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CMV matrices: Five years after ☆

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Abstract

CMV matrices are the unitary analog of Jacobi matrices; we review their general theory.

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1. Introduction

> *The Arnold Principle*: If a notion bears a personal name, then this name is not the name of the inventor.
>
> *The Berry Principle*: The Arnold Principle is applicable to itself. *V.I. Arnold*, *On Teaching Mathematics*, 1997 [8] (Arnold says that Berry formulated these principles.)

In 1848, Jacobi [45] initiated the study of quadratic forms $J(x_1, \ldots, x_n) = \sum_{k=1}^{n} b_k x_k^2 + 2\sum_{k=1}^{n-1} a_k x_k x_{k+1}$, that is, essentially $n \times n$ matrices of the form

$$J = \begin{pmatrix} b_1 & a_1 & 0 & \ldots & 0 \\ a_1 & b_2 & a_2 & \ldots & 0 \\ 0 & a_2 & b_3 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \ldots & \ldots & a_{n-1} & b_n \end{pmatrix} \tag{1.1}$$

and found that the eigenvalues of J were the zeros of the denominator of the continued fraction

$$\cfrac{1}{b_1 - z - \cfrac{a_1^2}{b_2 - z - \cfrac{a_2^2}{\cdots}}}. \tag{1.2}$$

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In the era of the birth of the spectral theorem, Toeplitz [79], Hellinger–Toeplitz [44], and especially Stone [75] realized that Jacobi matrices were universal models of self-adjoint operators, A, with a cyclic vector, φ_0.

To avoid technicalities, consider the case where A is bounded, and suppose initially that $\mathscr{H}$ is infinite-dimensional. By cyclicity, $\{A^k\varphi_0\}_{k=0}^\infty$ are linearly independent, so by applying Gram–Schmidt to $\varphi_0, A\varphi_0, A^2\varphi_0, \dots,$ we get polynomials $p_j(A)$ of degree exactly j with positive leading coefficients so that

$$\varphi_j = p_j(A)\varphi_0 \tag{1.3}$$

are an orthonormal basis for $\mathscr{H}$. By construction,

$$\varphi_j \perp \varphi_0, A\varphi_0, \dots, A^{j-1}\varphi_0$$

so

$$\langle \varphi_j, A\varphi_k\rangle = 0, \quad j \geqslant k+2. \tag{1.4}$$

Because A is self-adjoint, we see $\langle \varphi_j, A\varphi_k\rangle = 0$ also if $j \leqslant k-2$. Thus, the matrix $\langle \varphi_j, A\varphi_k\rangle$ has exactly form (1.1) where $a_j > 0$ (since $p_j(A)$ has leading positive coefficient).

Put differently, for all A, φ_0, there is a unitary $U : \mathscr{H} \to \ell^2$ (given by Fourier components in the φ_j basis), so UAU^{-1} has the form J and $\varphi_0 = (1, 0, 0, \dots)^{\mathrm{t}}$. The Jacobi parameters, $\{a_n, b_n\}_{n=1}^\infty$, are intrinsic, which shows there is exactly one J (with $\varphi_0 = (1, 0, 0, \dots)^{\mathrm{t}}$) in the unitary equivalence class of (A, φ_0).

There is, of course, another way of describing unitary invariants for (A, φ_0): the spectral measure $\mathrm{d}\mu$ defined by

$$\int x^n \,\mathrm{d}\mu(x) = \langle \varphi_0, A^n\varphi_0\rangle. \tag{1.5}$$

There is a direct link from $\mathrm{d}\mu$ to the Jacobi parameters: the $p_j(x)$ are orthonormal polynomials associated to $\mathrm{d}\mu$, and the Jacobi parameters are associated to the three-term recursion relation obeyed by the p's:

$$xp_j(x) = a_{j+1}p_{j+1} + b_{j+1}p_j(x) + a_j p_{j-1}(x) \tag{1.6}$$

(where $p_{-1} \equiv 0$).

Here we are interested in the analog of these structures for unitary matrices. We begin by remarking that for a general normal operator, N, the right form of cyclicity is that $\{N^k(N^*)^\ell\varphi_0\}_{k,\ell=0}^\infty$ is total. Since $A = A^*$, only $\{A^k\varphi_0\}_{k=0}^\infty$ enters. Since $U^* = U^{-1}$, for unitaries $U^k(U^*)^\ell = U^{k-\ell}$ and the right notion of cyclicity is that $\{U^k\varphi_0\}_{k=-\infty}^\infty$ is total.

Some parts of the above fourfold equivalence:

(1) unitary equivalence classes of (A, φ_0);
(2) spectral measures, that is, probability measures $\mathrm{d}\mu$ on $\mathbb{R}$ with bounded support and infinite support;
(3) Jacobi parameters;
(4) Jacobi matrices

are immediate for the unitary case. Namely, (1) $\Leftrightarrow$ (2) holds since there is a spectral theorem for unitaries, and so, a one–one correspondence between unitary equivalence classes of (U, φ_0) on infinite-dimensional spaces and probability measures on $\partial\mathbb{D}$ ($\mathbb{D} = \{z \mid |z| < 1\}$) with infinite support.

More subtle is the analog of Jacobi parameters. Starting from such a probability measure on $\partial\mathbb{D}$, one can form the monic orthogonal polynomials $\Phi_n(z)$ and find (see [77]; see also [69, Section 1.5]) $\{\alpha_n\}_{n=0}^\infty \in \mathbb{D}^\infty$, so

$$z\Phi_n(z) = \Phi_{n+1}(z) + \bar{\alpha}_n z^n\, \overline{\Phi_n(1/\bar{z})}. \tag{1.7}$$

While Verblunsky [81] defined the α_n in a different (albeit equivalent) way, he proved a theorem (called Verblusnky's theorem in [69]; see also [68]) that says this map $\mathrm{d}\mu \to \{\alpha_n\}_{n=0}^\infty$ is one–one and onto all of $\mathbb{D}^\infty$, so (1)–(3) for the unitary case have been well understood for 65 years.

Surprisingly, (4) (i.e., the canonical matrix form for unitaries) is of much more recent vintage. The key paper in [12] was submitted in April 2001—so we are witnessing five years of study in the area—it is reviewing these developments that is the main scope of this review article. Spectral theory of differential and difference operators has been an enduring theme of Des Evans' research and I am pleased to dedicate this review to him.

