2 + |q_{n+1}(z) r_{n+1}(z)|^2] + |1 - a_n r_{n+1}(z) q_n(z)|^2. \end{aligned}$$

Each term of the form $r_j(z) q_k(z)$ occurring on the right-hand side may be bounded by $||(zI - A)^{-1}||$, leading to (2.21).

If additional information on the sequence $(a_n)_{n \geq 0}$ is available, we may be even much more precise.

Corollary 2.15 *Let $(a_n)_{n \geq 0}$ be bounded. Then there exist continuous functions $\beta : \Omega(A) \to (0, +\infty)$ and $\delta : \Omega(A) \to (0, 1)$ such that for all $0 \leq j \leq k$ and for all $z \in \Omega(A)$*

$$|r_k(z) \cdot q_j(z)| \leq \beta(z) \cdot \delta(z)^{k-j}. \tag{2.23}$$

If in addition A is bounded, then the functions $\beta(z)$ and $|z| \cdot \delta(z)$ are continuous at infinity.

Here (2.23) follows from Theorem 2.12. The continuity of the involved functions β, δ has been discussed in [19, Lemma 3.3] and [17, Lemma 2.3] for bounded A, and implicitly in [18, Proof of Theorem 2.1] for bounded $(a_n)_{n \geq 0}$.

2.5 Some special cases

It is well-known (see, e.g., [10]) that a linear functional c having real moments is positive (i.e., $\det(c(x^{j+k}))_{j,k=0,\ldots,n} > 0$ for all $n \geq 0$) if and only if c has the representation

$$c(P) = \int P(x)\, d\mu(x) \quad \text{for any polynomial } P, \tag{2.24}$$

where μ is some positive Borel measure with real infinite support *supp* (μ). Under these assumptions, the support is a part of the positive real axis iff in addition $\det(c(x^{j+k+1}))_{j,k=0,\ldots,n} > 0$ for all $n \geq 0$. Furthermore, the sequence of moments is totally monotone (i.e., $\Delta^k c(x^n) > 0$ for all $n, k \geq 0$) iff (2.24) holds with μ some positive Borel measure with infinite support *supp* $(\mu) \subset [0, 1]$.

In all these cases, the corresponding Jacobi matrix is real, and the corresponding measure is unique (uniqueness of the moment problem) iff $\mathcal{A}$ is proper (in other words, A is self-adjoint). In this case, μ can be obtained by the Spectral Theorem, with *supp* $(\mu) = \sigma(A) \subset \mathbb{R}$, and

$$\phi(z) = \int \frac{d\mu(x)}{z - x} \tag{2.25}$$

holds for all $z \notin \sigma(A)$.

In case of complex bounded Jacobi matrices (or more general proper operators with $\Omega(A) \not\subset \Gamma(A)$), we may also obtain a complex-valued measure μ satisfying (2.24) and (2.25) via the Cauchy-integral formula; however, in general $\sigma(A) \neq \mathit{supp}(\mu)$. In all these cases, we recover the following well-known representation of functions of the second kind as Cauchy transforms.

Lemma 2.16 *Suppose that there exists some (real- or complex-valued) Borel measure μ such that (2.24) holds, and some set $U \subset \Omega(A)$ such that (2.25) is true for all $z \in U$. Then*

$$r_k(z)q_j(z) = \int \frac{q_j(x)q_k(x)}{z-x}\, d\mu(x), \quad 0 \le j \le k, \quad z \in U.$$

Proof: Consider the sequence of Cauchy transforms

$$\widetilde{r}_n(z) := \int \frac{q_n(x)}{z-x}\, d\mu(x), \quad n \ge 0,$$

and $\widetilde{r}_{-1} = 0$. One easily checks using (2.24) and (1.2) that $-a_n\widetilde{r}_{n+1}(z) + (z-b_n)\widetilde{r}_n(z) - a_{n-1}\widetilde{r}_{n-1}(z) = \int q_n(x)\, d\mu(x) = c(q_n) = \delta_{n,0}$ for $n \ge 0$. Moreover, $\widetilde{r}_0(z) = \phi(z) = r_0(z)$ for $z \in U$ by (2.25) and (2.19). Consequently, for $z \in U$, $(\tilde{r}_n(z))_{n\ge 0}$ satisfies the same recurrence and initialisation as the sequence $(r_n(z))_{n\ge 0}$, implying that $\tilde{r}_n(z) = r_n(z)$. Furthermore, for $j \le k$ there holds

$$r_k(z)q_j(z) - \int \frac{q_j(x)q_k(x)}{z-x}\, d\mu(x) = \int \frac{q_j(z)-q_j(x)}{z-x} q_k(x)\, d\mu(x).$$

Since the fraction on the right-hand side is a polynomial of degree $< j \le k$ in x, the right-hand integral vanishes by orthogonality and (2.24). □

If A is bounded, then any measure with compact support satisfying (2.24) will fulfil (2.25) with U being equal to the unbounded component of the complement of $\sigma(A) \cup \mathit{supp}(\mu)$, since the functions on both sides of (2.25) have the same Laurent expansion at infinity. It would be very interesting to prove for general non-real (unbounded but proper) Jacobi matrices that if (2.24) holds for some measure with compact support then also (2.25) is true for $z \in U$, where U is the intersection of $\Omega(A)$ with the unbounded connected component of $\mathbb{C} \setminus \mathit{supp}(\mu)$.

To the end of this section let us have a look at a different class of functionals which to our knowledge has not yet been studied in the context of complex Jacobi matrices: It is known from the work of Schoenberg and Edrei that the sequence of (real) moments $(c_n)_{n\ge 0}$, $c_n = c(x^n)$, $c_0 = 1$, $c_n = 0$ for $n < 0$, is totally positive (i.e., $\det(c_{m+j-k})_{j,k=0,\ldots,n} \ge 0$ for all $n, m \ge 0$) iff $\sum c_j z^j$ is the expansion at zero of a meromorphic function ψ having the representation

$$\psi(z) = e^{\gamma z} \prod_{j=1}^{\infty} \frac{1+\alpha_j z}{1-\beta_j z}, \quad \alpha_j, \beta_j, \gamma \ge 0, \quad \sum_{j=1}^{\infty} (\alpha_j + \beta_j) < \infty.$$

(including for instance the exponential function). Following [8], we exclude the case that ψ is rational. Many results about convergence of Padé approximants (at zero) of these functions have been obtained by Arms and Edrei [8], see also [10]. Let us consider the linear functionals $c^{[k]}$ defined by

$$c^{[k]}(x^n) = c_{n+k}, \quad n, k \ge 0, \quad \text{with symbol} \quad \phi^{[k]}(z) = z^{k-1}\Big(\psi(1/z) - \sum_{j=0}^{k-1} \frac{c_j}{z^j}\Big)$$

($c^{[0]} = c$), having symbols being meromorphic in $\mathbb{C} \setminus \{0\}$, and analytic around infinity. We have the following

Corollary 2.17 *The functionals $c^{[k]}$ as described above are regular for all $k \geq 0$. The associated complex Jacobi matrices $\mathcal{A}^{[k]}$ are compact, with Weyl function given by $\phi^{[k]}$, and spectrum $\{0\} \cup \{\beta_j : j \geq 1\}$. Finally, $(a_n^{[k]})^2 < 0$ for all $n, k \geq 0$.*

Proof: In [8, Theorem 1.I], the authors show that the Padé table of ψ (at zero) is normal. Denote by $Q_{m,n}$ the denominator of the Padé approximant of type $[m|n]$ at zero, normalized such that $Q_{m,n}(0) = 1$, and define

$$Q_n^{[k]}(z) := z^n Q_{n+k,n}(\frac{1}{z}) = z^n + Q_{n,1}^{[k]} z^{n-1} + Q_{n,2}^{[k]} z^{n-2} + \ldots .$$

It is well known and easily verified that $Q_n^{[k]}$ is an nth monic FOP of the linear functional $c^{[k]}$, and thus $c^{[k]}$ is regular. The sign of $(a_n^{[k]})^2$ follows from well-known determinantal representations for the recurrence coefficients, we omit the details. Precise asymptotics for $(Q_{n+k,n})_{n\geq 0}$ are given in [8, Theorem 1.II] (see also [10]), implying that

$$\lim_{n\to\infty} \frac{Q_n^{[k]}(z)}{z^n} = \exp(\frac{-\gamma}{2z}) \prod_{j=1}^{\infty} (1 - \frac{\beta_j}{z}) \tag{2.26}$$

for all $k \geq 0$ uniformly on closed subsets of $(\mathbb{C} \cup \{\infty\}) \setminus \{0\}$. In particular, the sequences $(Q_{n,1}^{[k]})_{n\geq 0}$ and $(Q_{n,2}^{[k]})_{n\geq 0}$ converge. On the other hand, we know from (1.2) that $Q_{n+1}^{[k]}(z) = (z - b_n^{[k]}) Q_n^{[k]}(z) - (a_{n-1}^{[k]})^2 Q_{n-1}^{[k]}(z)$. Thus

$$Q_{n+1,1}^{[k]} = Q_{n,1}^{[k]} - b_n^{[k]}, \quad Q_{n+1,2}^{[k]} = Q_{n,2}^{[k]} - b_n^{[k]} Q_{n,1}^{[k]} - (a_{n-1}^{[k]})^2, \tag{2.27}$$

implying that $b_n^{[k]} \to 0$ and $a_n^{[k]} \to 0$ for $n \to \infty$. Hence $\mathcal{A}^{[k]}$ is compact. Since its Weyl function ϕ has the same (convergent) Laurent expansion around infinity as $\phi^{[k]}$, we have $\phi = \phi^{[k]}$, and the rest of the assertion follows from Theorem 2.14 and the explicit knowledge of the singularities of $\phi^{[k]}$. □

3 Asymptotics of FOPs

3.1 nth root asymptotics of FOPs

In this subsection we will restrict ourselves to bounded Jacobi matrices A. We present some recent results of [6, 17, 19, 50, 51].

In their work on tridiagonal infinite matrices, Aptekarev, Kaliaguine and Van Assche also observed [6, Corollary 3] that

$$\limsup_{n\to\infty} |q_n(z)|^{1/n} > 1, \quad z \in \Omega(A).$$

Indeed, a combination of (2.23) for $j = 0$ and (2.21) yields the stronger relation

$$\liminf_{n\to\infty} [|q_n(z)|^2 + |q_{n+1}(z)|^2|]^{1/(2n)} > 1, \quad z \in \Omega(A). \tag{3.1}$$

For real bounded Jacobi matrices, this relation was already established by Szwarc [50, Corollary 1], who showed by examples [51] that there may be also exponential growth inside the spectrum.

Kaliaguine and Beckermann [19, Theorem 3.6] applied the maximum principle to the sequence of functions of the second kind and showed that, in the unbounded connected component $\Omega_0(A)$ of the resolvent set $\Omega(A)$, one may replace 1 on the right-hand side of (3.1) by $\exp(g_{\sigma(A)}(z))$. Here $g_{\sigma(A)}$ denotes the (generalized) Green function with pole at ∞ of the compact set $\sigma(A)$, being characterized by the three properties (see, e.g., [38, Section II.4])

(i) $g_{\sigma(A)}$ is nonnegative and harmonic in $\Omega_0(A) \setminus \{\infty\}$

(ii) $g_{\sigma(A)}(z) - \log|z|$ has a limit for $|z| \to \infty$

(iii) $\lim_{z\to\zeta, z\in\Omega_0(A)} g_{\sigma(A)}(z) = 0$ for quasi-every $\zeta \in \partial\Omega_0(A)$.

We also recall that the limit in (ii) equals $-\log cap\,(\sigma(A))$, where $cap\,(\cdot)$ is the logarithmic capacity.

A detailed study of nth root asymptotics of formal orthogonal polynomials with bounded recurrence coefficients has been given in [17]. We denote by k_n the leading coefficient of q_n, i.e.,

$$k_n = \frac{1}{a_0 \cdot a_1 \cdot \ldots \cdot a_{n-1}},$$

and define the quantities

$$\kappa_{\sup} := \limsup_{n\to\infty} |k_n|^{-1/n}, \quad \kappa_{\inf} := \liminf_{n\to\infty} |k_n|^{-1/n}.$$

Notice that $|a_n| \le ||A||$, and thus $||k_n|| \ge 1/||A||$, implying that $0 \le \kappa_{\inf} \le \kappa_{\sup} \le ||A||$.

Theorem 3.1 (see [17, Theorem 2.5 and Theorem 2.10])
Let A be bounded. Then there exist functions $g_{\inf}, g_{\sup}$ such that

$$\liminf_{n\to\infty} (|q_n(z)|^2 + |a_n q_{n+1}(z)|^2)^{-1/(2n)} = \exp(-g_{\sup}(z)), \tag{3.2}$$

$$\limsup_{n\to\infty} (|q_n(z)|^2 + |a_n q_{n+1}(z)|^2)^{-1/(2n)} = \exp(-g_{\inf}(z)), \tag{3.3}$$

holds locally uniformly in $\Omega(A)$ (i.e., uniformly on closed subsets of $\Omega(A)$).

Here $g_{\inf} = +\infty$ (and $g_{\sup} = +\infty$, respectively) if and only if $\kappa_{\sup} = 0$ (and $\kappa_{\inf} = 0$, respectively). Otherwise, $g_{\inf}$ is superharmonic, strictly positive, and continuous in $\Omega(A) \setminus \infty$, with

$$\lim_{|z|\to\infty} g_{\inf}(z) - \log|z| = \log\frac{1}{\kappa_{\sup}}.$$

Also, $g_{\sup}$ is subharmonic, strictly positive, and continuous in $\Omega(A) \setminus \infty$, with

$$\lim_{|z|\to\infty} g_{\sup}(z) - \log|z| = \log\frac{1}{\kappa_{\inf}}.$$

In addition,

$$0 \le \kappa_{\inf} \le \kappa_{\sup} \le \mathrm{cap}\,(\sigma(A)), \quad g_{\sigma(A)}(z) \le g_{\inf}(z) \le g_{\sup}(z), \quad z \in \Omega_0(A). \tag{3.4}$$

Various further properties and relations between $g_{\sigma(A)}$, $g_{\inf}$ and $g_{\sup}$ may be found in [17, Sections 2.2 and 2.3]. The proof of Theorem 3.1 is based on (2.22), Corollary 2.15, and applies tools from logarithmic potential theory. Instead of giving details, let us discuss some consequences and special cases. First, since $(a_n)_{n\geq 0}$ is bounded, we obtain from (3.2) that

$$\limsup_{n\to\infty} |q_n(z)|^{1/n} = \exp(g_{\sup}(z)) > 1, \quad z \in \Omega(A). \tag{3.5}$$

Furthermore, we will show below that (3.3) implies the relation

$$\liminf_{n\to\infty} |q_n(z)|^{1/n} = \exp(g_{\inf}(z)) > 1, \quad z \in F, \tag{3.6}$$

provided that the set $F \subset \Omega_0(A)$ does not contain any of the zeros of q_n for sufficiently large n. In addition, by combining (3.3) with (2.22) we get

$$\limsup_{n\to\infty} |r_n(z)|^{1/n} = \exp(-g_{\inf}(z)) < 1, \quad z \in \Omega(A). \tag{3.7}$$

Indeed, relation (2.22) allows us to restate Theorem 3.1 in terms of functions of the second kind.