There is an "obvious" matrix to try, namely, $\mathscr{G}_{k\ell} = \langle \varphi_k, z\varphi_\ell \rangle$ with $\varphi_k = \Phi_k/\|\Phi_k\|$ the orthonormal polynomials. This GGT matrix (as it is named in [69]; see Section 10) has two defects. First, $\{\varphi_k\}_{k=0}^{\infty}$ is a basis if and only if $\sum_{n=0}^{\infty} |\alpha_n|^2 = \infty$, and if it is not, $\mathscr{G}_{k\ell}$ is not unitary and is not conjugate to multiplication by z (in that case, one can look at the minimal dilation of $\mathscr{G}$, which is discussed in [15,69]). Second, it obeys (1.4), but in general, $\langle \varphi_j, U^* \varphi_k \rangle \neq 0$ for all $j \geqslant k+1$, that is, $\mathscr{G}$ is not of finite width measured from the diagonal. CMV [12] has the following critical ideas:

(a) The basis χ_k obtained by orthonormalizing $1, z, z^{-1}, z^2, z^{-2}, \ldots$ can be written in terms of $\varphi_\ell(z)$, $\overline{\varphi_\ell(1/\bar{z})}$, and powers of z.
(b) The matrix $\mathscr{C}_{k\ell} = \langle \chi_k, z\chi_\ell \rangle$ is unitary and five-diagonal.
(c) $\mathscr{C}$ can be factorized into $\mathscr{C} = \mathscr{L}\mathscr{M}$ where $\mathscr{L}$ is a direct sum of 2×2 unitary matrices and $\mathscr{M}$ the direct sum of a single 1×1 and 2×2 matrices.

It turns out that these key ideas appeared about 10 years earlier in the numeric matrix literature (still, of course, much later than the 1930's resolution of (1)–(3)). Intimately related to this history is what we will call the AGR factorization in Section 11—the ability to write $\mathscr{G}$ in the case of $n \times n$ matrices as a product $\widetilde{\Theta}_0 \cdots \widetilde{\Theta}_{n-1} \widetilde{\widetilde{\Theta}}_{n-1}$ of matrices with a single 2×2 block placed in **1** and a finite matrix which is diagonal, differing from **1** in a single place (see Section 11 for details).

In 1986, Ammar et al. [5] found the AGR factorization for orthogonal matrices—here the α_j are real and the $\Theta(\alpha_j)$ are reflections, so the AGR factorization can be viewed as an iteration of a Householder algorithm. In this paper, they also had a proof of the $\mathscr{L}\mathscr{M}$ factorization for this case. This proof (a variant of which appears in Section 10), which works in general to go from the AGR factorization of the GGT matrix to an $\mathscr{L}\mathscr{M}$ factorization, was only given in the orthogonal case since they did not yet have the AGR factorization for general unitaries.

In 1988 (published 1991), AGR [6] extended the AGR factorization to the general unitary case and realized the connection to Szegő recursion. While they could have proven an $\mathscr{L}\mathscr{M}$ factorization from this using the method in [5], they did not and the general $\mathscr{L}\mathscr{M}$ factorization only appeared in [11].

In 1991, Bunse-Gerstner and Elsner [11] found the $\mathscr{L}\mathscr{M}$ factorization for a general finite unitary and noted it was a five-diagonal representation. Watkins [82] codified and cleaned up those results and emphasized the connection to OPUC and found a proof of Szegő recursion from the $\mathscr{L}\mathscr{M}$ factorization. Virtually all the main results from [12] are already in Watkins [82].

We will continue to use the name CMV matrices, in part because the analytic revolution we discuss here was ushered in by their work and in part because the name has been used now in many, many publications.

Here is a summary of the rest of this review. Section 2 presents the basics, essentially notation and (a)–(c). Section 3 discusses "other" CMV matrices. In particular, we consider two kinds of finite variants. In the self-adjoint case, restricting the matrix by taking the first n rows and columns preserves self-adjointness but the analog for unitaries does not, and we have both the nonunitary cutoff CMV matrices obtained from the first n rows and columns and the unitary finite CMV matrices which are models of finite unitary matrices with a cyclic vector. Section 4 discusses CMV matrices for matrix-valued measures—something that is new here. Section 5 discusses the effect on Verblunsky coefficients of rank one multiplication perturbations, and Section 6 the formula for the resolvent of the CMV matrices, the analog of well-known Green's function formulae for Jacobi matrices. Sections 7 and 9 discuss perturbation results, and Section 8 a general theorem on the essential spectrum of CMV matrices. Section 10 discusses the AGR factorization discussed above as preparation for the Killip–Nenciu discussion of five-diagonal models for β-distribution of eigenvalues, the subject of Section 11. Section 12 discusses the defocusing AL flows, which bear the same relation to CMV matrices as Toda flows do to Jacobi matrices. Finally, Section 13 discusses a natural reduction of CMV matrices to a direct sum of two Jacobi matrices when all Verblunsky coefficients are real.

We do not discuss the use of CMV matrices to compute the zeros of OPUC. These zeros are the eigenvalues of the cutoff CMV matrix. We note that this method of computing zeros was used in the recent paper of Martínez-Finkelshtein et al. [57]. Numerical aspects of CMV matrices deserve further study.

While this is primarily a review article, there are numerous new results, including:

(1) an analysis of what matrices occur as cutoff CMV matrices (Section 3);
(2) an analysis following Watkins [82] of the $\mathcal{LM}$ factorization without recourse to Szegő recursion (Section 3);
(3) the basics of CMV matrices for matrix-valued measures (Section 4);
(4) a new proof of AGR factorization using intermediate bases (Section 10);
(5) a new trace class estimate for GGT matrices that relies on AGR factorization (Section 10);
(6) a reworked proof of the Killip–Nenciu [50] theorem on the measure that Haar measure on $\mathbb{U}(n)$ induces on Verblunsky coefficients (Section 11);
(7) an argument of AGR is made explicit and streamlined to go from AGR to $\mathcal{LM}$ factorization (Section 10).

2. CMV matrices: the basics

In this section, we define the CMV basis, the CMV matrix, and the $\mathcal{LM}$ factorization.

CMV matrices can be thought of in terms of unitary matrices or OPUC. We start with the OPUC point of view. A measure $d\mu$ in $\partial\mathbb{D}$ is called nontrivial if it is not supported on a finite set; equivalently, if every polynomial, which is not identically zero, is nonzero in $L^2(\partial\mathbb{D}, d\mu)$. Then one can define *orthonormal polynomials*, $\varphi_n(z)$ (or $\varphi_n(z, d\mu)$), by

$$\text{(i)} \quad \varphi_n(z) = \kappa_n z^n + \text{lower order}, \quad \kappa_n > 0, \tag{2.1}$$

$$\text{(ii)} \quad \varphi_n \perp \{1, z, z^2, \ldots, z^{n-1}\}. \tag{2.2}$$

We define the monic polynomials $\Phi_n(z)$ by $\Phi_n(z) = \varphi_n(z)/\kappa_n$.

The *Szegő dual* is defined by

$$P_n^*(z) = z^n \overline{P_n(1/\bar{z})} \tag{2.3}$$

that is,

$$P_n(z) = \sum_{j=0}^{n} c_j z^j \Rightarrow P_n^*(z) = \sum_{j=0}^{n} \bar{c}_{n-j} z^j. \tag{2.4}$$

The symbol * is n-dependent and is sometimes applied to polynomials of degree at most n, making the notation ambiguous!

Then there are constants $\{\alpha_n\}_{n=0}^{\infty}$ in $\mathbb{D}$, called *Verblunsky coefficients*, (sometimes we will write $\alpha_n(d\mu)$) so that

$$\rho_n \varphi_{n+1}(z) = z\varphi_n(z) - \bar{\alpha}_n \varphi_n^*(z), \tag{2.5}$$

where

$$\rho_n = (1 - |\alpha_n|^2)^{1/2}. \tag{2.6}$$

Moreover, $\mu \to \{\alpha_n\}_{n=0}^{\infty}$ sets up a one–one correspondence between nontrivial measures on $\partial\mathbb{D}$ and points of $\mathbb{D}^\infty$ (as we will show below). Eq. (2.5) (called Szegő recursion after [77]) and this one–one correspondence are discussed in [69,70]; see also [68]. Applying * for P_{n+1} to (2.5), we get

$$\rho_n \varphi_{n+1}^*(z) = \varphi_n^*(z) - \alpha_n z \varphi_n(z). \tag{2.7}$$

If one defines (of course, $\rho = (1 - |\alpha|^2)^{1/2}$)

$$A(\alpha) = \frac{1}{\rho} \begin{pmatrix} z & -\bar{\alpha} \\ -\alpha z & 1 \end{pmatrix} \tag{2.8}$$

then (2.5)/(2.7) can be written as

$$\begin{pmatrix} \varphi_{n+1} \\ \varphi_{n+1}^* \end{pmatrix} = A(\alpha_n) \begin{pmatrix} \varphi_n \\ \varphi_n^* \end{pmatrix}. \tag{2.9}$$

Since $\det(A) = z$, we have

$$A(\alpha)^{-1} = \frac{1}{\rho z}\begin{pmatrix} 1 & \bar{\alpha} \\ \alpha z & z \end{pmatrix} \tag{2.10}$$

and thus

$$\rho_n \varphi_n(z) = \frac{\varphi_{n+1}(z) + \bar{\alpha}_n \varphi^*_{n+1}(z)}{z}, \tag{2.11}$$

$$\rho_n \varphi^*_n(z) = (\varphi^*_{n+1}(z) + \alpha_n \varphi_{n+1}(z)). \tag{2.12}$$

Introduce the notation $[y_1, \ldots, y_k]$ for the span of the vectors $y_1, \ldots, y_k$ and $P_{[y_1,\ldots,y_k]}$ for the projection onto the space $[y_1, \ldots, y_k]$. For $x \notin [y_1, \ldots, y_k]$, define

$$[x; y_1, \ldots, y_k] = \frac{(1 - P_{[y_1,\ldots,y_k]})x}{\|(1 - P_{[y_1,\ldots,y_k]})x\|} \tag{2.13}$$

the normalized projection of x onto $[y_1, \ldots, y_k]^\perp$, that is, the result of adding x to a Gram–Schmidt procedure.

We define π_n to be $P_{[1,\ldots,z^{n-1}]}$.

By the definition of φ_n and the fact that * is anti-unitary on $\operatorname{Ran} \pi_n$ and takes z^j to z^{n-j}, we have

$$\varphi_n = [z^n; 1, \ldots, z^{n-1}], \quad \varphi^*_n = [1; z, \ldots, z^n]. \tag{2.14}$$

With this notation out of the way, we can define the *CMV basis* $\{\chi_n\}_{n=0}^\infty$ and *alternate CMV basis* $\{x_n\}_{n=0}^\infty$ as the Laurent polynomials (i.e., polynomials in z and z^{-1}) obtained by applying Gram–Schmidt to $1, z, z^{-1}, z^2, z^{-2}, \ldots$ and $1, z^{-1}, z, z^{-2}, z^2, \ldots$, that is, for $k = 0, 1, \ldots$,

$$\chi_{2k} = [z^{-k}; 1, z, \ldots, z^{-k+1}, z^k], \quad \chi_{2k-1} = [z^k; 1, z, \ldots, z^{k-1}, z^{-k+1}], \tag{2.15}$$

$$x_{2k} = [z^k; 1, z^{-1}, \ldots, z^{k-1}, z^{-k}], \quad x_{2k-1} = [z^{-k}; 1, z^{-1}, \ldots, z^{-k+1}, z^{k-1}]. \tag{2.16}$$