The simplest case which may illustrate these findings is the Toeplitz operator $\mathcal{A}$ with $a_n = 1/2$, $b_n = 0$, $n \geq 0$, see [35, Section II.9.2]. [5] Here one may write down explicitly q_n and r_n in terms of the Joukowski function, in particular one finds that $\sigma(A) = [-1,1]$, and $g_{\inf} = g_{\sup} = g_{[-1,1]}$. Of course, in the generic case there will be no particular relation between $g_{\sup}$, $g_{\inf}$, and $g_{\sigma(A)}$. Some extremal cases of Theorem 3.1 have been discussed in [17, Example 2.9] (see also [23, Example 4.1 and Example 4.2]). For instance, there are operators with $\sigma(A) = [-1,3]$, and $g_{\inf} = g_{\sup} = g_{[-1,1]}$. Also, the case $\sigma(A) = [-2,2]$, $\kappa_{\inf} = \kappa_{\sup} = 1/2 < cap\,(\sigma(A)) = 1$, and $g_{\inf} \neq g_{\sup}$ may occur. In addition there is an example where $g_{\sup}(z) - g_{\inf}(z) = \log(\kappa_{\sup}/\kappa_{\inf}) \neq 0$ for all $z \in \Omega(A)$.

The nth root asymptotic of general orthogonal polynomials are investigated by Stahl and Totik [48]. Of course, in case of orthogonality on the real line (i.e., real Jacobi matrices) results as (3.4), (3.6), (3.5) have been known before, see, e.g., [48, Theorem 1.1.4 and Corollary 1.1.7].

In this context we should mention the deep work of Stahl concerning the convergence of Padé approximants and asymptotics of the related formal orthogonal polynomials. He considers linear functionals as in (2.24), where μ is some (real- or complex-valued but not positive) Borel measure with compact support. Of course, such functionals are not necessarily regular, but we can always consider the asymptotics of the subsequence of (unique) FOPs corresponding to normal points. In [43, Corollary of Theorem 1] Stahl constructs a measure μ supported on $[-1,1]$ such that the sequence of normalized zero counting measures is weakly dense in the set of positive Borel measures of total mass ≤ 1 supported on $\mathbb{C}$! In contrast, in the case of regular functionals and bounded recurrence coefficients, it is shown in [17, Theorem 2.5] that the support of any partial weak limit of the sequence of normalized zero counting measures is a subset of $\mathbb{C} \setminus \Omega_0(A)$.

Another very interesting class has been considered by Stahl in a number of papers (see for instance [46]), here the symbols (the Cauchy transform of μ) are multivalued functions having, e.g., a countable number of branchpoints. Here it follows from [46, Theorems 1.7 and 1.8] that (3.5) and (3.7) hold quasi-everywhere outside of $supp\,(\mu)$, with $g_{\inf} = g_{supp}$ being the Green function of $supp\,(\mu)$. Again, it is not clear whether the functional is regular, and the corresponding recurrence coefficients are bounded.

[5] See also the case of periodic complex Jacobi matrices discussed in Section 4.3 below.

Linear functionals of the form

$$c_w(P) = \int_{-1}^{1} \frac{w(x)P(x)}{\sqrt{1-x^2}}\, dx, \tag{3.8}$$

with some possibly complex-valued weight function w have been discussed by a number of authors, see, e.g., the introduction of [43]. Nuttall [37], Nuttall and Wherry [36], Baxter [16], Magnus [31], and Baratchart [11] suggested conditions on w insuring that all (at least sufficiently large) indices n are normal, and that there are only "few" zeros outside of $[-1, 1]$. In particular, nth root asymptotics for the sequence of FOPs are derived.

3.2 Ratio asymptotics and zeros of FOP

It is well-known that the monic polynomial q_n/k_n is the characteristic polynomial of the finite section $\mathcal{A}_n$ obtained by taking the first n rows and columns of $\mathcal{A}$. In this section we will be concerned with the location of zeros of FOPs, i.e., of eigenvalues of $\mathcal{A}_n$. In Numerical Linear Algebra, one often refers to these zeros as Ritz values. The motivation for our work is the idea that the sequence of matrices $\mathcal{A}_n$ approximates in some sense the infinite matrix $\mathcal{A}$ and thus the corresponding difference operator A; therefore the corresponding spectra should be related. In the sequel we will try to make this statement more precise.

An important tool in our investigations is the rational function[6]

$$\begin{aligned} u_n(z) \;&:=\; \frac{q_n(z)}{a_n q_{n+1}(z)} = \frac{q_n(z)/k_n}{q_{n+1}(z)/k_{n+1}} \\ &=\; \frac{\det(z\mathcal{I}_n - \mathcal{A}_n)}{\det(z\mathcal{I}_{n+1} - \mathcal{A}_{n+1})} = (e_n, (z\mathcal{I}_{n+1} - \mathcal{A}_{n+1})^{-1} e_n). \end{aligned}$$

Here and in the sequel we denote by $e_0, ..., e_n$ also the canonical basis of $\mathbb{C}^{n+1}$, the length of the vectors being clear from the context. In the theory of continued fractions, the sequence $(1/u_n)_{n\geq 0}$ of meromorphic functions is referred to as a tail sequence of the J-fraction (1.3) [30, Section II.1.2, Eqn. (1.2.7)]. Using (1.2), one easily verifies that

$$\frac{1}{z u_n(z)} = \frac{a_n q_{n+1}(z)}{z \cdot q_n(z)} = 1 - \frac{b_n}{z} - \frac{a_{n-1}^2}{z^2} + \mathcal{O}(\frac{1}{z^3})_{z\to\infty}. \tag{3.9}$$

In order to motivate our results presented below, let us shortly recall some properties of orthogonal polynomials, i.e., real Jacobi matrices. It is well known that here the zeros of q_n are simple, and lie in the convex hull $\mathcal{S}$ of $\sigma(A)$. Also, they interlace with the zeros of q_{n+1}, and thus u_n has positive residuals. These two elements allow to conclude that $(u_n)_{n\geq 0}$ is bounded uniformly in closed subsets of $\mathbb{C} \setminus \mathcal{S}$. Finally, q_n can have at most one zero in a *gap* of the form $(a, b) \subset \mathcal{S} \setminus \sigma(A)$.

[6]Most of the results presented in this paper for the sequence (u_n) are equally valid for the ratio

$$\phi^{(n+1)}(z) := \frac{r_{n+1}(z)}{a_n r_n(z)}$$

which can be shown to have a meromorphic continuation in $\mathbb{C} \setminus \sigma_{ess}(A)$, and coincides with the Weyl function of the associated Jacobi matrix $\mathcal{A}^{(n+1)}$. Some additional interesting properties are presented in a futur publication.

We should mention first that none of these properties remain valid for FOPs. Classical counter examples known from Padé approximation (such as the examples of Perron and of Gammel-Wallin, see [10]) use linear functionals c which are highly non regular. But there also exist other ones.

Example 3.2 (a) *The linear functional (3.8) with weight* $w(x) = (x - \cos(\alpha_1 \pi))(x - \cos(\alpha_2 \pi))$ *has been studied in detail by Stahl [44]. Provided that* $1, \alpha_1, \alpha_2$ *are rationally independent, Stahl showed that* c *is regular, but (two) zeros of the sequence of FOPs cluster everywhere in* $\mathbb{C}$.

(b) *Beckermann [17, Example 5.7] investigated the linear functional with generating function*

$$\phi_d(z) = (z - d) \cdot [\exp(\frac{1}{z^2 - 1}) - 1].$$

Here the coefficients of the recurrence relation are given by $a_0^2 = 3/2 - d^2$, *and*

$$b_{2n} = -d, \; b_{2n+1} = d, \; -a_{2n}^2 a_{2n+1}^2 = \frac{1}{4(2n+1)(2n+3)}, \; a_{2n+2}^2 + a_{2n+1}^2 = 1 - d^2$$

for $n \geq 0$ *(provided that there is no division by zero, which can for instance been insured if* $d \in (-\infty, -\sqrt{3/2}) \cup [-1, 1] \cup (\sqrt{3/2}, +\infty)$*). One may show that* $a_{2n-1} \to 0$*, and thus* $\mathcal{A}$ *is bounded but not real. Also,* $\sigma(A) = \sigma_{ess}(A) = \{\pm 1\}$*. Furthermore,* $q_{2n-1}(-d) = 0$ *for all* $n \geq 0$*, and* $-d$ *may be far from the convex hull of* $\sigma(A)$.

Below we will see however that many of the properties for OPs remain valid for FOPs outside[7] the numerical range $\Gamma(A)$. An important tool in these investigations is the notion of normal families as introduced by Montel: a sequence of functions analytic in some domain D is called a normal family if from each subsequence we may extract a subsequence which converges locally uniformly in D (i.e., uniformly on closed subsets of D), with limit being different from the constant ∞. By a Theorem of Montel [39, Section 2.2 and Theorem 2.2.2], a family of functions analytic in D is normal in D if and only if it is uniformly bounded on any closed subset of D. More generally, we will also consider sequences of functions being meromorphic in D. Such a sequence is called normal in D if, given a subsequence, we may extract a subsequence converging locally uniformly in D with respect to the chordal metric $\chi(\cdot)$ on the Riemann sphere [39, Definition 3.1.1]. Notice that normal families of analytic functions are also normal families of meromorphic functions, but the converse is clearly not true.

Theorem 3.3 (a) *The sequence* $(u_n)_{n \geq 0}$ *is bounded above uniformly on compact subsets of* $\mathbb{C} \setminus \Gamma(A)$.

(b) *The sequence* $(u_n)_{n \geq 0}$ *of meromorphic functions is normal around infinity iff* A *is bounded.*

(c) (compare with [17, Proposition 2.2]) *Let* Λ *be some infinite set of integers such that* $(a_n)_{n \in \Lambda}$ *is bounded. Then the sequence* $(u_n)_{n \in \Lambda}$ *of meromorphic functions is normal in* $\Omega(A)$.

[7] Notice that, for real $\mathcal{A}$, $\Gamma(A)$ coincides with the convex hull $\mathcal{S}$ of the spectrum. It is known from examples [19] that this property is not true for general complex Jacobi matrices.

Proof: (a) We first observe that there is a connection between the numeical range of the difference operator and the numerical range of the finite sections $\mathcal{A}_n$, namely[8]

$$\Gamma(\mathcal{A}_n) = \Theta(\mathcal{A}_n) = \{\frac{(y, Ay)}{(y, y)} : y \in \mathcal{C}_0, \Pi_n y = y\} \subset \Theta(A) \subset \Gamma(A).$$

Since

$$\frac{1}{||(z\mathcal{I}_n - \mathcal{A}_n)^{-1}||^2} = \min_{y \in \mathbb{C}^n} \frac{||(z\mathcal{I}_n - \mathcal{A}_n)y||^2}{||y||^2} \le \min_{y \in \mathbb{C}^n} |\frac{(y, (z\mathcal{I}_n - \mathcal{A}_n)y)}{(y, y)}| = \text{dist}(z, \Theta(\mathcal{A}_n)),$$

we may conclude that

$$|u_n(z)| = |(e_n, (z\mathcal{I}_{n+1} - \mathcal{A}_{n+1})^{-1} e_n)| \le ||(z\mathcal{I}_{n+1} - \mathcal{A}_{n+1})^{-1}|| \le \frac{1}{\text{dist}(z, \Gamma(A))},$$

leading to the claim of part (a).

(b) If A is bounded then $\Gamma(A)$ is compact. Hence its complement contains a neighborhood D of infinity (for instance the set $|z| > ||A||$), and $(u_n)_{n \ge 0}$ is a normal family of analytic functions in U according to part (a) and the Theorem of Montel. Conversely, suppose that $(u_n)_{n \ge 0}$ is a normal family of meromorphic functions in a neighborhood D of infinity. Then $(u_n)_{n \ge 0}$ is equicontinuous in D (with respect to the chordal metric). Since $u_n(\infty) = 0$ for all $n \ge 0$, there exists some $R > 0$ such that

$$\chi(u_n(z), 0) = \frac{|u_n(z)|}{\sqrt{1 + |u_n(z)|^2}} \le \frac{1}{2}, \quad n \ge 0, \quad |z| \ge R.$$

It follows that $|u_n(z)| \le 1$ for all $n \ge 0$ and $|z| \ge R$. Applying the maximum principle for analytic functions, we obtain $|\tilde{u}_n(z)| \le R$ for all $n \ge 0$ and $|z| \ge R$, where $\tilde{u}_n(z) = z \cdot u_n(z)$. Consequently, both $(\tilde{u}_n)_{n \ge 0}$ and $(1/\tilde{u}_n)_{n \ge 0}$ are normal families of meromorphic functions in $|z| > R$. Since $\tilde{u}_n(\infty) = 1$, it follows again from equicontinuity that $(1/\tilde{u}_n)_{n \ge 0}$ is bounded above by some constant M for $|z| > R'$ with some suitable $R' > R$. Using the Cauchy formula we obtain

$$|(1/\tilde{u}_n)'(\infty)| \le M \cdot R', \quad |(1/\tilde{u}_n)''(\infty)| \le \frac{M \cdot (R')^2}{2}, \quad n \ge 0.$$

Taking into account (3.9), we may conclude that both sequences $(b_n)_{n \ge 0}$, $(a_n)_{n \ge 0}$ are bounded, and thus the operator A is bounded.

(c) Here we closely follow arguments from [17, Proof of Proposition 2.2]. By the Marty Theorem [39, Section 3], the sequence $(u_n)_{n \in \Lambda}$ is a normal family of meromorphic functions in some domain $D \subset \mathbb{C}$ if and only if the spherical derivative

$$\rho(u_n) := \frac{|u_n'|}{1 + |u_n|^2}$$

is bounded uniformly with respect to $n \in \Lambda$ on compact subsets of D. Using the confluent limit of the Christoffel-Darboux formula

$$a_n \cdot \frac{q_n(x) q_{n+1}(z) - q_n(z) q_{n+1}(x)}{z - x} = \sum_{j=0}^{n} q_j(x) \cdot q_j(z),$$

[8] Indeed, using (2.2) one immediately obtains the more precise relation

$$\Gamma(A) = \text{Clos}\Big(\bigcup_{n \ge 0} \Gamma(\mathcal{A}_n)\Big).$$

one obtains

$$|\rho(u_n)(z)| = \frac{|\sum_{j=0}^{n} q_j(z)^2|}{|q_n(z)|^2 + |a_n q_{n+1}(z)|^2}.$$

According to (2.14), the right-hand side is bounded above by $\max(1,|a_n|^2)\cdot||(zI-A)^{-1}||$, and this quantity is bounded on closed subsets of $\Omega(A)$ uniformly for $n\in\Lambda$ by assumption on (a_n). □

Let us shortly comment on Theorem 3.3. Part (c) has been stated in [17, Proposition 2.2] for bounded difference operators. Then of course the whole sequence (u_n) is normal in $\Omega(A)$, and from the proof of part (b) we see that any partial limit of (u_n) is different from the constants $0,\infty$ in the unbounded connected component $\Omega_0(A)$ of $\Omega(A)$. If A is no longer bounded then things become much more involved. However, for real Jacobi matrices we still obtain from part (a) the normality in $\mathbb{C}\setminus\mathbb{R}$. On the other hand, we see from part (b) that the expansion (3.9) can be only exploited for bounded difference operators.