So, in particular, as functions in $L^2(\partial\mathbb{D}, d\mu)$,

$$x_n = \bar{\chi}_n \tag{2.17}$$

and as Laurent polynomials,

$$x_n(z) = \overline{\chi_n(1/\bar{z})}. \tag{2.18}$$

As realized in [12], the $\{\chi_n\}_{n=0}^\infty$ and $\{x_n\}_{n=0}^\infty$ are always a basis of $L^2(\partial\mathbb{D}, d\mu)$ since the Laurent polynomials are dense on $C(\partial\mathbb{D})$, while $\{\varphi_n\}_{n=0}^\infty$ may or may not be a basis (it is known that this is a basis if and only if $\sum_n |\alpha_n|^2 = \infty$; see [69, Theorem 1.5.7]). On the other hand, the χ and x bases can be expressed in terms of φ and φ^* by (2.14) and the fact that multiplication by z^ℓ is unitary. For example,

$$\begin{aligned} x_{2k} &= z^{-k}[z^{2k}; z^k, z^{k-1}, \ldots, z^{2k-1}, 1] \\ &= z^{-k}[z^{2k}; 1, \ldots, z^{2k-1}] \\ &= z^{-k}\varphi_{2k}(z). \end{aligned}$$

The full set is

$$\chi_{2k}(z) = z^{-k}\varphi^*_{2k}(z), \quad \chi_{2k-1}(z) = z^{-k+1}\varphi_{2k-1}(z), \tag{2.19}$$

$$x_{2k}(z) = z^{-k}\varphi_{2k}(z), \quad x_{2k-1}(z) = z^{-k}\varphi^*_{2k-1}(z). \tag{2.20}$$

Since χ and x are bases, the matrices of multiplication by z in these bases are unitary. So we have the unitary matrices

$$\mathcal{C}_{m\ell} = \langle \chi_m, z\chi_\ell \rangle, \tag{2.21}$$

$$\tilde{\mathcal{C}}_{m\ell} = \langle x_m, z x_\ell \rangle \tag{2.22}$$

called the *CMV matrix* and the *alternate CMV matrix*, respectively. By (2.18), the unitarity of $\mathcal{C}$ and $\bar{z}=z^{-1}$, we see

$$\tilde{\mathcal{C}}_{mk}=\mathcal{C}_{km} \tag{2.23}$$

that is, $\mathcal{C}$ and $\tilde{\mathcal{C}}$ are transposes of each other. We will see shortly that $\mathcal{C}$ is five-diagonal, but this follows now by noting that both z and z^{-1} map $[\chi_0,\dots,\chi_k]$ into $[\chi_0,\dots,\chi_{k+2}]$.

CMV [12], Ammar–Gragg–Reichel [5], Bunse-Gerstner and Elsner [11], and Watkins [82] also discussed the important factorization $\mathcal{C}=\mathcal{L}\mathcal{M}$ as follows:

$$\mathcal{L}_{mk}=\langle\chi_m, zx_k\rangle,\qquad \mathcal{M}_{mk}=\langle x_m,\chi_k\rangle. \tag{2.24}$$

Since $\{x_k\}_{k=1}^{\infty}$ is a basis, $\langle f,g\rangle=\sum_{k=0}^{\infty}\langle f,x_k\rangle\langle x_k,g\rangle$, and thus

$$\mathcal{C}=\mathcal{L}\mathcal{M},\qquad \tilde{\mathcal{C}}=\mathcal{M}\mathcal{L}. \tag{2.25}$$

The point of this factorization is that $\mathcal{L}$ and $\mathcal{M}$ have a simpler structure than $\mathcal{C}$. Indeed, $\mathcal{L}$ is a direct sum of 2×2 blocks and $\mathcal{M}$ of a single 1×1 block and then 2×2 blocks.

One can (and we will) see this based on calculations, but it is worth seeing why it is true in terms of the structure of the CMV and alternate CMV basis. Notice that χ_{2n-1} and χ_{2n} span the two-dimensional space $[1,z,z^{-1},\dots,z^n,z^{-n}]\cap[1,z,z^{-1},\dots,z^{n-1},z^{-n+1}]^{\perp}$ and so do x_{2n-1} and x_{2n}. This shows that $\mathcal{M}$ is a direct sum of $\mathbf{1}_{1\times 1}$ and 2×2 matrices. Similarly, χ_{2n} and χ_{2n+1} span $[1,\dots,z^{-n},z^{n+1}]\cap[1,\dots,z^{-n+1},z^{n}]^{\perp}$, as do zx_{2n} and zx_{2n+1} (even for $n=0$). Thus $\mathcal{L}$ has a 2×2 block structure.

In fact, we can use Szegő recursion in form (2.5), (2.7), (2.11), (2.12) to find the 2×2 matrices explicitly. For example, taking (2.12) for $n=2m-1$, we get

$$\varphi_{2m}^{*}=\rho_{2n-1}\varphi_{2m-1}^{*}-\alpha_{2m-1}\varphi_{2m}$$

and multiplying by z^{-m} yields (by (2.20)/(2.20)),

$$\chi_{2m}=-\alpha_{2m-1}x_{2m}+\rho_{2m-1}x_{2m-1}$$

This plus similar calculations imply

Theorem 2.1 (*Ammar et al. [5], Bunse-Gerstner and Elsner [11], Cantero et al. [12], Watkins [82]*). *Let*

$$\Theta(\alpha)=\begin{pmatrix}\bar{\alpha} & \rho\\ \rho & -\alpha\end{pmatrix}. \tag{2.26}$$

Then $\mathcal{C}=\mathcal{L}\mathcal{M}$ *and*

$$\mathcal{L}=\Theta(\alpha_0)\oplus\Theta(\alpha_2)\oplus\Theta(\alpha_4)\oplus\cdots\oplus\Theta(\alpha_{2m})\oplus\cdots \tag{2.27}$$

and

$$\mathcal{M}=\mathbf{1}_{1\times 1}\oplus\Theta(\alpha_1)\oplus\Theta(\alpha_3)\oplus\cdots\oplus\Theta(\alpha_{2m+1})\oplus\cdots \tag{2.28}$$

Doing the multiplication yields

$$\mathcal{C}=\begin{pmatrix}\bar{\alpha}_0 & \bar{\alpha}_1\rho_0 & \rho_1\rho_0 & 0 & 0 & \dots\\ \rho_0 & -\bar{\alpha}_1\alpha_0 & -\rho_1\alpha_0 & 0 & 0 & \dots\\ 0 & \bar{\alpha}_2\rho_1 & -\bar{\alpha}_2\alpha_1 & \bar{\alpha}_3\rho_2 & \rho_3\rho_2 & \dots\\ 0 & \rho_2\rho_1 & -\rho_2\alpha_1 & -\bar{\alpha}_3\alpha_2 & -\rho_3\alpha_2 & \dots\\ 0 & 0 & 0 & \bar{\alpha}_4\rho_3 & -\bar{\alpha}_4\alpha_3 & \dots\\ \dots & \dots & \dots & \dots & \dots & \dots\end{pmatrix} \tag{2.29}$$

$\mathcal{C}$ is five-diagonal, that is, only nonzero in those diagonals $\mathcal{C}_{k\,k+j}$ with $j=0,\pm 1,\pm 2$. Notice that half of the elements with $j=\pm 2$ are zero, so it is only "barely" five-diagonal—and it cannot be tridiagonal or even four-diagonal since

Proposition 2.2 (*Cantero et al. [13]*). *If* $\{A_{jk}\}_{1\leqslant j,k<\infty}$ *is a semi-infinite unitary matrix and*

$$k-j\notin\{-1,\ldots,n\}\Rightarrow A_{jk}=0$$

then A is a direct sum of finite blocks of size at most $n+1$.