A different proof of part (b) can be based of the observation that, for unbounded operators, it is interesting to consider the so-called contracted zero distribution (for real Jacobi matrices see, e.g., [23, 53]): Since the eigenvalues of $\mathcal{A}_n/||\mathcal{A}_n||$ are all in the unit disk, one easily verifies that $\tilde{q}_n(z) = q_n(||\mathcal{A}_n||\cdot z)$ has its zeros in the unit disk. As a consequence, one may derive nth root asymptotics for $(\tilde{q}_n)$. Indeed, for particular families of recurrence coefficients (Hermite, Laguerre, or Freud polynomials) even stronger asymptotics have been derived in the last years, see, e.g., [29]. In our context, one may verify that the rational functions

$$\tilde{u}_n(z) = ||\mathcal{A}_{n+1}||\cdot u_n(||\mathcal{A}_{n+1}||\cdot z) = \frac{||\mathcal{A}_{n+1}||\cdot q_n(||\mathcal{A}_{n+1}||\cdot z)}{a_n\cdot q_{n+1}(||\mathcal{A}_{n+1}||\cdot z)}$$

form a normal family in $|z|>1$, which has at least one partial limit being different from the constant 0. Then the assertion of Theorem 3.3(b) follows by applying a criterion of Zalcman [57]. Indeed, the contracted zero distribution has shown be very useful in describing properties of OPs for unbounded supports, and it seems to be interesting to explore the implications for complex Jacobi matrices and FOPs.

In the following statement we summarize some implications for the zeros of FOPs.

Theorem 3.4 **(a)** *There are no zeros of FOPs outside* $\Gamma(A)$.

(b) *Let* Λ *be some infinite set of integers such that* $(a_n)_{n\in\Lambda}$ *is bounded. Then for each closed* $F\subset\Omega(A)$ *there exists a* $\delta=\delta(F)$ *such that, for all* $n\in\Lambda$*, the zeros of* q_n *in* F *have at least the distance* δ *from the zeros of* q_{n+1} *in* F*. If* $\mathcal{A}$ *is real, then* $\Omega(A)$ *is the largest open set with this property.*

(c) **(compare with [17, Proposition 2.1])** *Let* Λ *be some infinite set of integers such that* $(a_n)_{n\in\Lambda}$ *is bounded, and denote by* Ω *a connected component of* $\Omega(A)$ *which is not a subset of* $\Gamma(A)$*. Then for each closed* $F\subset\Omega$ *there exists a constant* $\nu=\nu(F)$ *such that, for all* $n\in\Lambda$*, the number of zeros of* q_{n+1} *in* F *(counting multiplicities) is bounded by* $\nu(F)$*. If* $\mathcal{A}$ *is real, then* Ω *is the largest open connected set with this property.*

Proof: Part (a) follows immediately from Theorem 3.3(a) by observing that zeros of q_{n+1} are poles of u_n. In order to show part (b), recall from Theorem 3.3(c) that $(u_n)_{n\in\Lambda}$ is normal and thus equicontinuous in closed subsets of $\Omega(A)$. Given F as above, we hence find a $\delta > 0$ such that $\chi(u_n(z'), u_n(z'')) \leq 1/2$ for all $n \in \Lambda$ and for all $z', z'' \in F$ satisfying $|z' - z''| < \delta$. If now $z', z'' \in F$ with $q_n(z') = 0 = q_{n+1}(z'')$, then

$$\chi(u_n(z'), u_n(z'')) = \chi(0, \infty) = 1,$$

and thus $|z' - z''| \geq \delta$, showing that the zeros in F of q_n and of q_{n+1} are separated.

Suppose now that $\mathcal{A}$ is real. Then, according to, e.g., Example 2.7, the corresponding difference operator A is self-adjoint, and the corresponding moment problem has a unique solution μ, with $supp(\mu) = \sigma(A)$. It follows that, for any function f continuous on $\mathbb{R}$ with compact support, we have $I_n(f) \to \int f(x)\, d\mu(x)$, where $I_n(\cdot)$ denotes the nth Gaussian quadrature rule. Given any $z_0 \notin \Omega(A)$ (i.e., $z_0 \in supp(\mu)$) and $\delta > 0$, there exists a continuous function f with support in $U = (z_0 - \delta, z_0 + \delta)$ such that $\int f(x)\, d\mu(x) > 0$. In particular, there exists some N such that $I_n(f) > 0$, $n \geq N$, showing that all polynomials q_n must have at least one zero in U. This terminates the proof of part (b).

If the assertion of part (c) is not true, then using Theorem 3.3(c) we may construct a closed set $F \subset \Omega$ and a subsequence $(v_n)_{n \geq 0}$ of $(u_n)_{n \in \Lambda}$, v_n having at least n poles in F, with $(v_n)_{n \geq 0}$ converging to some function v locally uniformly in Ω. Notice that v is meromorphic in Ω. From Theorem 3.3(a) we know that v is different from the constant ∞ in $\Omega \setminus \Gamma(A)$, and thus in Ω. Clearly, poles of (v_n) only accumulate in the set $F' := \{z \in F : |v(z)| \geq 2\}$, and thus we may suppose without loss of generality that there exists an open set $U \supset F$ with its closure U' contained in Ω such that $|v(z)| \geq 1$ for $z \in U'$, and $v(z) \neq \infty$ on the boundary $\partial U'$ of U'. As a consequence, for a sufficiently large N, the sequence $(1/v_n)_{n \geq N}$ consists of functions being analytic in U', and tends to $1/v$ uniformly in U' with respect to the Euclidean metric. Applying the principle of argument to the connected components of U, we may conclude that, for sufficiently large n, the number of poles of v_n in U' coincides with the number of poles of v in U'. Since the latter number is finite, we have a contradiction to the construction of v_n. A proof for the final sentence of part (c) follows the same lines as the second part of the proof of (b), we omit the details. $\square$

Of course, for real Jacobi matrices, assertions related to Theorem 3.4 have been known before, see [3, Corollary 2] for part (b), and [52, Theorem 6.1.1] for part (c). Part (a) for complex Jacobi matrices has already been mentioned in [19, Theorem 3.10]. For complex bounded Jacobi matrices, $\Gamma(A)$ is bounded and contains $\sigma(A)$, and thus Ω necessarily coincides with the unbounded connected component $\Omega_0(A)$ of $\Omega(A)$. Consequently, for bounded A, part (c) gives a bound for the number of zeros of (all) FOPs in closed subsets of $\Omega_0(A)$, and this statement has been already established in [17, Proposition 2.1].

We terminate this section with a discussion of the closed convex set

$$\Gamma_{ess}(A) = \bigcap_{k \geq 0} \Gamma(A^{(k)}),$$

where $A^{(k)}$ denotes the difference operator of the associated Jacobi matrix $\mathcal{A}^{(k)}$ introduced before Theorem 2.8, $A^{(0)} = A$. This set has been considered before in [14, 15]. In the next statement we collect some properties of this set. Our main purpose is to generalize Theorem 3.3(a) and Theorem 3.4(a).

Theorem 3.5 **(a)** *There holds* $\Gamma_{ess}(A) \subset \Gamma(A^{(k+1)}) \subset \Gamma(A^{(k)})$ *for all* $k \geq 0$, *and* $\Gamma_{ess}(A) \neq \mathbb{C}$ *iff* $\Gamma(A) \neq \mathbb{C}$.

(b) *For any compact difference operator* B *we have* $\Gamma_{ess}(A) = \Gamma_{ess}(A+B)$.

(c) *Let* $\mathcal{A}$ *be proper. Then* $\sigma(A) \subset \Gamma(A)$ *and* $\sigma_{ess}(A) \subset \Gamma_{ess}(A)$. *Furthermore,* $\sigma(A) \setminus \Gamma_{ess}(A)$ *consists of isolated points which only accumulate on* $\Gamma_{ess}(A)$.

(d) *The sequence* $(u_n)_{n\geq 0}$ *of meromorphic functions is normal in* $\Omega(A)\setminus\Gamma_{ess}(A)$, *and any partial limit is different from the constant* ∞.

(e) *For any compact subset* F *of* $\Omega(A) \setminus \Gamma_{ess}(A)$ *there exists a constant* $N = N(F)$ *such that none of the FOPs* q_n *for* $n \geq N$ *has a zero in* F.

Proof: (a) The first inclusions follow immediately from the definition of the numerical range. It remains to discuss the case $\Gamma_{ess}(A) \neq \mathbb{C}$. Then at least for one $k \geq 0$ we must have $\Gamma(A^{(k)}) \neq \mathbb{C}$. Since $\Gamma(A^{(k)})$ is convex, it must be contained in some halfplane. Furthermore, one easily checks that any $z \in \Theta(A)$ may be written as $z = z_1 + z_2$, with $z_2 \in \Gamma(A^{(k)})$, and $|z_1| \leq 2||\mathcal{A}_k||$. Thus $\Theta(A)$ and $\Gamma(A)$ are contained in some halfplane, and $\Gamma(A) \neq \mathbb{C}$.

(b) This assertion follows from the fact that any $z \in \Gamma(A^{(k)} + B^{(k)})$ may be written as $z = z_A + z_B$, with $z_A \in \Gamma(A^{(k)})$, $|z_B| \leq ||B^{(k)}||$, and $||B^{(k)}|| \to 0$.

(c) It is known [28, Theorem V.3.2] that, in connected components of $\mathbb{C}\setminus\Gamma(A)$, $\mathcal{R}(zI - A)$ is closed and $\dim(zI - A) = 0$. Since $\mathcal{A}$ is proper, it follows from Lemma 2.4(d) that $\mathcal{R}(zI - A)^{\perp} = \mathcal{N}((zI - A)^*) = \{0\}$, and thus $\mathcal{R}(zI - A) = \ell^2$. Consequently, $\mathbb{C} \setminus \Gamma(A) \subset \Omega(A)$. Also, it follows (implicitly) from [28, Theorem IV.5.35] that $\sigma_{ess}(A) = \sigma_{ess}(A^{(k)})$ for all $k \geq 0$, and $\sigma_{ess}(A^{(k)}) \subset \Gamma(A^{(k)})$ by [28, Problem V.3.6]. Thus we have also established the second inclusion $\sigma_{ess}(A) \subset \Gamma_{ess}(A)$.

In order to see the last sentence of part (c), denote by D a connected component of $\mathbb{C} \setminus \sigma_{ess}(A)$. From [28, Section IV.5.6] we know that either $D \subset \sigma(A)$, or the elements of $\sigma(A)$ in D are isolated and accumulate only in $\sigma_{ess}(A) \subset \Gamma_{ess}(A)$. If now $\sigma(A)\setminus\Gamma_{ess}(A) \subset \mathbb{C}\setminus\sigma_{ess}(A)$, there is nothing to show. Otherwise, suppose that D contains a point $z \in \sigma(A) \setminus \Gamma_{ess}(A)$. Then the assertion follows by showing that $D \not\subset \sigma(A)$. Indeed, we know from part (a) and the preceding paragraph that there exists a $\zeta \in \mathbb{C} \setminus \Gamma(A) \subset \Omega(A)$. By convexity of $\Gamma_{ess}(A)$, it follows that the segment $[z, \zeta]$ is a subset of $\mathbb{C} \setminus \Gamma_{ess}(A) \subset \mathbb{C} \setminus \sigma_{ess}(A)$. Hence $[z, \zeta] \subset D$, which implies that $D \not\subset \sigma(A)$.

(d),(e) We show in Corollary 4.4(a) below that for any compact subset F of $\Omega(A) \setminus \Gamma_{ess}(A)$ there exists a constant $N = N(F)$ such that

$$\sup_{n\geq N} \max_{z\in F} ||(z\mathcal{I}_n - \mathcal{A}_n)^{-1}|| < \infty.$$

Since $u_n(x) = (e_n, (z\mathcal{I}_{n+1} - \mathcal{A}_{n+1})^{-1} e_n)$, it follows that

$$\sup_{n\geq N} \max_{z\in F} |u_n(z)| < \infty.$$

Then assertions (d),(e) follow immediately. □

A particularly interesting case contained in Theorem 3.5 has been discussed by Barrios, López, Martínez and Torrano, see [12, 13, 14, 15]: here $A = G + C$, where G is a self-adjoint difference operator (resulting from a real proper Jacobi matrix) and C is a compact complex difference operator. Then $\mathcal{A}$ is proper (and determined), and

$$\sigma_{ess}(A) = \sigma_{ess}(G) \subset \Gamma_{ess}(A) = \Gamma_{ess}(G) \subset \Gamma(G) = \mathrm{conv}(\sigma(G)) \subset \mathbb{R}$$

by (2.12) and parts (a),(b), and (c). Several of the results given in the present paper for general complex Jacobi matrices have been shown for the above class already earlier, see, e.g. [14, Lemma 3 and Lemma 4] and [15]. In particular, Theorem 3.5(e) for this class was established in [14, Corollary 1].

3.3 An open problem concerning zero-free regions

We have seen above that, for bounded operators A, the zeros of all FOPs are contained in the convex compact set $\Gamma(A)$, and most of them are "close" to the polynomial convex hull[9] of the spectrum $\sigma(A)$.

Let us have a closer look at an inverse problem: Suppose that c is some regular linear functional and Γ is some compact[10] convex set containing **all** zeros of **all** FOPs. Can we give some (spectral) properties of the underlying difference operator, or the sequence (u_n)?

Zero-free regions can be obtained from the recurrence relation, e.g., by applying techniques from continued fractions. There are for instance Cassini ovals [55, Corollary 4.1], or the Worpitski set (see [56, Theorem V.26.2] and [19, Section 3.1]).

A related question in Padé approximation has been discussed by Gonchar [26] who showed that the sequence of rational functions $(p_n/q_n)_{n\geq 0}$ converges locally uniformly in $\mathbb{C} \setminus \Gamma$ to some function f with a geometric rate. In other words, the absence of poles in sets (with a particular shape) is already sufficient to insure convergence of Padé approximants. Let us recall here some of his intermediate findings: writing a_n, b_n in terms of the coefficients of q_n/k_n (compare with (2.27)), and taking into account that the zeros of q_n/k_n are bounded, one finds the relation (see [26, Proof of Proposition 4])

$$\sup_{n\geq 0} \frac{|a_n|}{n+1} < \infty, \quad \sup_{n\geq 0} \frac{|b_n|}{n+1} < \infty. \tag{3.10}$$

Notice that combining this result with Example 2.7 shows that the underlying complex Jacobi matrix is proper. A combination of [26, Proposition 2 and Proposition 4] leads to the relations

$$\begin{aligned}
&\liminf_{n\to\infty} |q_n(z)|^{1/n} = \liminf_{n\to\infty} (|q_n(z)|^2 + |a_n q_{n+1}(z)|^2)^{1/(2n)} \geq \exp(g_\Gamma(z)), \quad z \in \mathbb{C} \setminus \Gamma \\
&\kappa_{\sup} = \limsup_{n\to\infty} |a_0 \cdot a_1 \cdot \ldots \cdot a_{n-1}|^{1/n} \leq \mathit{cap}\,(\Gamma), \\
&\limsup_{n\to\infty} |\widetilde{r}_n(z)|^{1/n} = \liminf_{n\to\infty} (|\widetilde{r}_n(z)|^2 + |a_n \widetilde{r}_{n+1}(z)|^2)^{1/(2n)} \leq \exp(-g_\Gamma(z)), \quad z \in \mathbb{C} \setminus \Gamma
\end{aligned}$$

[9] Indeed, it is also unclear whether there is an example of a (complex) operator A where the number of zeros of FOPs in some compact subset of a bounded component of $\Omega(A)$ is unbounded.