This was proven for $n=1$ in [10] and conjectured for $n=2$ in a draft of [69] before motivating [13].

While our construction has been for α_n's which come from a $d\mu$ and, in particular, which obey

$$|\alpha_j(d\mu)|<1 \tag{2.30}$$

Θ defines a unitary so long as $|\alpha_n|\leqslant 1$. We thus define a *CMV matrix* to be a matrix of form (2.25)–(2.29) for any $\{\alpha_n\}_{n=0}^{\infty}$ with $|\alpha_n|\leqslant 1$. If $|\alpha_n|<1$ for all n, we call $\mathscr{C}$ a *proper CMV matrix*, and if $|\alpha_n|=1$ for some n, we call it an *improper CMV matrix*.

To state the analog of Stone's self-adjoint cyclic model theorem, we need another definition. A *cyclic unitary model* is a unitary operator, U, on a (separable) Hilbert space, $\mathscr{H}$, with a distinguished unit vector, v_0, which is cyclic, that is, finite linear combinations of $\{U^n v_0\}_{n=-\infty}^{\infty}$ are dense in $\mathscr{H}$. We call the model *proper* if $\dim(\mathscr{H})=\infty$ and *improper* if $\dim(\mathscr{H})<\infty$. It is easy to see that the model is improper if and only if $P(U)=0$ for some polynomial, P, which can be taken to have degree $\dim(\mathscr{H})-1$. Two cyclic unitary models, $(\mathscr{H},U,v_0)$ and $(\widetilde{\mathscr{H}},\widetilde{U},\tilde{v}_0)$, are called equivalent if and only if there is a unitary W from $\mathscr{H}$ onto $\widetilde{\mathscr{H}}$ so that

$$Wv_0=\tilde{v}_0,\quad WUW^{-1}=\widetilde{U}. \tag{2.31}$$

Theorem 2.3. *There is a one–one correspondence between proper cyclic unitary models and proper CMV matrices,* $\mathscr{C}$, *in that* $\delta_0=(1,0,0,\ldots)^{\mathrm{t}}$ *is cyclic for any such* $\mathscr{C}$ *and every equivalence class contains exactly one proper CMV model*: $(\ell^2,\mathscr{C},\delta_0)$.

Remark 1. There is behind this a fourfold equivalence:

(i) equivalence classes of proper cyclic unitary models;
(ii) nontrivial probability measures on $\partial\mathbb{D}$;
(iii) Verblunsky coefficients $\{\alpha_n(d\mu)\}_{n=0}^{\infty}$ in $\mathbb{D}^{\infty}$;
(iv) proper CMV matrices.

The spectral theorem sets up a one–one correspondence between (i) and (ii), while the definition of CMV matrices between (iii) and (iv). Szegő recursion sets up a map from $d\mu$ to $\{\alpha_n(d\mu)\}_{n=1}^{\infty}$. As we will show, each $(\ell^2,\mathscr{C},\delta_0)$ is a cyclic model, so the key remaining fact is the uniqueness.

2. A corollary of this is Verblunsky's theorem (also called "Favard's theorem for the unit circle") that each $\{\alpha_n\}_{n=0}^{\infty}\in\mathbb{D}$ is the Verblunsky coefficient for some $d\mu$. See [69,68] for further discussion and other proofs.

Proof. As explained in Remark 1, we need only prove that any proper CMV matrix has δ_0 as a cyclic vector, and that if $\{\alpha_n^{(0)}\}_{n=0}^{\infty}$ are the Verblunsky coefficients for $\mathscr{C}$ and $d\mu$ the spectral measure for δ_0, then

$$\alpha_n(d\mu)=\alpha_n^{(0)}. \tag{2.32}$$

Let δ_n be the unit vector in ℓ^2 with coefficient 1 in place n and 0 elsewhere; index labeling for our vectors starts at 0. By direct calculations using the $\mathscr{L}\mathscr{M}$ representation,

$$\mathscr{C}^{n+1}\delta_0-\rho_0^{(0)}\rho_1^{(0)}\ldots\rho_{2n}^{(0)}\delta_{2n+1}\in[\delta_0,\ldots,\delta_{2n}], \tag{2.33}$$

$$(\mathscr{C}^*)^n\delta_0-\rho_0^{(0)}\ldots\rho_{2n-1}^{(0)}\delta_{2n}\in[\delta_0,\ldots,\delta_{2n-1}]. \tag{2.34}$$

It follows that δ_0 is cyclic and

$$\chi_n(d\mu)=W\delta_n, \tag{2.35}$$

where W is the spectral representation from ℓ^2 to $L^2(\partial\mathbb{D}, \mathrm{d}\mu)$. Eq. (2.35) follows from (2.33)–(2.34), induction, and the Gram–Schmidt definition of χ.

By (2.35) and

$$\langle\delta_0, \mathscr{C}\delta_0\rangle = \bar{\alpha}_0^{(0)}, \quad \langle\chi_0, z\chi_0\rangle = \alpha_0(\mathrm{d}\mu),$$
$$\langle\delta_{2n-2}, \mathscr{C}\delta_{2n-1}\rangle = \bar{\alpha}_{2n-1}^{(0)}\rho_{2n-2}^{(0)}, \quad \langle\chi_{2n-2}, z\chi_{2n-1}\rangle = \bar{\alpha}_{2n-1}\rho_{2n-2},$$
$$\langle\delta_{2n}, \mathscr{C}\delta_{2n-1}\rangle = \bar{\alpha}_{2n}^{(0)}\rho_{2n-1}^{(0)}, \quad \langle\chi_{2n}, z\chi_{2n-1}\rangle = \bar{\alpha}_{2n}(\mathrm{d}\mu)\rho_{2n-1}(\mathrm{d}\mu)$$

we obtain (2.32) by induction. □

3. Cutoff, finite, two-sided, periodic, and floquet CMV matrices

In this section, we will discuss various matrices constructed from or related to CMV matrices. Some are finite, and in that case, we will also discuss the associated characteristic polynomial which turns out to be equal or related to the basic ordinary or Laurent polynomials of OPUC: the monic orthogonal and paraorthogonal polynomials and the discriminant. The basic objects we will discuss are:

(i) *Cutoff CMV matrices*, that is, $\tilde{\pi}_n\mathscr{C}\tilde{\pi}_n$ where $\tilde{\pi}_n$ is projection onto the span of the first n of $1, z, z^{-1}, \ldots$.
(ii) *Finite CMV matrices*, the upper $n \times n$ block of an improper CMV matrix with $\alpha_{n-1} \in \partial\mathbb{D}$.
(iii) *Two-sided CMV matrices* defined for $\{\alpha_n\}_{n=-\infty}^{\infty}$ via extending $\mathscr{L}$ and $\mathscr{M}$ in the obvious way to a two-sided form.
(iv) *Periodic CMV matrices*. The special case of two-sided CMV matrices when $\alpha_{n+p} = \alpha_n$ for some p.
(v) *Floquet CMV matrices*. Periodic CMV matrices have a direct integral decomposition whose fibers are $p \times p$ matrices that are finite CMV matrices with a few changed matrix elements.

Cutoff CMV matrices: A *cutoff CMV matrix* is the restriction of a proper CMV matrix to the upper $n \times n$ block, that is, top n rows and leftmost n columns. We use $\mathscr{C}^{(n)}$ to denote the cutoff matrix associated to $\mathscr{C}$. A glance at (2.29) shows that $\mathscr{C}^{(n)}$ depends on $\{\alpha_j\}_{j=0}^{n-1}$. Here is a key fact:

Proposition 3.1. *Let $\Phi_n(z)$ be the monic orthogonal polynomial associated to $\mathscr{C}$ (i.e., $\Phi_n = \kappa_n^{-1}\varphi_n$). Then*

$$\Phi_n(z) = \det(z\mathbf{1} - \mathscr{C}^{(n)}). \tag{3.1}$$

Proof. If π_n is the projection onto $[1, \ldots, z^{n-1}]$ and $\tilde{\pi}_n$ on the span of the first n of $1, z, z^{-1}, \ldots$, then π_n and $\tilde{\pi}_n$ are unitarily equivalent under a power of z. So if $M_z f = zf$, then $\pi_n M_z \pi_n$ and

$$\tilde{\pi}_n M_z \tilde{\pi}_n \equiv \mathscr{C}^{(n)} \tag{3.2}$$

are unitarily equivalent, and thus, (3.1) is equivalent to

$$\Phi_n(z) = \det(z\mathbf{1} - \pi_n M_z \pi_n). \tag{3.3}$$

Let z_j be a zero of Φ_n of multiplicity k_j and let $P_j(z) = \Phi_n(z)/(z - z_j)^{k_j}$. Then with $A = \pi_n M_z \pi_n$, we have

$$(A - z_j)^{k_j} P_j = 0, \quad (A - z_j)^{k_j - 1} P_j \neq 0.$$

Thus, as z_j runs through the distinct zeros, $\{(A - z_j)^{\ell} P_j \mid \ell = 0, 1, \ldots, k_j - 1\}$ gives us a Jordan basis in which A has a $k_j \times k_j$ block for each z_j of the form

$$\begin{pmatrix} z_j & 1 & \ldots & \ldots & 0 \\ 0 & z_j & 1 & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & \ldots & 1 \\ 0 & 0 & \ldots & \ldots & z_j \end{pmatrix}$$

and thus

$$\det(z - A) = \prod (z - z_j)^{k_j} = \Phi_n(z). \qquad \square$$

Corollary 3.2. *The zeros of $\Phi_n(z)$ lie in $\mathbb{D}$.*

Remark. See [69, Section 1.7] for six other proofs of this theorem.

Proof. Let $A = \pi_n M_z \pi_n$. Then $\|A\| \leqslant 1$, so obviously, eigenvalues lie in $\overline{\mathbb{D}}$. If $A\eta = z_0\eta$ with $\eta \in \operatorname{Ran} \pi_n$ and $z_0 \in \partial\mathbb{D}$, then $\|A\eta\| = \|\eta\|$, so $\pi_n z\eta = z\eta$ and thus as polynomials $(z - z_0)\eta = 0$. Since the polynomials are a division ring, $\eta = 0$, that is, there are no eigenvalues on $\partial\mathbb{D}$. $\square$

To classify cutoff CMV matrices, we need to understand how $\Theta(\alpha)$ arises from a 2×2 change of basis.

Lemma 3.3. *Let f, g be two independent unit vectors with*

$$\langle f, g \rangle = \alpha. \tag{3.4}$$

Let φ_1, φ_2 be the result of applying Gram–Schmidt to f, g and ψ_1, ψ_2 to g, f. Let M be the matrix of change of basis

$$\varphi_1 = m_{11}\psi_1 + m_{12}\psi_2, \tag{3.5}$$

$$\varphi_2 = m_{21}\psi_1 + m_{22}\psi_2. \tag{3.6}$$

Then $\alpha \in \mathbb{D}$ and $M = \Theta(\alpha)$.