[10] Example 3.2(a) of Stahl shows that there exist regular functionals induced by some measure on $[-1, 1]$ where all but two zeros stay in $[-1, 1]$, but the sequence of exceptional zeros is not bounded (and thus the underlying operator also is unbounded). Thus the restriction to bounded Γ seems to be natural.

where $\widetilde{r}_n(z) = q_n(z)f(z) - p_n(z)$. Of course, in the case $\sigma(A) \subset \Gamma$, these relations (with $f(z) = \phi(z)$ and $\widetilde{r}_n(z) = r_n(z)$) would follow from our Theorem 3.1. But this is exactly our problem: does it follow only from the knowledge about zeros of FOPs that $\sigma(A) \subset \Gamma$? Clearly, for real Jacobi matrices the answer is yes, but for complex Jacobi matrices?

Since an operator A with compact spectrum is necessarily bounded, a first step in this direction would be to sharpen (3.10) and to show that A is bounded. According to Theorem 3.3(b), this is equivalent to the fact that $(u_n)_{n\geq 0}$ (or $(z \cdot u_n)_{n\geq 0}$) is normal in some neighborhood of infinity.

Notice that $(z \cdot u_n)_{n\geq 0}$ does not take the values $0, \infty$ in $\overline{\mathbb{C}} \setminus \Gamma$. Moreover, by a theorem of Montel [39], any sequence of meromorphic functions which does not take three different values in some region D is normal. It would be interesting to know whether, for our particular sequence of (rational) functions, the information on the zeros of FOPs is already sufficient for normality.

Another interesting approach to our problem would be to impose in addition that A is bounded. If this implies $\sigma(A) \subset \Gamma$, then we would have at least a partial answer to the following problem raised by Aptekarev, Kaliaguine and Van Assche [6]: does the convergence of the whole sequence of Padé approximants with a geometric rate at a fixed point z implies that $z \in \Omega(A)$?

3.4 Compact perturbations of Jacobi matrices and ratio asymptotics

An important element in the study of FOPs is the detection of so-called *spurious zeros* (or spurious poles in Padé approximation). We have seen in the preceding section that the absence of zeros in some region has some important consequences concerning, e.g., the convergence of Padé approximants. Roughly speaking, we call *spurious* the zeros of FOPs which are not related to the spectrum of the underlying difference operator. To give an example, consider a real Jacobi matrix induced by a measure supported on $[-2,-1] \cup [1,2]$ which is symmetric with respect to the origin. Then the zeros of the OPs q_{2n} lie all in the spectrum of A, and also $2n$ of the zeros of the OPs q_{2n+1} lie in the spectrum of A, but $q_{2n+1}(0) = 0$ by symmetry.

We will not give a proper definition of spurious zero in the general case, see [47, Section 4] for a more detailed discussion. Here we will restrict ourselves to bounded complex Jacobi matrices: a sequence $(z_n)_{n\in\Lambda}$ is said to consist of spurious zeros if $q_n(z_n) = 0$, $n \in \Lambda$, and $(z_n)_{n\in\Lambda}$ lies in some closed subset of the unbounded connected component $\Omega_0(A)$ of the resolvent set. Notice that $|z_n| \leq ||A||$ by Theorem 3.4(a), implying that $(z_n)_{n\in\Lambda}$ remains in some compact subset of $\Omega_0(A)$. We therefore may (and will) assume that $(z_n)_{n\in\Lambda}$ converges to some $\zeta \in \Omega_0(A)$.

From Theorem 3.4(c) and the remarks after Theorem 3.4 we see that there are only "few" such spurious zeros, and that the set of their limits ζ just coincide with the set of zeros (or poles) in $\Omega_0(A)$ of partial limits of the normal family (u_n). Also, $\zeta \in \sigma(A) \cup \Gamma_{ess}(A)$ by Theorem 3.5(e).

One motivation for the considerations of this section is to show that the set of limits of spurious zeros remains invariant with respect to compact perturbations. This follows as a corollary from the following

Theorem 3.6 *Let A, $\widetilde{A}$ be two complex Jacobi matrices with entries a_n, b_n, and $\widetilde{a}_n, \widetilde{b}_n$, respec-*

tively. Suppose that $\mathcal{A}, \widetilde{\mathcal{A}}$ are bounded, and[11] *that $\arg(\widetilde{a}_n/a_n) \in (-\pi/2, \pi/2]$ for $n \geq 0$.*

Then the difference $A - \widetilde{A}$ of the corresponding difference operators is compact iff

$$\lim_{n\to\infty} \chi(u_n, \widetilde{u}_n) = 0 \tag{3.11}$$

uniformly in closed subsets of $\Omega_0(A) \cap \Omega_0(\widetilde{A})$.

Theorem 3.6 has been known before (at least partially) for real Jacobi matrices. Take as reference system the entries $\widetilde{a}_n = a \neq 0$, $\widetilde{b} = b$, $n \geq 0$. Then

$$\widetilde{u}_n(z) = \frac{\widetilde{q}_n(z)}{\widetilde{a}_n \widetilde{q}_{n+1}(z)} \to \frac{2}{z - b + \sqrt{(z-b)^2 - 4a^2}}$$

uniformly on closed subsets of $\mathbb{C} \setminus [b - 2a, b + 2a] = \mathbb{C} \setminus \sigma(\widetilde{A})$ (we choose a branch of the square root such that the right-hand side vanishes at infinity). Thus Theorem 3.6 includes as a special case the well-known description of the Nevai–Blumenthal class $\mathcal{M}(a; b)$, see, e.g., [33]. This description is usually shown by applying the Poincaré Theorem, and a similar description is known for compact perturbations of (real) periodic Jacobi matrices (being considered more detailed in Subsection 4.3 below). Finally, Nevai and Van Assche [34] showed that a relation similar to (3.11) holds provided that $\widetilde{\mathcal{A}}$ is a real compact perturbation of a real $\mathcal{A}$.

Before proving Theorem 3.6, let us motivate and state a related more general result. Given any (not necessarily regular) linear functional c acting on the space of polynomials, the (unique) *monic* FOPs Q_{n_j} corresponding to normal indices n_j together with some auxiliary monic polynomials Q_n, $n \neq n_j$ are known to satisfy a recurrence of the form

$$z \cdot Q_n(z) = Q_{n+1}(z) + \sum_{j=n-\gamma_n}^{n} b_{n,j} Q_j(z), \quad n \geq 0, \quad Q_0(z) = 1, \tag{3.12}$$

where $b_{n,j}$ are some complex numbers, and the integer $\gamma_n \geq 0$ is bounded above by some multiple of the maximal distance of two succeeding normal indices. We may rewrite the recurrence formally as

$$(z\mathcal{I} - \mathcal{B}) \cdot \begin{bmatrix} Q_0(z) \\ Q_1(z) \\ Q_2(z) \\ \vdots \end{bmatrix}, \quad \mathcal{B} = \begin{bmatrix} b_{0,0} & 1 & 0 & 0 & \cdots & \cdots \\ b_{1,0} & b_{1,1} & 1 & 0 & & \\ b_{2,0} & b_{2,1} & b_{2,2} & 1 & 0 & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \end{bmatrix}, \tag{3.13}$$

i.e., $\mathcal{B}$ is a lower Hessenberg matrix. If in addition the distance of two succeeding normal indices is uniformly bounded, then $\mathcal{B}$ is banded. This occurs for instance for symbols like $\sin(1/z)$, or for functionals c which are *asymptotically regular*, i.e., all sufficiently large indices are normal. Notice that, by (3.13), Q_n is the characteristic polynomial of the finite principal submatrix $\mathcal{B}_n$ of order n.

A class of asymptotically regular functionals was studied by Magnus [31] who considered c_w of (3.8) with a complex and continuous w which is different from 0 in $[-1, 1]$ (in fact, his class is larger). By, e.g., the Theorem of Rakhmanov, the real Jacobi matrix associated to $c_{|w|}$ is a compact perturbation of the Toeplitz operator having 1/2 on the super- and the subdiagonal

[11] Such a normalisation is known from orthogonal polynomials where usually $a_n, \widetilde{a}_n > 0$. It can be insured by possibly multiplying $\widetilde{q}_n$ by -1.

and else 0. The functional c_w may be not regular, but is asymptotically regular by [31, Theorem 6.1(i)]. Therefore the corresponding matrix $\mathcal{B}$ will in general not be tridiagonal, but is a compact perturbation of the Toeplitz operator having 1 on the super-, 1/4 on the subdiagonal and else 0 (see [31, Theorem 6.1(iii)] and Theorem 3.7 below).

For regular functionals, recurrence (3.13) holds with

$$b_{n,n} = b_n, \quad b_{n+1,n} = a_n^2, \quad b_{k,n} = 0, \quad k-1 \geq n \geq 0, \tag{3.14}$$

showing that $\mathcal{B}$ is bounded iff the corresponding Jacobi matrix is bounded. Recurrences of the above form are also valid for more general sequences of polynomials. For instance, for monic OPs with respect to the hermitian scalar product

$$(f,g)_\mu = \int \overline{f(z)} g(z)\, d\mu(z),$$

μ being some positive measure with compact infinite support, we always have a recurrence (3.12) with $b_{n,k} = (Q_k, zQ_n)_\mu/(Q_k,Q_k)_\mu$. We have the following complement of Theorem 3.6.

Theorem 3.7 *Let $\mathcal{B}$ be a tridiagonal matrix as in (3.14), with coefficients $b_{n,k}$ and associated monic FOPs Q_n and let $\widetilde{\mathcal{B}}$ be a lower Hessenberg matrix as in (3.13) with coefficients $\widetilde{b}_{n,k}$ and associated polynomials $\widetilde{Q}_n$, Provided that $\mathcal{B}$ and $\widetilde{\mathcal{B}}$ are bounded, we have*

$$\lim_{n\to\infty} \Big(\frac{Q_n(z)}{Q_{n+1}(z)} - \frac{\widetilde{Q}_n(z)}{\widetilde{Q}_{n+1}(z)} \Big) = 0 \tag{3.15}$$

uniformly for $|z| \geq R$ for sufficiently large R iff[12]

$$\lim_{n\to\infty} (b_{n+j,n} - \widetilde{b}_{n+j,n}) = 0, \quad j = 0,1,2,\dots. \tag{3.16}$$

Proof: Suppose that (3.15) holds. Since $Q_n, \widetilde{Q}_n$ are monic and of degree exactly n, we have the expansions

$$\frac{Q_n(z)}{Q_{n+1}(z)} = \sum_{j=0}^{\infty} \frac{u_{n,j}}{z^{j+1}}, \quad \frac{\widetilde{Q}_n(z)}{\widetilde{Q}_{n+1}(z)} = \sum_{j=0}^{\infty} \frac{\widetilde{u}_{n,j}}{z^{j+1}},$$

where $u_{n,0} = \widetilde{u}_{n,0} = 1$, and $u_{n,j} - \widetilde{u}_{n,j}$ tends to zero for $n \to \infty$ for all fixed $j \geq 1$ by (3.15). From (3.13) we obtain

$$z\frac{Q_n(z)}{Q_{n+1}(z)} = 1 + b_{n,n}\frac{Q_n(z)}{Q_{n+1}(z)} + b_{n,n-1}\frac{Q_{n-1}(z)}{Q_n(z)}\frac{Q_n(z)}{Q_{n+1}(z)} + \dots + b_{n,n-j}\prod_{\ell=0}^{j}\frac{Q_{n-\ell}(z)}{Q_{n+1-\ell}(z)} + \mathcal{O}(\frac{1}{z^{j+2}})_{z\to\infty}$$

for any $n \geq j \geq 0$, and a similar equation for the quantities related to $\widetilde{\mathcal{B}}$. Inserting the expansions at infinity and comparing coefficients leads to

$$u_{n,1} - \widetilde{u}_{n,1} = b_{n,n} - \widetilde{b}_{n,n} \to 0, \quad u_{n,2} - \widetilde{u}_{n,2} = (b_{n,n-1} + b_{n,n}^2) - (\widetilde{b}_{n,n-1} + \widetilde{b}_{n,n}^2) \to 0,$$

and similarly $u_{n,j+1} - \widetilde{u}_{n,j+1} = b_{n,n-j} - \widetilde{b}_{n,n-j} + C_{n,j} - \widetilde{C}_{n,j}$ for $j \geq 2$, where $C_{n,j}$ is a polynomial expression of the quantities $b_{n-\ell,n-i}$ for $0 \leq \ell \leq i < j$, and $\widetilde{C}_{n,j}$ is obtained from $C_{n,j}$ by

[12] If $\mathcal{B}$ is in addition banded, then this second condition is equivalent to the fact that $\mathcal{B} - \widetilde{\mathcal{B}}$ is compact.

replacing the quantities $b_{n-\ell,n-i}$ by $\widetilde{b}_{n-\ell,n-i}$. One concludes by recurrence on j that the claimed limit relation (3.16) for the recurrence coefficients holds.

The other implication of Theorem 3.7 is slightly more involved. We choose

$$|z| \geq R := 2 \cdot \max\{||\mathcal{B}||, ||\widetilde{\mathcal{B}}||\}.$$

Then $|z| \geq 2 \cdot \max\{||\mathcal{B}_n||, ||\widetilde{\mathcal{B}}_n||\}$ for all n, implying that

$$||(z\mathcal{I}_n - \mathcal{B}_n)^{-1}|| \leq \frac{2}{|z|}, \quad ||(z\mathcal{I}_n - \widetilde{\mathcal{B}}_n)^{-1}|| \leq \frac{2}{|z|}, \quad n \geq 0.$$

It follows from (3.13) that

$$(z\mathcal{I}_n - \widetilde{\mathcal{B}}_n) \cdot (\widetilde{Q}_0(z), ..., \widetilde{Q}_{n-1}(z))^T = (0, ..., 0, \widetilde{Q}_n(z))^T,$$

and thus $\widetilde{Q}_n(z)/\widetilde{Q}_{n+1}(z) = (e_n, (z\mathcal{I}_{n+1} - \widetilde{\mathcal{B}}_{n+1})^{-1} e_n)$, as well as

$$\sum_{j=0}^{n} |\widetilde{Q}_j(z)|^2 \leq ||(z\mathcal{I}_{n+1} - \widetilde{\mathcal{B}}_{n+1})^{-1}||^2 |\widetilde{Q}_{n+1}(z)|^2 \leq \frac{4|\widetilde{Q}_{n+1}(z)|^2}{|z|^2}.$$

From the latter relation one deduces by recurrence on $n - j$ that

$$|(e_j, (z\mathcal{I}_{n+1} - \widetilde{\mathcal{B}}_{n+1})^{-1} e_n)|^2 = |\frac{\widetilde{Q}_j(z)}{\widetilde{Q}_{n+1}(z)}|^2 \leq \frac{4}{|z|^2 \cdot (1 + |z|^2/4)^{n-j}}, \quad 0 \leq j \leq n. \tag{3.17}$$

We claim that also

$$|(e_n, (z\mathcal{I}_{n+1} - \mathcal{B}_{n+1})^{-1} e_j)|^2 \leq \frac{4}{|z|^2 \cdot (1 + |z|^2/(4a^2))^{n-j}}, \quad 0 \leq j \leq n, \tag{3.18}$$

where $a = \max\{1, \sup |b_{n+1,n}|\} \leq ||\mathcal{B}|| < \infty$. This inequality is based on the observation that the polynomials $Q_n^L(z) := k_n q_n(z) = k_n^2 Q_n(z)$ satisfy

$$(Q_0^L(z), ..., Q_{n-1}^L(z)) \cdot (z\mathcal{I}_n - \mathcal{B}_n) = b_{n,n-1} \cdot (0, ..., 0, Q_n^L(z)).$$

Thus a proof for (3.18) follows the same lines as the proof of (3.17), we omit the details.

Given an $\epsilon > 0$, by assumption (3.16) on the recurrence coefficients we may find an $L > 0$ and an $N > 0$ such

$$\lambda := (1 + R^2/(4a^2))^{-1/2} < \epsilon^{1/L}, \quad \text{and} \quad |b_{n+\ell,n} - \widetilde{b}_{n+\ell,n}| < \epsilon, \quad n \geq N, \quad \ell = 0, ..., L.$$

For all other indices we have the trivial upper bound $|b_{n+\ell,n} - \widetilde{b}_{n+\ell,n}| \leq (||\mathcal{B}|| + ||\widetilde{\mathcal{B}}||) =: b$. Using (3.17), (3.18) we obtain for $|z| \geq R$, $n \geq N + L$,

$$\begin{aligned}
&\left|\frac{Q_n(z)}{Q_{n+1}(z)} - \frac{\widetilde{Q}_n(z)}{\widetilde{Q}_{n+1}(z)}\right| = \left|(e_n, [(z\mathcal{I}_{n+1} - \mathcal{B}_{n+1})^{-1} - (z\mathcal{I}_{n+1} - \widetilde{\mathcal{B}}_{n+1})^{-1}]e_n)\right| \\
&= \left|(e_n, (z\mathcal{I}_{n+1} - \mathcal{B}_{n+1})^{-1}(\widetilde{\mathcal{B}}_{n+1} - \mathcal{B}_{n+1})(z\mathcal{I}_{n+1} - \widetilde{\mathcal{B}}_{n+1})^{-1} e_n)\right| \\
&\leq \frac{2}{R} \sum_{j=0}^{n} \sum_{k=0}^{j} \lambda^{n-j+n-k} \cdot |b_{j,k} - \widetilde{b}_{j,k}| \\
&\leq \frac{2b}{R} \sum_{j=0}^{n} \sum_{k=0}^{\min\{j,n-L\}} \lambda^{n-j+n-k} + \frac{2\epsilon}{R} \sum_{j=n-L}^{n} \sum_{k=n-L}^{j} \lambda^{n-j+n-k} \leq \frac{2(b+1)}{R(1-\lambda)^2} \cdot \epsilon,
\end{aligned}$$

Since $\epsilon > 0$ was arbitrary, we have established (3.15). Hence the second implication of Theorem 3.7 is shown. □

Proof of Theorem 3.6: We apply Theorem 3.7 with

$$\widetilde{b}_{n,n} = \widetilde{b}_n, \quad \widetilde{b}_{n+1,n} = \widetilde{a}_n^2, \quad \widetilde{b}_{k,n} = 0, \quad k-1 \geq n \geq 0.$$

Since $q_n/(a_n q_{n+1}) = Q_n/Q_{n+1}$ is bounded around infinity by Theorem 3.3(a), and similarly for the tilde quantities, we see that (3.11) implies (3.15). In order to show that also the converse is true, suppose that (3.15) holds but not (3.11). Then there is some infinite set Λ and some $z_n \in \Omega_0(A) \cap \Omega_0(\widetilde{A})$, $(z_n)_{n\in\Lambda}$ tending to some $\zeta \in \Omega_0(A) \cap \Omega_0(\widetilde{A})$, such that $(\chi(u_n(z_n), \widetilde{u}_n(z_n)))_{n\in\Lambda}$ does not converge to zero. Using the normality established in Theorem 3.3(c), we find a subset also denoted by Λ such that $(u_n)_{n\in\Lambda}$ (and $(\widetilde{u}_n)_{n\in\Lambda}$, respectively) tends to some meromorphic function u (and $\widetilde{u}$, respectively) locally uniformly in $\Omega_0(A)$ (and in $\Omega_0(\widetilde{A})$, respectively). Notice that $u(\zeta) \neq \widetilde{u}(\zeta)$ by construction of ζ, and $u = \widetilde{u}$ in some neighborhood of infinity by (3.15), which is impossible for meromorphic functions. Hence (3.11) and (3.15) are equivalent.

Notice that (3.16) may be rewritten in our setting as $\widetilde{b}_n - b_n \to 0$, and $\widetilde{a}_n^2 - a_n^2 \to 0$. The normalization $\arg(\widetilde{a}_n/a_n) \in (-\pi/2, \pi/2]$ of Theorem 3.6 allows to conclude that $|a_n - \widetilde{a}_n| \leq |a_n + \widetilde{a}_n|$, showing that $(a_n^2 - \widetilde{a}_n^2)_{n\geq 0}$ tends to zero iff $(a_n - \widetilde{a}_n)_{n\geq 0}$ does. Thus $A - \widetilde{A}$ is compact iff (3.16) holds, and Theorem 3.6 follows from Theorem 3.7. □

It is known for many examples (see, e.g., [47, Proposition 4.2]) that spurious poles of Padé approximants p_n/q_n are accompanied by a "close" zero. As a further consequence of Theorem 3.7, we can be more precise. In fact, consider $\widetilde{\mathcal{B}}$ obtained from $\mathcal{B}$ by changing the values $\widetilde{b}_{1,0} = 0$ and $\widetilde{b}_{0,0} \in \sigma(A)$. Comparing with (1.2) one easily sees that $\widetilde{Q}_n(z) = (z - \widetilde{b}_{0,0}) p_n(z)/k_n$, and as in the above proof it follows that

$$\chi(\frac{p_n}{a_n p_{n+1}}, \frac{q_n}{a_n q_{n+1}}) \to 0$$

locally uniformly in $\Omega_0(A) \cap \Omega_0([\widetilde{\mathcal{B}}]_{\min}) = \Omega_0(A) \cap \Omega_0(A^{(1)})$, which according to Theorem 2.8 coincides with $\Omega := \{z \in \Omega_0(A) : \phi(z) \neq 0\}$. In particular, applying the argument principle we may conclude that, for every sequence $(z_n)_{n\in\Lambda}$ tending to $\zeta \in \Omega_0(A)$ with $q_n(z_n) = 0$, there exists a sequence $(z_n')_{n\in\Lambda}$ tending to ζ with $p_n(z_n') = 0$.

3.5 Trace class perturbations and strong asymptotics

It is known for real Jacobi matrices [34] that if $A - \tilde{A}$ is not only compact but of trace class then we may have a stronger form of convergence. A similar assertion is true for complex Jacobi matrices

Theorem 3.8 *Let $\mathcal{A}$, $\widetilde{\mathcal{A}}$ be two bounded complex Jacobi matrices. Provided that the difference $A - \widetilde{A}$ of the corresponding difference operators is of trace class, i.e.,*

$$\sum_{n=0}^{\infty} |a_n - \widetilde{a}_n| + |b_n - \widetilde{b}_n| < \infty,$$

the corresponding monic FOPs verify

$$\lim_{n\to\infty} \frac{\widetilde{Q}_n(z)}{Q_n(z)} = \det(I + (A - \widetilde{A})(zI - A)^{-1})$$

uniformly on closed subsets of subdomains D of $\Omega_0(A) \cap \Omega_0(\widetilde{A})$ which are (asymptotically) free of zeros of the FOPs q_n and $\widetilde{q}_n$, $n \geq 0$.

Proof: Define the projections $E_n : \ell^2 \to \mathbb{C}^n$ by $E_n(y_j)_{j\geq 0} = (y_j)_{0\leq j<n}$. We start by establishing for $z \in \Omega(A)$ the formula

$$E_n(zI - A)^{-1}E_n^* - (z\mathcal{I}_n - \mathcal{A}_n)^{-1} = (q_0(z), ..., q_{n-1}(z))^T \frac{r_n(z)}{q_n(z)}(q_0(z), ..., q_{n-1}(z)). \qquad (3.19)$$

Indeed, by (2.19),

$$\begin{aligned} I_n &= E_n(zI - A)(zI - A)^{-1}E_n^* \\ &= E_n(zI - A)E_n^*E_n(zI - A)^{-1}E_n^* - (0, ..., 0, a_{n-1})^T r_n(z)(q_0(z), ..., q_{n-1}(z)). \end{aligned}$$

Taking into account that $E_n(zI - A)E_n^* = z\mathcal{I}_n - \mathcal{A}_n$, and

$$(0, ..., 0, a_{n-1})^T = \frac{1}{q_n(z)}(z\mathcal{I}_n - \mathcal{A}_n)(q_0(z), ..., q_{n-1}(z))^T,$$

identity (3.19) follows. In a similar way one obtains for $z \in \Omega(A)$ using (3.19)

$$\begin{aligned} &E_n(zI - \widetilde{A})(zI - A)^{-1}E_n^* - (z\mathcal{I}_n - \widetilde{\mathcal{A}}_n)(z\mathcal{I}_n - \mathcal{A}_n)^{-1} \\ &= (z\mathcal{I}_n - \widetilde{\mathcal{A}}_n)[E_n(zI - A)^{-1}E_n^* - (z\mathcal{I}_n - \mathcal{A}_n)^{-1}] + E_n(zI - \widetilde{A})(I - E_n^*E_n)(zI - A)^{-1}E_n^* \\ &= \Big((z\mathcal{I}_n - \widetilde{\mathcal{A}}_n)(q_0(z), ..., q_{n-1}(z))^T \frac{r_n(z)}{q_n(z)} - (0, ..., 0, \widetilde{a}_{n-1})^T r_n(z)\Big)(q_0(z), ..., q_{n-1}(z)) \\ &= a_{n-1} r_n(z) q_n(z)(z\mathcal{I}_n - \widetilde{\mathcal{A}}_n)\Big(\frac{q_0(z)}{q_n(z)} - \frac{\widetilde{q}_0(z)}{\widetilde{q}_n(z)}, ..., \frac{q_{n-1}(z)}{q_n(z)} - \frac{\widetilde{q}_{n-1}(z)}{\widetilde{q}_n(z)}\Big)^T \Big(0, ..., 0, 1\Big)(z\mathcal{I}_n - \mathcal{A}_n)^{-1}. \end{aligned}$$

Consequently,

$$\begin{aligned} &\det(E_n(zI - \widetilde{A})(zI - A)^{-1}E_n^*) = \det((z\mathcal{I}_n - \widetilde{\mathcal{A}}_n)(z\mathcal{I}_n - \mathcal{A}_n)^{-1}) \\ &\cdot \det\Big(I_n - a_{n-1} r_n(z) q_n(z)\Big(\frac{q_0(z)}{q_n(z)} - \frac{\widetilde{q}_0(z)}{\widetilde{q}_n(z)}, ..., \frac{q_{n-1}(z)}{q_n(z)} - \frac{\widetilde{q}_{n-1}(z)}{\widetilde{q}_n(z)}\Big)^T \Big(0, ..., 0, 1\Big)\Big) \\ &= \frac{\widetilde{Q}_n(z)}{Q_n(z)} \cdot \Big[1 - a_{n-1} r_n(z) q_n(z)\Big(\frac{q_{n-1}(z)}{q_n(z)} - \frac{\widetilde{q}_{n-1}(z)}{\widetilde{q}_n(z)}\Big)\Big]. \end{aligned} \qquad (3.20)$$

Using the projector $\Pi_n = E_n^*E_n$ introduced in Section 2, the term on the left-hand side may be rewritten as

$$\det(E_n(zI - \widetilde{A})(zI - A)^{-1}E_n^*) = \det(I_n + E_n(A - \widetilde{A})(zI - A)^{-1}E_n^*) = \det(I + \Pi_n(A - \widetilde{A})(zI - A)^{-1}),$$

where the term of the right is the determinant of a finite rank perturbation of the identity, see, e.g., [28, Section III.4.3]. Since $A - \widetilde{A}$ is a trace class operator, the same is true for $(A - \widetilde{A})(zI - A)^{-1}$ and thus

$$\lim_{n\to\infty} \det(I + \Pi_n(A - \widetilde{A})(zI - A)^{-1}) = \det(I + (A - \widetilde{A})(zI - A)^{-1})$$

uniformly in closed subsets of $\Omega(A)$. It remains to see whether the term in brackets on the right-hand side of (3.20) tends to 1. Let F be some closed subset of the zero–free region $D \subset \Omega := \Omega_0(A) \cap \Omega_0(\widetilde{A})$. According to Theorem 3.3(c), both (u_n) and $(\widetilde{u}_n)$ are normal families of meromorphic functions in Ω, and the functions are analytic in the subdomain D. Furthermore, we know from Theorem 3.3 that any partial limit is different from the constant infinity. It is known (see, e.g., [17, Lemma 2.4(d)]) that then (u_n) and $(\widetilde{u}_n)$ are bounded on F uniformly in n. Combining this with Theorem 3.6 we find that $|u_n - \widetilde{u}_n| \to 0$ uniformly in F, and

$$\max_{z\in F} \left|\frac{q_{n-1}(z)}{q_n(z)} - \frac{\widetilde{q}_{n-1}(z)}{\widetilde{q}_n(z)}\right| \le |a_{n-1}| \cdot \max_{z\in F} |u_{n-1}(z) - \widetilde{u}_{n-1}(z)| + |a_{n-1} - \widetilde{a}_{n-1}| \cdot \max_{z\in F} |\widetilde{u}_{n-1}(z)|$$

tends to zero for $n \to \infty$. Moreover, the remaining term $a_{n-1}r_n(z)q_n(z)$ is bounded uniformly for $z \in F$ and $n \ge 0$ according to (2.23). This terminates the proof of Theorem 3.8. □

We conclude this section by some general remarks concerning the strong asymptotics

$$\max_{z\in U} \left|\frac{\widetilde{Q}_n(z)}{Q_n(z)} - g(z)\right| = 0, \quad \text{where } U \text{ is some closed disk around } \infty.$$

Indeed, by examining the proof we see that this assertion is true also for the more general matrices $\mathcal{B}, \widetilde{\mathcal{B}}$ of Theorem 3.7 provided that $\mathcal{B} - \widetilde{\mathcal{B}}$ is of trace class. Finally, already from the real case it is known that for this form of strong asymptotic it is necessary that $\mathcal{A} - \widetilde{\mathcal{A}}$ is compact, but it does not need to be of trace class. Indeed, a necessary and sufficient condition seems to be that $\mathcal{A} - \widetilde{\mathcal{A}}$ is compact, and that

$$\sum_{j=0}^{n-1} [r_j(z)q_j(z) - \widetilde{r}_j(z)\widetilde{q}_j(z)] = \operatorname{trace} \Pi_n[(zI - A)^{-1} - (zI - \widetilde{A})^{-1}]\Pi_n$$

converges for $n \to \infty$ uniformly in U (to g'/g). It would be very interesting to explore the connection to some complex counterpart of the Szegő condition.

4 Approximation of the resolvent and the Weyl function

The goal of this section is to investigate the question whether we may approximate the resolvent $(zI - A)^{-1}$ by means of inverses $(z\mathcal{I}_n - \mathcal{A}_n)^{-1}$ of finite sections of $z\mathcal{I} - \mathcal{A}$. This question is of interest, e.g., for discrete Sturm-Liouville problems on the semiaxis: for solving in ℓ^2 the equation $(zI - A)y = f$ for given $f \in \ell^2$ via a projection methods, one considers instead the finite-dimensional problems $(z\mathcal{I}_n - \mathcal{A}_n)y^{(n)} = E_n f$.