Proof. $|\alpha| < 1$ by the Schwarz inequality and the independence of f and g. Note that

$$\begin{aligned} \|g - \langle f, g \rangle f\|^2 &= \|g\|^2 + |\langle f, g \rangle|^2 \|f\|^2 - 2\operatorname{Re}[\langle f, g \rangle \langle g, f \rangle] \\ &= 1 - |\alpha|^2 \equiv \rho^2 \end{aligned}$$

so

$$\varphi_2 = \rho^{-1}(g - \alpha f), \tag{3.7}$$

$$\psi_2 = \rho^{-1}(f - \bar{\alpha} g). \tag{3.8}$$

From this, a direct calculation shows that

$$m_{11} = \langle \psi_1, \varphi_1 \rangle = \langle g, f \rangle = \bar{\alpha},$$

$$m_{12} = \langle \psi_2, \varphi_1 \rangle = \rho^{-1}(1 - |\alpha|^2) = \rho,$$

$$m_{21} = \langle \psi_1, \varphi_2 \rangle = \rho^{-1}(1 - |\alpha|^2) = \rho,$$

$$m_{22} = \langle \psi_2, \varphi_2 \rangle = \rho^{-2}(\alpha + \alpha|\alpha|^2 - 2\alpha) = -\alpha. \qquad \square$$

Remark. One can use this lemma to deduce the form of $\mathcal{L}$ and $\mathcal{M}$ in the $\mathcal{L}\mathcal{M}$ factorization without recourse to Szegő recursion, and then use their form to deduce the Szegő recursion. This is precisely Watkins' approach [82] to the factorization and Szegő recursion.

Given any matrix A and vector δ_0, define

$$V_k = \operatorname{span}(\delta_0, A\delta_0, A^*\delta_0, \ldots, A^k\delta_0, (A^*)^k\delta_0) \tag{3.9}$$

which has dimension $2k + 1$ if and only if the vectors are independent.

Here is a complete classification of cutoff CMV matrices analogous to Theorem 2.3:

Theorem 3.4. *Let A be an $n \times n$ cutoff CMV matrix with $\delta_0 = (1, 0, \dots, 0)^{\mathrm{t}}$. Then*:

(i) *If $n = 2k + 1$, V_k has dimension n. If $n = 2k$, then* $\operatorname{span}[V_{k-1} \cup \{A^k \delta_0\}]$ *has dimension n.*
(ii) *If $n = 2k + 1$, A^* is an isometry on* $\operatorname{span}(V_{k-1} \cup \{(A)^k \delta_0\})$ *and A is an isometry on* $\operatorname{span}(V_{k-1} \cup \{(A^*)^k \delta_0\})$. *If $n = 2k$, A^* is an isometry on* $\operatorname{span}(V_{k-2} \cup \{A^{k-1}\delta_0, A^k \delta_0\})$ *and A is an isometry on V_{k-1}.*
(iii) $\|A\| \leqslant 1$.
(iv) *A is not unitary.*

Conversely, if A_0, δ_0 are a pair of an $n \times n$ matrix and vector δ_0 obeying (i)–(iv), *then there is a basis in which $\delta_0 = (1, 0, \dots, 0)^{\mathrm{t}}$ and A is a cutoff CMV matrix.*

(A, δ_0) determine the Verblunsky coefficients $(\alpha_0, \dots, \alpha_{n-1})$ uniquely. In particular, two cutoff CMV matrices with distinct $\{\alpha_j\}_{j=0}^n$ are not unitarily equivalent by a unitary preserving δ_0.

Proof. Suppose first that A is a cutoff CMV matrix, that is, $A = \tilde{\pi}_n \mathscr{C} \tilde{\pi}_n$. By definition of $\tilde{\pi}_n$,

$$\tilde{\pi}_n \mathscr{C}^j \delta_0 = \mathscr{C}^j \delta_0, \quad \tilde{\pi}_n (\mathscr{C}^*)^\ell \delta_0 = (\mathscr{C}^*)^\ell \delta_0$$

for $j = 0, 1, \dots, k$ and $\ell = 0, 1, \dots, k$ (resp., $k - 1$) if $n = 2k + 1$ (resp., $2k$). It follows that for those values of j and ℓ,

$$\mathscr{C}^j \delta_0 = A^j \delta_0, \quad (\mathscr{C}^*)^\ell \delta_0 = (A^*)^\ell \delta_0 \tag{3.10}$$

so that (i) holds.

This also shows that $A^* A^j \delta_0 = A^{j-1} \delta_0$ for $j = 1, \dots, k$, and from this and (3.10), it follows that A^* is unitary on $\operatorname{span}\{A^j \delta_0\}_{j=0}^k \cup \{(A^*)^\ell \delta_0\}_{\ell=0}^{k-1 \text{ (or } k-2)}$. Similarly, we get the unitarity result for A.

(iii) is obvious since $\|\tilde{\pi}_n\| = \|\mathscr{C}\| = 1$ and (iv) follows since there is a vector φ in $\operatorname{Ran}(\tilde{\pi}_n)$ with $\tilde{\pi}_n \mathscr{C} \varphi \neq \mathscr{C} \varphi$. This completes the proof of the first paragraph of the theorem.

As a preliminary to the converse, we note that $\tilde{\pi}_n$ commutes with either $\mathscr{L}$ or $\mathscr{M}$, so a finite CMV matrix has the form $\mathscr{L}_n \mathscr{M}_n$ where if $n = 2k + 1$ is odd ($\mathbf{1} = 1 \times 1$ identity matrix),

$$\mathscr{L}_n = \Theta(\alpha_0) \oplus \cdots \oplus \Theta(\alpha_{2k-2}) \oplus \alpha_{2k} \mathbf{1}, \tag{3.11}$$

$$\mathscr{M}_n = \mathbf{1} \oplus \Theta(\alpha_1) \oplus \cdots \oplus \Theta(\alpha_{2k-1}) \tag{3.12}$$

and if $n = 2k$ is even,

$$\mathscr{L}_n = \Theta(\alpha_0) \oplus \cdots \oplus \Theta(\alpha_{2k-2}), \tag{3.13}$$

$$\mathscr{M}_n = \mathbf{1} \oplus \Theta(\alpha_1) \oplus \cdots \oplus \Theta(\alpha_{2k-3}) \oplus \alpha_{2k-1} \mathbf{1}. \tag{3.14}$$

We will prove that when A obeys (i)–(iv), then A has an $\mathscr{L}_n \mathscr{M}_n$ factorization with parameter α_j given intrinsically by A. This will not only prove the converse but the uniqueness of the map from $\{\alpha_j\}_{j=0}^{N-1}$ to cutoff CMV matrices, and so it will complete the proof of the theorem.