Another motivation comes from convergence questions for Padé approximation and continued fractions: With p_n, q_n as in (1.2), (1.4) we define the rational function

$$\pi_n(z) = \frac{p_n(z)}{q_n(z)} = (e_0, (z\mathcal{I}_n - \mathcal{A}_n)^{-1}e_0).$$

It is known [56] that $\pi_n(z)$ has the J–fraction expansion

$$\pi_n(z) = \frac{1|}{|z - b_0} + \frac{-a_0^2|}{|z - b_1} + \frac{-a_1^2|}{|z - b_2} + \frac{-a_2^2|}{|z - b_3} + \cdots + \frac{-a_{n-2}^2|}{|z - b_{n-1}}$$

being the nth convergent of the J–fraction (1.3) . In addition, the (formal) expansion at infinity of this J-fraction is known to coincide with (2.18), and one also shows that π_n is its nth Padé approximant (at infinity). The question is whether we may insure the convergence of $\pi_n(z) = (e_0, (z\mathcal{I}_n - \mathcal{A}_n)^{-1} e_0)$ to the Weyl function $\phi(z) = (e_0, (zI - A)^{-1} e_0)$.

This question has been studied by means of operators by many authors, see [56, Section 26] and [6, 12, 13, 17, 19] for bounded A and [14, 15] for bounded perturbations of possibly unbounded self-adjoint A. Our aim is to show that most of these results about the approximation of the Weyl function are in fact results about the approximation of the resolvent $(zI - A)^{-1}$ by $(z\mathcal{I}_n - \mathcal{A}_n)^{-1}$.

4.1 Approximation of the resolvent

Different kinds of resolvent convergence may be considered for $z \in \Omega(A)$, for instance *norm convergence*

$$\lim_{\substack{n\to\infty \\ n\in\Lambda}} ||(z\mathcal{I}_n - \mathcal{A}_n)^{-1} - E_n(zI - A)^{-1}E_n^*|| = 0, \tag{4.1}$$

strong resolvent convergence

$$\lim_{\substack{n\to\infty \\ n\in\Lambda}} E_n^*(z\mathcal{I}_n - \mathcal{A}_n)^{-1}E_n y = (zI - A)^{-1} y \quad \forall\, y \in \ell^2, \tag{4.2}$$

or *weak resolvent convergence*

$$\lim_{\substack{n\to\infty \\ n\in\Lambda}} (E_n y', (z\mathcal{I}_n - \mathcal{A}_n)^{-1}E_n y) = (y', (zI - A)^{-1} y) \quad \forall\, y, y' \in \ell^2. \tag{4.3}$$

The interested reader may easily check that (4.1) implies (4.2), and the latter implies (4.3). Notice also that (pointwise) convergence results for Padé approximation of the Weyl function are obtained by choosing in (4.3) the vectors $y = y' = e_0$. In all these forms of convergence we assume implicitly that $z\mathcal{I}_n - \mathcal{A}_n$ is invertible for (sufficiently large) $n \in \Lambda$. We also mention the related condition

$$\limsup_{\substack{n\to\infty \\ n\in\Lambda}} ||(z\mathcal{I}_n - \mathcal{A}_n)^{-1}|| =: C < \infty. \tag{4.4}$$

A Kantorovitch type theorem gives connections between properties (4.2) and (4.4). For complex (possibly unbounded) Jacobi matrices we have the following result.

Theorem 4.1 *Let A be a difference operator resulting from a complex Jacobi matrix, Λ some infinite set of integers, and $z \in \mathbb{C}$. The following assertions are equivalent:*

(*a*) $z \in \Omega(A)$, *and (4.2) holds.*

(*b*) $z \in \Omega(A)$, *and (4.3) holds.*

(*c*) $\mathcal{A}$ *is proper, and (4.4) holds.*

In addition, if property (c) holds for some $z = z_0$, then the limit relations (4.2), (4.3) take place uniformly for $|z - z_0| \leq 1/(2C)$.

Proof: Trivially, (b) follows from (a). Also, $\Omega(A) \neq \emptyset$ implies that $\mathcal{A}$ is proper by Theorem 2.6. In addition, (b) makes only sense if $z\mathcal{I}_n - \mathcal{A}_n$ is invertible for sufficiently large $n \in \Lambda$.

Furthermore, a sequence of weakly converging bounded linear operators is necessarily uniformly bounded, see, e.g., [28, Section III.3.1]. Thus (b) implies (c).

Suppose now that (c) holds. By possibly dropping some elements from Λ we may replace condition (4.4) by

$$\sup_{n\in\Lambda} ||(z\mathcal{I}_n - \mathcal{A}_n)^{-1}|| \leq C' := 3C/2 < \infty. \tag{4.5}$$

For any $y \in \mathcal{C}_0$, say, $y = \Pi_k y$, we find an index $n \in \Lambda$, $n > k$, with

$$||(zI - A)y|| = ||E_{k+1}(zI - A)\Pi_k y|| = ||(z\mathcal{I}_n - \mathcal{A}_n)E_n y|| \geq \frac{||E_n y||}{||(z\mathcal{I}_n - \mathcal{A}_n)^{-1}||} \geq \frac{||y||}{C'}.$$

As in the second part of the proof of Theorem 2.10 we obtain

$$\inf_{y\in\mathcal{D}(A)} \frac{||(zI - A)y||}{||y||} = \inf_{y\in\mathcal{C}_0} \frac{||(zI - A)y||}{||y||} \geq \frac{1}{C'} > 0.$$

Consequently, $\mathcal{N}(zI - A) = \{0\}$. Since $\mathcal{A}$ is proper, it follows from Lemma 2.4(a),(d) that $\mathcal{N}((zI - A)^*) = \{0\}$. Furthermore, by [28, Theorem IV.5.2], $\mathcal{R}(zI - A)$ is closed. Since its orthogonal complement is given by $\mathcal{N}((zI - A)^*)$, we may conclude that $\mathcal{R}(zI - A) = \ell^2$, and thus $z \in \Omega(A)$.

In order to show the second part of (a), let $y \in \ell^2 = \mathcal{R}(zI - A)$, and $x \in \mathcal{D}(A)$ with $(zI - A)x = y$. Let $\epsilon > 0$. By (2.2), we find $\tilde{x} \in \mathcal{C}_0$, $\tilde{y} = (zI - A)\tilde{x}$, such that

$$C'||y - \tilde{y}|| \leq \epsilon/3, \quad \text{and} \quad ||x - \tilde{x}|| \leq \epsilon/3.$$

Also, since $y \in \ell^2$ and $\tilde{x} \in \mathcal{C}_0$, we find an $N \geq 0$ such that

$$\Pi_n \tilde{x} = \tilde{x}, \quad \text{and} \quad C'||(I - \Pi_n)y|| \leq \epsilon/3, \quad n \geq N.$$

Recalling that $E_n E_n^* = \mathcal{I}_n$ and $E_n^* E_n = \Pi_n$, we obtain

$$\begin{aligned}
& ||E_n^*(z\mathcal{I}_n - \mathcal{A}_n)^{-1}E_n y - (zI - A)^{-1}y|| \\
\leq\; & ||E_n^*(z\mathcal{I}_n - \mathcal{A}_n)^{-1}E_n[y - E_n^*(z\mathcal{I}_n - \mathcal{A}_n)E_n\tilde{x}]|| \\
& + ||E_n^*(z\mathcal{I}_n - \mathcal{A}_n)^{-1}E_n E_n^*(z\mathcal{I}_n - \mathcal{A}_n)E_n\tilde{x} - x|| \\
\leq\; & C'||y - \Pi_n(zI - A)\Pi_n\tilde{x}|| + ||\Pi_n\tilde{x} - x|| \\
=\; & C'||y - \Pi_n(zI - A)\tilde{x}|| + ||\tilde{x} - x|| \\
\leq\; & C'(||(I - \Pi_n)y|| + ||\Pi_n(y - \tilde{y})||) + ||\tilde{x} - x|| \leq \epsilon
\end{aligned}$$

for all $n \geq N$, $n \in \Lambda$, and thus (4.2) holds.

It remains to show the last sentence. We first mention that if $z_0 \in \mathbb{C}$ verifies (4.5) then for any z with $|z - z_0| \leq \epsilon \leq 1/(2C)$ and for any $n \in \Lambda$ there holds

$$||(z\mathcal{I}_n - \mathcal{A}_n)^{-1}|| \leq ||(z_0\mathcal{I}_n - \mathcal{A}_n)^{-1}|| \cdot ||(\mathcal{I}_n + (z - z_0)(z_0\mathcal{I}_n - \mathcal{A}_n)^{-1})^{-1}|| \leq 4C' = 6C, \tag{4.6}$$

and

$$||(z\mathcal{I}_n - \mathcal{A}_n)^{-1} - (z_0\mathcal{I}_n - \mathcal{A}_n)^{-1}|| = |z - z_0|||(z\mathcal{I}_n - \mathcal{A}_n)^{-1}(z_0\mathcal{I}_n - \mathcal{A}_n)^{-1}|| \leq \epsilon \cdot 9C'^2.$$

The same estimates are obtained for the resolvent. Thus, given $\epsilon > 0$ and $y \in \ell^2$, we may cover $U := \{z \in \mathbb{C} : |z - z_0| < 1/(2C)\}$ by a finite number of closed disks of radius $\epsilon' \leq \epsilon/(9C'^2 \cdot ||y||)$ centred at $z_1, ..., z_K \in U$, and find an N such that

$$||E_n^*(z_k\mathcal{I}_n - \mathcal{A}_n)^{-1}E_n y - (z_k I - A)^{-1}y|| < \epsilon, \quad n \in \Lambda, \quad n \geq N, \quad k = 1, ..., K.$$

Then for each $z \in U$ we find a k with $|z - z_k| \le \epsilon'$, and

$$\begin{aligned}&||E_n^*(z\mathcal{I}_n - \mathcal{A}_n)^{-1}E_n y - (zI - A)^{-1}y||\\ &\le 2\epsilon' \cdot (9C^2) \cdot ||y|| + ||E_n^*(z_k\mathcal{I}_n - \mathcal{A}_n)^{-1}E_n y - (z_k I - A)^{-1}y|| \le 3\epsilon\end{aligned}$$

for all $n \ge N$, $n \in \Lambda$, showing that the convergence in (4.2) (and thus in (4.3)) takes place uniformly in U. □

Different variants of the Kantorovitch Theorem have been discussed before in the context of FOPs and Padé approximation, see [31, Theorem 4.1 and Theorem 4.2] or [15, Lemma 4 and Lemma 5]. Usually, the condition $z \in \Omega(A)$ is imposed for all equivalencies; then the proof simplifies considerably, and also applies to general proper matrices.

We see from Theorem 4.1 that the notion of weak and strong resolvent convergence are equivalent for proper complex Jacobi matrices. On the other hand, by (3.19),

$$||(z\mathcal{I}_n - \mathcal{A}_n)^{-1} - E_n(zI - A)^{-1}E_n^*|| = |\frac{r_n(z)}{q_n(z)}| \cdot \sum_{j=0}^{n-1} |q_j(z)|^2 = |\phi(z) - \pi_n(z)| \cdot \sum_{j=0}^{n-1} |q_j(z)|^2, \quad (4.7)$$

and at least for particular examples it is known that the right-hand side of (4.7) does not tend to zero. Thus we may not expect to have norm convergence.

If $\mathcal{A}$ is not proper then Theorem 4.1 does not give any information (notice that $\Omega(A) = \emptyset$ by Theorem 2.6(c)). However, at least in the indeterminated case we clearly understand what happens.

Theorem 4.2 *Let $\mathcal{A}$ be indeterminated. If Λ is some infinite set of integers and $\zeta \in \mathbb{C}$ such that*

$$\lim_{\substack{n\to\infty\\ n\in\Lambda}} (e_0, (\zeta\mathcal{I}_n - \mathcal{A}_n)^{-1}e_0) =: \pi, \quad (4.8)$$

then with the unique $\eta \in \mathbb{C} \cup \{\infty\}$ satisfying $\phi_{[\eta]}(\zeta) = \pi$ (see Theorem 2.11) there holds

$$\lim_{\substack{n\to\infty\\ n\in\Lambda}} ||(z\mathcal{I}_n - \mathcal{A}_n)^{-1} - E_n(zI - A_{[\eta]})^{-1}E_n^*|| = 0$$

uniformly on compact subsets of $\Omega(A_{[\eta]})$.

Proof: We will only show pointwise norm convergence for $z \in \Omega(A_{[\eta]})$, the extension to uniform convergence follows as in the proof of Theorem 4.1. First one shows as in (3.19) and (4.7) that

$$||(z\mathcal{I}_n - \mathcal{A}_n)^{-1} - E_n(zI - A_{[\eta]})^{-1}E_n^*|| = |\phi_{[\eta]}(z) - \pi_n(z)| \cdot \sum_{j=0}^{n-1} |q_j(z)|^2, \quad z \in \Omega(A_{[\eta]}).$$

Since $\mathcal{A}$ is indeterminated, the sum is bounded uniformly in n for all $z \in \mathbb{C}$, and $\phi_{[\eta]}(z) \neq \infty$. Therefore it remains only to show that $\pi_n(\zeta) \to \pi$ for $n \to \infty$, $n \in \Lambda$ implies $\pi_n(z) \to \phi_{[\eta]}(z)$

for $n \to \infty$, $n \in \Lambda$ and $z \in \mathbb{C}$. Here we follow [56, Proof of Theorem 23.2]: According to [56, Theorem 23.1 and equations (23.2),(23.6)], there exist polynomials $a_{j,n}$, $j = 1, 2, 3, 4$ with

$$\lim_{n\to\infty} a_{j,n}(z) = a_j(z), \quad j = 1, 2, 3, 4, \quad z \in \mathbb{C}, \tag{4.9}$$

$$a_{1,n}(z)a_{4,n}(z) - a_{2,n}(z)a_{3,n}(z) = 1, \quad n \geq 0, \quad z \in \mathbb{C}, \tag{4.10}$$

$$p_n(z) = p_n(0)a_{2,n}(z) - q_n(0)a_{1,n}(z), \quad q_n(z) = p_n(0)a_{4,n}(z) - q_n(0)a_{3,n}(z), \tag{4.11}$$

with $a_1, ..., a_4$ as in Theorem 2.11. Combining (4.10), (4.11) we get

$$p_n(0) = -p_n(\zeta)a_{3,n}(\zeta) + q_n(\zeta)a_{1,n}(\zeta), \quad q_n(0) = -p_n(\zeta)a_{4,n}(\zeta) + q_n(\zeta)a_{2,n}(\zeta),$$

and by assumption on $\pi_n(\zeta) = p_n(\zeta)/q_n(\zeta)$ we may conclude from (4.9) that

$$\lim_{\substack{n\to\infty \\ n\in\Lambda}} \pi_n(0) = \frac{a_1(\zeta) - \pi a_3(\zeta)}{a_2(\zeta) - \pi a_4(\zeta)}.$$

Here the right-hand side equals η by definition. Applying again (4.9), (4.11), we obtain for $z \in \mathbb{C}$ the desired relation

$$\lim_{\substack{n\to\infty \\ n\in\Lambda}} \pi_n(z) = \frac{a_1(z) - \eta a_2(z)}{a_3(z) - \eta a_4(z)} = \phi_{[\eta]}(z).$$

□

Theorem 4.2 implies that in the indeterminated case we obtain weak and strong resolvent convergence to $(zI - A_{[\eta]})^{-1}$. Since (4.8) follows from weak convergence, we may conclude that here all three notions of convergence are equivalent. Notice that (4.8) is equivalent to the convergence of a subsequence of Padé approximants at one point.

Let us return to the more interesting case of proper complex Jacobi matrices. In order to be able to exploit Theorem 4.1, we need to know whether there exist infinite sets Λ (possibly depending on z) satisfying (4.4). In the following Theorem we show that, under some additional assumptions, the existence can be insured.

Theorem 4.3 **(a)** *Suppose that the infinite sequence $(a_n)_{n\in\Lambda'}$ is bounded. Then $z \in \Omega(A)$ iff there exists an infinite set of integers Λ satisfying (4.4).*

(b) *Suppose that $(a_{n-1})_{n\in\Lambda'}$ is bounded, $\Lambda \subset \Lambda'$, and let $z \in \Omega$, where Ω is a connected component of $\Omega(A)$ which is not a subset of $\Gamma(A)$. Then (4.4) holds iff z is not an accumulation point of $\{$zeros of q_n: $n \in \Lambda\}$.*

(c) *Suppose that $(a_{n-1})_{n\in\Lambda}$ tends to zero. Then $z \in \Omega(A)$ iff (4.4) holds.*

(d) *Let $A, \widetilde{A}$ be two difference operators with compact $A - \widetilde{A}$, and $z \in \Omega(A) \cap \Omega(\widetilde{A})$. Then (4.4) for A implies (4.4) for $\widetilde{A}$.*

(e) *Relation (4.4) with $\Lambda = \{0, 1, 2, ...\}$ holds for $z \in \Omega(A) \setminus \Gamma_{ess}(A)$.*

It seems that the assertions of Theorem 4.3 have been unnoticed so far for general possibly unbounded complex Jacobi matrices. For bounded or compact perturbations of self-adjoint Jacobi matrices, results related to Theorem 4.3(e) may be found in [15, Sections 1 and 2].

Combining Theorem 4.3 with Theorem 4.1 (especially the last sentence) and using classical compactness arguments, we may get uniform counterparts of (4.1) and (4.4). Since these results play an important role for the convergence of Padé approximants, we state the result explicitly in

Corollary 4.4 *We have*

$$\limsup_{\substack{n\to\infty\\ n\in\Lambda}} \max_{z\in F} ||(z\mathcal{I}_n - \mathcal{A}_n)^{-1}|| < \infty$$

and

$$\limsup_{\substack{n\to\infty\\ n\in\Lambda}} \max_{z\in F} ||E_n^*(z\mathcal{I}_n - \mathcal{A}_n)^{-1}E_n y - (zI - A)^{-1}y|| = 0$$

for a compact set F and $y \in \ell^2$ provided that one of the following conditions is satisfied:

(a) $\Lambda = \{0, 1, 2, ...\}$ *and* $F \subset \Omega(A) \setminus \Gamma_{ess}(A)$.

(b) $(a_{n-1})_{n\in\Lambda}$ *tends to zero and* $F \subset \Omega(A)$.

(c) $(a_{n-1})_{n\in\Lambda}$ *is bounded,* $F \subset \Omega$, *with* $\Omega \not\subset \Gamma(A)$ *being some subdomain of* $\Omega(A)$, *and* F *does not contain accumulation points of zeros of* q_n, $n \in \Lambda$.

For the proof of Theorem 4.3(d),(e) we will need the following lemma which for bounded operators was already stated before by Magnus [31].

Lemma 4.5 (compare with [31, Theorem 4.4])
Let $\mathcal{B}$ be some infinite proper matrix, and write $B = [\mathcal{B}]_{\min}$. Furthermore, let $\widetilde{B}$ be an operator in ℓ^2, with $\mathcal{C}_0 \subset \mathcal{D}(\widetilde{B})$, $0 \in \Omega(B) \cap \Omega(\widetilde{B})$, and $B - \widetilde{B}$ being compact. Then for any infinite set of integers Λ we have the implication

$$\sup_{n\in\Lambda} ||(E_n B E_n^*)^{-1}|| = C' < \infty \quad \Longrightarrow \quad \limsup_{\substack{n\to\infty\\ n\in\Lambda}} ||(E_n \widetilde{B} E_n^*)^{-1}|| < \infty.$$

Proof: We claim that there exist N, C such that, for all $n \geq N$, $n \in \Lambda$, the system

$$(E_n \widetilde{B} E_n^*) x_n = y_n$$

admits a unique solution x_n for all $y_n \in \mathbb{C}^n$, with $||x_n|| \leq C \cdot ||y_n||$. Then the assertion follows. For proving this claim, we rewrite the system as

$$[\mathcal{I}_n + (E_n B E_n^*)^{-1}(E_n(\widetilde{B} - B)E_n^*]x_n = (E_n B E_n^*)^{-1} y_n$$

Recalling that $E_n E_n^* = \mathcal{I}_n$, $E_n^*\mathcal{I}_n = E_n^*$, $E_n^* E_n = \Pi_n$, the system takes the form

$$[I + B^{-1}(\widetilde{B} - B) + \Delta_n](E_n^* x_n) = E_n^*(E_n^* B E_n)^{-1} y_n \tag{4.12}$$

where

$$\begin{aligned}\Delta_n &= E_n^*(E_n B E_n^*)^{-1} E_n(\widetilde{B} - B) - B^{-1}(\widetilde{B} - B)\\ &= [E_n^*(E_n B E_n^*)^{-1} E_n - B^{-1}](I - \Pi_m)(\widetilde{B} - B) + [E_n^*(E_n B E_n^*)^{-1} E_n - B^{-1}]\Pi_m(\widetilde{B} - B)\end{aligned}$$

for every integer m. Here the expression in brackets is bounded in norm by $C' + ||B^{-1}||$. Since $(B - \widetilde{B})$ is compact, it is known that $||(I - \Pi_m)(\widetilde{B} - B)|| \to 0$ for $m \to \infty$. Hence we may find a m such that

$$||(I - \Pi_m)(\widetilde{B} - B)|| \leq \frac{1}{4||\widetilde{B}^{-1}B|| \cdot (C' + ||B^{-1}||)}.$$

Since $\mathcal{B}$ is proper, with $0 \in \Omega(B)$, one shows as in the proof of Theorem 4.1 that

$$\lim_{\substack{n\to\infty \\ n\in\Lambda}} E_n^*(E_n B E_n^*)^{-1} E_n y = B^{-1} y, \quad y \in \ell^2.$$

In particular, we may find for $\epsilon := 1/(4\sqrt{m}||\widetilde{B}^{-1}B|| \cdot ||E_m(\widetilde{B} - B)||)$ an $N \geq m$ such that

$$||[E_n^*(E_n B E_n^*)^{-1} E_n - B^{-1}]e_j|| \leq \epsilon, \quad j = 0, ..., m-1, \quad n \geq N, \quad n \in \Lambda.$$

implying that $||[E_n^*(E_n B E_n^*)^{-1} E_n - B^{-1}]E_m^*|| \leq \sqrt{m} \cdot \epsilon$. Collecting the individual terms, we may conclude that $||\Delta_n|| \leq 1/(2 \cdot ||\widetilde{B}^{-1}B||)$. In particular, $B^{-1}\widetilde{B} + \Delta_n$ is invertible, with inverse having a norm bounded by $2||\widetilde{B}^{-1}B||$. Thus the system (4.12) has a unique solution for $n \geq N$, $n \in \Lambda$, with

$$||x_n|| \leq 2||\widetilde{B}^{-1}B|| \cdot ||E_n^*(E_n^* B E_n)^{-1}|| \cdot ||y_n|| \leq 2||\widetilde{B}^{-1}B|| \cdot C' \cdot ||y_n||,$$

as claimed above. □

Proof of Theorem 4.3: (a) By Example 2.7, $\mathcal{A}$ is proper. Thus (4.4) implies that $z \in \Omega$. In order to show the converse, let $z \in \Omega(A)$. According to (4.7), it will be sufficient to give a suitable error estimate for the error of Padé approximation. For $n \in \Lambda'$, define $\epsilon_n = 1$ if $|u_n(z)| \leq 1$, and $\epsilon_n = 0$ otherwise. Furthermore, let $\Lambda = \{n + \epsilon_n : n \in \Lambda'\}$. Then we get for $n \in \Lambda'$

$$|a_n|^{2\epsilon_n} |q_{n+\epsilon_n}(z)|^2 \geq \frac{1}{2}(|q_n(z)|^2 + |a_n q_{n+1}(z)|^2)$$

by construction of ϵ_n, and trivially

$$|a_n|^{2\epsilon_n} |r_{n+\epsilon_n}(z)|^2 \leq (|r_n(z)|^2 + |a_n r_{n+1}(z)|^2).$$

Using the left-hand estimate of (2.22), we may conclude that

$$\begin{aligned}
&|\frac{r_{n+\epsilon_n}(z)}{q_{n+\epsilon_n}(z)}| \cdot \sum_{j=0}^{n} |q_j(z)|^2 \leq \sqrt{2\frac{|r_n(z)|^2 + |a_n r_{n+1}(z)|^2}{|q_n(z)|^2 + |a_n q_{n+1}(z)|^2}} \cdot \sum_{j=0}^{n} |q_j(z)|^2 \\
&\leq \sqrt{2} \cdot (|r_n(z)|^2 + |a_n r_{n+1}(z)|^2) \cdot \sum_{j=0}^{n} |q_j(z)|^2 \\
&= \sqrt{2} \cdot (||\Pi_{n+1}(zI - A)e_n||^2 + |a_n|^2 ||\Pi_{n+1}(zI - A)e_{n+1}||^2)
\end{aligned}$$

where in the last equality we have applied (2.19). Notice that the term on the right-hand side is bounded by $\sqrt{2}(1 + |a_n|^2)||(zI - A)^{-1}||^2$. Hence, using (4.7) we obtain

$$\begin{aligned}
&||(z\mathcal{I}_{n+\epsilon_n} - \mathcal{A}_{n+\epsilon_n})^{-1}|| \\
&\leq ||E_n(zI - A)^{-1}E_n^*|| + ||(z\mathcal{I}_{n+\epsilon_n} - \mathcal{A}_{n+\epsilon_n})^{-1} - E_n(zI - A)^{-1}E_n^*|| \\
&\leq ||(zI - A)^{-1}|| + \sqrt{2}(1 + |a_n|^2)||(zI - A)^{-1}||^2,
\end{aligned}$$

being bounded in n by assumption on (a_n). Thus (4.4) holds.

(b) We first show that (4.4) implies that z may not be an accumulation point of zeros of q_n, $n \in \Lambda$. In fact, as in (4.6) we may find some $N > 0$ such that

$$||(\zeta\mathcal{I}_n - \mathcal{A}_n)^{-1}|| \leq 6C, \quad n \in \Lambda, \quad n \geq N, \quad |z - \zeta| < \frac{1}{2C},$$

showing that eigenvalues of $\mathcal{A}_n$ (i.e., zeros of q_n) have to stay away from z for sufficiently large $n \in \Lambda$. Suppose now that $\Lambda \subset \Lambda'$ is as described in part (b). Then there exists an open neighborhood $U \subset \Omega$ of z such that u_{n-1} is analytic in U for $n \in \Lambda$ (at least after dropping a finite number of elements of Λ). Also, from Theorem 3.3(c) we know that $(u_{n-1})_{n\in\Lambda}$ is a normal family of meromorphic functions in Ω, with any partial limit being different from the constant ∞ by Theorem 3.3(a). It follows from [17, Lemma 2.4(d)] that then $(u_{n-1})_{n\in\Lambda}$ is bounded uniformly on compact subsets of U, in particular,

$$d := \sup_{n\in\Lambda} |u_{n-1}(z)| < \infty.$$

Consequently,

$$|a_{n-1}q_n(z)|^2 = \frac{|q_{n-1}(z)|^2 + |a_{n-1}q_n(z)|^2}{|u_{n-1}(z)|^2 + 1} \geq \frac{|q_{n-1}(z)|^2 + |a_{n-1}q_n(z)|^2}{d^2 + 1}.$$

As in the proof of part (a) (with $\epsilon_n = 1$ and n replaced by $n - 1$) we may conclude that

$$||(z\mathcal{I}_n - \mathcal{A}_n)^{-1}|| \leq ||(zI - A)^{-1}|| + \sqrt{1 + d^2}(1 + |a_{n-1}|^2)||(zI - A)^{-1}||^2,$$

and thus (4.4) is true.

(c) As in part (a), it is sufficient to show that $z \in \Omega(A)$ implies (4.4). Denote by $\mathcal{B}^{[n]}$ the infinite matrix obtained from $\mathcal{A}$ by replacing a_{n-1} by 0, and write $B^{[n]} := [\mathcal{B}^{[n]}]_{\min}$. Let $z \in \Omega(A)$. By assumption on $(a_{n-1})_{n\in\Lambda}$, we find an $N > 0$ such that

$$||A - B^{[n]}|| \leq \frac{1}{2||(zI - A)^{-1}||}, \quad n \in \Lambda, \quad n \geq N.$$

Thus $z \in \Omega(B^{[n]})$ and $||(zI - B^{[n]})^{-1}|| \leq 2||(zI - A)^{-1}||$. On the other hand, $\mathcal{B}^{[n]}$ is block diagonal, with $E_n(zI - B^{[n]})^{-1}E_n^* = (z\mathcal{I}_n - \mathcal{A}_n)^{-1}$. Thus $||(z\mathcal{I}_n - \mathcal{A}_n)^{-1}|| \leq 2||(zI - A)^{-1}||$ for all $n \in \Lambda$, $n \geq N$, implying (4.4).

(d) This part follows immediately from Lemma 4.5.

(e) The complex Jacobi matrix $\mathcal{A}$ is proper by Theorem 2.6(c), and one easily deduces that the same is true for all associated Jacobi matrices $\mathcal{A}^{(k)}$. By Definition of $\Gamma_{ess}(A)$, there exist a $k > 0$ with $z \in \mathbb{C} \setminus \Gamma(A^{(k)})$, the latter being a subset of $\Omega(A^{(k)})$ by Theorem 3.5(c). From the proof of Theorem 3.3(a) we know that

$$||(z\mathcal{I}_n - \mathcal{A}_n^{(k)})^{-1}|| \leq \frac{1}{\text{dist}(z, \Gamma(A^{(k)}))} < \infty, \quad n \geq 0.$$

Let $\mathcal{B}$ be obtained from $\mathcal{A}$ by keeping the elements from $\mathcal{A}^{(k)}$, putting $\zeta \neq z$ on the first k diagonal positions, and zero else. One easily verifies that then

$$||(z\mathcal{I}_n - \mathcal{B}_n)^{-1}|| \leq \frac{1}{\text{dist}(z, \{\zeta\} \cup \Gamma(A^{(k)}))} < \infty, \quad n \geq 0.$$

Writing $B = [\mathcal{B}]_{\min}$, we trivially have $z \in \Omega(B)$, and $A - B$ is compact (and even of finite rank). Thus the assertion follows from Lemma 4.5. $\square$

4.2 Some consequences for the approximation of the Weyl function

We summarize some consequences of the preceding section for the convergence of Padé approximants $\pi_n(z) = (e_0, (z\mathcal{I}_n - \mathcal{A}_n)^{-1} e_0)$ (i.e., Weyl functions of the finite sections $\mathcal{A}_n$) to the Weyl function $\phi(z) = (e_0, (zI - A)^{-1} e_0)$ in the following statement which is an immediate consequence of Corollary 4.4.

Corollary 4.6 *The subseqence $(\pi_n)_{n\in\Lambda}$ converges to the Weyl function ϕ uniformly in the compact set F provided that one of the following conditions is satisfied:*

(a) $\Lambda = \{0, 1, 2, ...\}$ *and* $F \subset \Omega(A) \setminus \Gamma_{ess}(A)$.

(b) $(a_{n-1})_{n\in\Lambda}$ *tends to zero and* $F \subset \Omega(A)$.

(c) $(a_{n-1})_{n\in\Lambda}$ *is bounded,* $F \subset \Omega$, *with* $\Omega \not\subset \Gamma(A)$ *being some subdomain of* $\Omega(A)$, *and F does not contain accumulation points of zeros of* q_n, $n \in \Lambda$.

For convergence outside $\Gamma(A)$ (which is included in Corollary 4.6(a)) we refer the reader to [56, Theorem 26.2 and Theorem 26.3] and [19, Theorem 3.10] in case of bounded $\mathcal{A}$, and [56, Theorem 25.4] in case of determined $\mathcal{A}$. For the special case of a compact perturbation of a self-adjoint Jacobi operator, Corollary 4.6(a) may be found in [15, Corollary 6] and [14, Theorem 2]. The latter assertion applies a different technique of proof, and contains additional information about the number of poles at isolated points of $\Omega(A) \setminus \Gamma_{ess}(A)$. Assertion [15, Theorem 2] on bounded perturbations of a self-adjoint Jacobi operator is contained in Corollary 4.6(a).

For bounded complex Jacobi matrices, Corollary 4.6(b) may be found in [17, Corollary 4.2]. As shown in [17, Corollary 5.6], this statement can be used to prove the Baker-Gammel-Wills conjecture for Weyl functions of operators with countable compact spectrum. Corollary 4.6(c) for bounded complex Jacobi matrices was established in [17, Theorem 4.1] (containing additional results on the rate on convergence in terms of the functions $g_{\inf}$ and g_{sup} of Theorem 3.1). Here as set Ω we may choose the unbounded connected component $\Omega_0(A)$ of $\Omega(A)$. Notice that a connected component Ω of $\Omega(A)$ with $\Omega \not\subset \Gamma(A)$ is unbounded also for unbounded $\mathcal{A}$. Thus Corollary 4.6(c) has to be compared with the result of Gonchar [26] mentioned in Section 3.3.

In their work on bounded tridiagonal infinite matrices, Aptekarev, Kaliaguine and Van Assche observed [6, Theorem 2] that

$$\liminf_{n\to\infty} |\pi_n(z) - \phi(z)| = 0, \quad z \in \Omega(A). \tag{4.13}$$

Notice that this relation also holds for unbounded $\mathcal{A}$ since otherwise a nontrivial multiple of the sequence $(|q_n(z)|)_{n\geq 0} \notin \ell^2$ would minorize the sequence $(|r_n(z)|)_{n\geq 0} = (|\phi(z) - \pi_n(z)| \cdot |q_n(z)|)_{n\geq 0} \in \ell^2$. If a subsequence of (a_n) is bounded, then by combining Theorem 4.3(a) with Theorem 4.1 we see that relation (4.13) even holds uniformly in some neighborhood of any $z \in \Omega(A)$. This was observed before in [17, Theorem 4.4] for bounded complex and in [3, Corollaries 3 and 4] for bounded real Jacobi matrices.

In this context, let us discuss the related question whether (pointwise) convergence of (a subsequence of) Padé approximants at some z implies that $z \in \Omega(A)$. Clearly, the answer is no, see for instance the counterexamples presented in the last paragraph of [6]. If we replace however Padé convergence by weak (or strong) resolvent convergence, and we limit ourselves to sequences (a_n) containing a bounded subsequence, then the answer is yes: we have $z \in \Omega(A)$ iff there exists an infinite set Λ of indices such that

$$\lim_{\substack{n\to\infty \\ n\in\Lambda}} (E_n y', (z\mathcal{I}_n - \mathcal{A}_n)^{-1} E_n y) \quad \text{exists } \forall\, y, y' \in \ell^2. \tag{4.14}$$

Indeed, if $z \in \Omega(A)$ then we may use Theorem 4.3(a) and Theorem 4.1 to establish (4.14). Conversely, (4.14) implies (4.4) by [28, Problem V.1.6], and thus $z \in \Omega(A)$ by Theorem 4.3(a).

We terminate this section with a generalization of [17, Theorem 3.1] where convergence in (logarithmic) capacity of (π_n) is established for bounded $\mathcal{A}$ on compact subsets of the unbounded connected component of the resolvent set.

Theorem 4.7 *Let $(a_n)_{n\in\Lambda}$ be bounded, and denote by Ω a connected component of $\Omega(A)$. Then there exist $\epsilon_n \in \{0, 1\}$ such that, for each compact $F \subset \Omega$ and for each $\epsilon > 0$, we have*

$$\lim_{\substack{n\to\infty \\ n\in\Lambda}} \text{cap}\,\{z \in F : |\phi(z) - \pi_{n+\epsilon_n}(z)| \geq \epsilon\} = 0.$$

If in addition $\Omega \not\subset \Gamma(A)$ then we may choose $\epsilon_n = 1$ for all $n \in \Lambda$.

Proof: From Theorem 3.3(c) we know that $(u_n)_{n\in\Lambda}$ is a normal family of meromorphic functions in Ω. If in addition $\Omega \not\subset \Gamma(A)$, then any partial limit is different from the constant ∞ by Theorem 3.3(a), and we put $v_n = u_n$, $\epsilon_n = 1$. Otherwise, let $\zeta \in \Omega$. If $|u_n(\zeta)| \leq 1$ then again $v_n = u_n$, $\epsilon_n = 1$, and otherwise $v_n = 1/u_n$, $\epsilon_n = 0$. In this way we have constructed a normal family $(v_n)_{n\in\Lambda}$ of meromorphic functions in Ω, with any partial limit being different from the constant ∞.

Let $F, F' \subset \Omega$ be compact, the interior of F' containing F. Let ω_n, $n \in \Lambda$ be a monic polynomial of minimal degree such that $\omega_n v_n$ is analytic in F'. From the proof of Theorem 3.4(c) we know that the degree ν_n of ω_n is bounded by some $\nu(F')$ uniformly for $n \in \Lambda$. We claim that

$$\sup_{n\in\Lambda} C_n =: C(F) < \infty, \quad C_n := \max_{z\in F} |\omega_n(z) \cdot v_n(z)|. \tag{4.15}$$

Otherwise, there would be integers $n_k \in \Lambda$ such that $C_{n_k} > k$. By normality, we may assume without loss of generality that $(v_{n_k})_k$ converges to some meromorphic v uniformly in F'. Since $v \not\equiv \infty$, we find some open set D, $F \subset D \subset F'$, having a finite number of open components, and $v(z) \neq \infty$ for $z \in \partial D$. By uniform convergence on ∂D it follows that

$$\limsup_{k\to\infty} \max_{z\in\partial D} |v_{n_k}(z)| < \infty.$$

Since D is bounded and the degrees of the ω_n are uniformly bounded, we may conclude that the above relation remains true after multiplication of v_{n_k} with ω_{n_k}. Using the maximum principle for analytic functions we obtain a bound for $\omega_{n_k} \cdot v_{n_k}$ on F uniformly in k, in contradiction to the construction of n_k. Thus (4.15) holds.

From (4.15) we conclude that, for any $d > \max\{2, 2C(F)\}$ and $n \in \Lambda$,

$$\begin{aligned} &\mathit{cap}\,\{z \in F : \sqrt{1 + |v_n(z)|^2} > d\} \leq \mathit{cap}\,\{z \in F : |v_n(z)| > d/2\} \\ &\leq \mathit{cap}\,\{z \in F : |\omega_n(z)| \leq \frac{2C(F)}{d}\} = (\frac{2C(F)}{d})^{1/\nu_n} \leq (\frac{2C(F)}{d})^{1/\nu(F')}. \end{aligned}$$

Notice that by construction (compare with the proof of Theorem 4.3(a))

$$\phi(z) - \pi_{n+\epsilon_n}(z) = \frac{a_n^{\epsilon_n} r_{n+\epsilon_n}(z) \cdot \sqrt{1+|v_n(z)|^2}}{\sqrt{|q_n(z)|^2 + |a_n q_{n+1}(z)|^2}} \leq \sqrt{1+|v_n(z)|^2} \cdot [|r_n(z)|^2 + |a_n r_{n+1}(z)|^2|].$$

Since the term in brackets tends to zero uniformly in F by (2.19), we obtain the claimed convergence by combining the last two formulas. □

Combining the reasoning of the proofs of Theorem 4.3(a) and Theorem 4.7, we may also show that with $\Omega, \Lambda, \epsilon_n$ as in Theorem 4.7 there holds for any compact $F \subset \Omega$

$$\lim_{\epsilon \to 0} cap \left(\left\{ z \in F : \limsup_{\substack{n\to\infty \\ n \in \Lambda}} ||(z\mathcal{I}_{n+\epsilon_n} - \mathcal{A}_{n+\epsilon_n})^{-1}|| > \frac{1}{\epsilon} \right\} \right) = 0.$$

Thus our result on convergence in capacity of Padé approximants is again connected to a type of strong resolvent convergence in capacity.

In [45], Stahl suggested to replace in the Baker-Gammel-Wills conjecture [10] locally uniform convergence of a subsequence by convergence in capacity of a subsequence. Theorem 4.7 confirms (under assumptions on the regularity of the underlying function and assumptions on some of the coefficients of its J-fraction expansion) that this is true in the resolvent set. Of course, this open set does not need to contain the maximal disk of analyticity of the Weyl function, but it might be helpful in investigating the above conjecture for special classes of functions. We refer the reader to Baker's survey [9] for further recent developments in convergence questions for Padé approximation.

4.3 An application to asymptotically periodic Jacobi matrices

A complex Jacobi–matrix $\mathcal{A}$ is called m–periodic if $a_{jm+k} = a_k, b_{jm+k} = b_k$, $k = 0, 1, ..., m-1$, $j \geq 0$, and $\widetilde{\mathcal{A}}$ is called *asymptotically periodic* if it is a compact perturbation of a m–periodic matrix, i.e.,

$$\lim_{j\to\infty} \widetilde{a}_{jm+k} = a_k, \quad \lim_{j\to\infty} \widetilde{b}_{jm+k} = b_k, \quad k = 0, 1, ..., m-1.$$

Real periodic and asymptotically periodic Jacobi matrices have been studied by a number of authors, see, e.g., [24, 22, 32]. Complex perturbations of real periodic Jacobi matrices are investigated in [12, 13], and complex (asymptotically) periodic Jacobi matrices in [19, Sections 2.2 and 2.3] and [18, Example 3.6]

It is well–known (see, e.g., [19, Section 2.2]) that here the sequences $(p_n(z))_{n\geq -1}$ and $(q_n(z))_{n\geq -1}$ verify the recurrence relation[13]

$$y_{(j+1)m+k} = h(z) \cdot y_{jm+k} - y_{(j-1)m+k}, \quad j \geq 0, \quad k \geq -1 \tag{4.16}$$

with some polynomial h for which we have several representations

$$h(z) = \frac{q_{2m-1}(z)}{q_{m-1}(z)} = \frac{p_{2m}(z)}{p_m(z)} = q_m(z) - a_{m-1}p_{m-1}(z).$$

[13]Here we need to put $a_{-1} = a_{m-1}$, and thus $1 = -a_{m-1}p_{-1}(z) = a_{m-1}r_{-1}(z)$. This slight modification does not change the other elements of the sequences $(p_n(z))_{n\geq -1}$ or $(r_n(z))_{n\geq -1}$.

In [19, Section 2.3], the authors show (see also [18, Example 3.6]) that $\sigma_{ess}(A) = \{z \in \mathbb{C} : h(z) \in [-2, 2]\}$, which by [19, Lemma 2.5] has empty interior and connected complement. The Weyl function of $\mathcal{A}$ is an algebraic function, meromorphic (and single-valued) in $\mathbb{C} \setminus \sigma_{ess}(A)$, with possible poles at the zeros of q_{m-1} [19, Section 2.2], and $\sigma(A)$ is just the extremal set of Stahl [46], i.e., the set of minimal capacity outside of which the Weyl function has a single-valued analytic continuation from infinity [19, Remark 2.9].

Let us show here that we may localize the spurious zeros of the FOPs associated to $\mathcal{A}$ (and to $\widetilde{\mathcal{A}}$). First, using (1.2) and (2.20) one easily verifies the well-known fact that

$$q_n^{(k+1)}(z) := a_k(q_{n+k+1}(z)r_k(z) - r_{n+k+1}(z)q_k(z)) \tag{4.17}$$

is the nth FOP of the associated Jacobi matrix $\mathcal{A}^{(k+1)}$. For $z \notin \sigma_{ess}(A)$, the equation $y^2 = h(z)y - 1$ has one solution $w(z)$ of modulus $|w(z)| < 1$, and the second solution $1/w(z)$. From (4.16), (3.7) we may conclude that there exist (algebraic) functions $\alpha_k, \beta_k, \gamma_k$ such that

$$r_{jm+k}(z) = \alpha_k(z) \cdot w(z)^j, \quad q_{jm+k}(z) = \beta_k(z) \cdot w(z)^j + \gamma_k(z) \cdot w(z)^{-j} \tag{4.18}$$

for all $k \geq -1$, $j \geq 0$ and $z \in \Omega(A)$. Injecting this information in (2.20) we obtain

$$a_k(\gamma_{k+1}(z)\alpha_k(z) - \gamma_k(z)\alpha_{k+1}(z)) = 1, \tag{4.19}$$

showing that $|\gamma_k(z)| + |\gamma_{k+1}(z)| \neq 0$ for all $z \in \Omega(A)$. We may deduce that

$$\lim_{j\to\infty} \chi\Big(\frac{q_{jm+k}(z)}{a_{jm+k}q_{jm+k+1}(z)}, \frac{\gamma_k(z)}{a_k\gamma_{k+1}(z)}\Big) = 0, \quad k = 0, 1, ..., m-1, \quad z \in \Omega(A). \tag{4.20}$$

Also, by periodicity, $q_n^{(k)}(z) = q_n^{(k+m)}(z)$, and by combining (4.18) with (4.17) we may conclude that

$$q_{m-1}^{(k+1)}(z) = a_k[w(z)^{-1} - w(z)]\alpha_k(z)\gamma_k(z). \tag{4.21}$$

From (4.20) and (4.21) we see that spurious zeros of $(q_{jm+k})_{j\geq 0}$ accumulating in $\zeta \in \Omega(A)$ verify $\gamma_k(\zeta) = 0$ and thus $q_{m-1}^{(k+1)}(\zeta) = 0$.

Combining this finding with Theorem 3.6 and Corollary 4.6(c), the following statement is obtained

Corollary 4.8 *Let $\widetilde{\mathcal{A}}$ be an asymptotically periodic complex Jacobi matrix, denote by $\mathcal{A}$ the corresponding m-periodic Jacobi matrix, and let $k \in \{0, ..., m-1\}$. Then for each compact subset F of $\Omega(A) \cap \Omega(\widetilde{A})$ which does not contain zeros of $q_{m-1}^{(k+1)}$ there exists an $J = J(F)$ such that $\widetilde{q}_{mj+k}$ has no zeros in F for $j \geq J$, and*

$$\lim_{j\to\infty} \max_{z\in F} |\widetilde{\phi}(z) - \widetilde{\pi}_{mj+k}(z)| = 0.$$

Notice that pointwise convergence for asymptotically periodic complex Jacobi matrices was already obtained in [19, Theorem 2.11]. If $\mathcal{A}$ is real then clearly $\sigma_{ess}(A)$ consists of at most m real intervals. Barrios, López, and Torrano [12, 13] showed that then the zeros of all $q_{m-1}^{(k+1)}$ lie in the convex hull $\mathcal{S}$ of $\sigma_{ess}(A)$, and obtained uniform convergence of $(\widetilde{\pi}_n)_{n\geq 0}$ on compact subsets of $\mathbb{C} \setminus \mathcal{S}$.

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