We first consider the case $n = 2k + 1$ odd. Define χ_ℓ to be the basis obtained by Gram–Schmidt on $\delta_0, A\delta_0, A^*\delta_0, \dots, A^k \delta_0, (A^*)^k \delta_0$ (this is possible because (i) implies these vectors are linearly independent) and define x_ℓ to be the result of Gram–Schmidt on $\delta_0, A^*\delta_0, A\delta_0, \dots, (A^*)^k \delta_0, A^k \delta_0$. Then if A is written in χ_ℓ basis,

$$A = \mathscr{L} \mathscr{M}, \tag{3.15}$$

where

$$\mathscr{M}_{k\ell} = \langle x_k, \chi_\ell \rangle, \quad \mathscr{L}_{k\ell} = \langle \chi_k, A x_\ell \rangle. \tag{3.16}$$

We need to show that $\mathscr{L}$, $\mathscr{M}$ have form (3.11)/(3.12).

If P_m is the projection to the orthogonal complement of V_{m-1} and $f = P_{m-1}(A^*)^m \delta_0 / \|P_{m-1}(A^*)^m \delta_0\|$ and $g = P_{m-1} A^m \delta_0 / \|P_{m-1} A^m \delta_0\|$, then $\{\chi_\ell, x_\ell\}_{\ell=m,m+1}$ are given by Lemma 3.3. So M has the form $1 \oplus \Theta(\alpha_1) \oplus \cdots \oplus \Theta(\alpha_{2k-1})$ as required.

Let W_ℓ be the projection onto the span of the first 2ℓ of $\delta_0, A\delta_0, A^*\delta_0, A^2\delta_0, \ldots$ and $\widetilde{W}_\ell$ the span of the first 2ℓ of $\delta_0, A^*\delta_0, A\delta_0, (A^*)^2\delta_0, \ldots$. By hypothesis (ii), A is an isometry on $\widetilde{W}_1, \widetilde{W}_2, \ldots, \widetilde{W}_k$, and by the same hypothesis, $AA^*\varphi = \varphi$ for $\varphi = \delta_0, A^*\delta_0, \ldots, (A^*)^k\delta_0$. So it follows that A maps $\widetilde{W}_\ell$ to W_ℓ for $\ell = 1, \ldots, k$. Thus, by Lemma 3.3, the $2k \times 2k$ upper block of L is $\Theta(\alpha_0) \oplus \Theta(\alpha_2) \oplus \cdots \oplus \Theta(\alpha_{2k-2})$. Since A and A^* are contractions, L must have 0's in the bottom and rightmost column, except for the lower corner. That corner value, call it α_{2k}, must have $|\alpha_{2k}| \leqslant 1$ by (iii) and $|\alpha_{2k}| < 1$ by (iv). Thus, we have the required $\mathscr{L}\mathscr{M}$ factorization if $n = 2k + 1$.

Now let $\ell = 2k$ be even. Define χ_ℓ as before, but define $\tilde{x}_\ell$ by Gram–Schmidt on $A\delta_0, \delta_0, A^2\delta_0, A^*\delta_0, \ldots, A^k\delta_0, (A^*)^{k-1}\delta_0$. Then A written in χ_ℓ basis has form (3.15) where

$$\mathscr{M}_{k\ell} = \langle \tilde{x}_k, A\chi_\ell\rangle, \quad \mathscr{L}_{k\ell} = \langle \chi_k, \tilde{x}_\ell\rangle. \tag{3.17}$$

We need to show that $\mathscr{L}$, $\mathscr{M}$ have form (3.13)/(3.14).

Define W_ℓ to be the span of $\delta_0, A\delta_0, A^*\delta_0, \ldots, A^\ell\delta_0, (A^\ell)^*\delta_0$ and $\widetilde{W}_\ell$ the span of $A\delta_0, \delta_0, \ldots, (A^*)^{\ell-1}\delta_0, A^{\ell+1}\delta_0$. As above, A is an isometry of W_ℓ to $\widetilde{W}_\ell$, so M has the form $\mathbf{1} \oplus \Theta(\alpha_1) \oplus \cdots \oplus \Theta(\alpha_{2k-3}) \oplus \alpha_{2k-1}\mathbf{1}$ where $|\alpha_{2k-1}| < 1$ by condition (iv). Similarly, L has a $\Theta(\alpha_0) \oplus \cdots \oplus \Theta(\alpha_{2k-2})$ block structure. This proves (3.13)/(3.14) and completes the case $n = 2k$. □

Remark. This theorem sets up a one–one correspondence between $\{\alpha_j\}_{j=0}^{n-1} \in \mathbb{D}^n$ and cutoff CMV matrices.

Finite CMV matrices: As discussed in Section 2, $\mathscr{C}$, originally defined for $|\alpha_j| < 1$, has an extension to $|\alpha_j| \leqslant 1$ via the Θ formula for $\mathscr{L}$, $\mathscr{M}$. Since $|\alpha_{j_0}| = 1$ implies $\rho_{j_0} = 0$ and $\Theta(\alpha_{j_0})$ is diagonal, if $|\alpha_{j_0}| = 1$, $\mathscr{C}(\{\alpha_j\})$ leaves $\mathbb{C}^{j_0+1}$ (i.e., vectors φ with $\varphi_k = 0$ if $k \geqslant j_0 + 1$) invariant and $\mathscr{C} \restriction \mathbb{C}^{j_0+1}$ is a $(j_0+1) \times (j_0+1)$ unitary matrix. If $|\alpha_0|, \ldots, |\alpha_{n-2}| < 1$ and $|\alpha_{n-1}| = 1$, the corresponding $n \times n$ matrix is called a *finite $n \times n$ CMV matrix*, $\mathscr{C}_n(\{\alpha_0, \ldots, \alpha_{n-2}, \alpha_{n-1}\})$. $\mathscr{C}_n$ has the form $\mathscr{L}_n\mathscr{M}_n$ where (3.11)/(3.12) or(3.13)/(3.14) hold, and now $\alpha_{n-1} \in \partial\mathbb{D}$.

If U is an $n \times n$ matrix and δ_0 a cyclic vector in the sense that $\{U^m\delta_0\}_{m=-\infty}^{\infty}$ is total, δ_0 cannot be orthogonal to any eigenvector. So U has to have n distinct eigenvalues $\{\lambda_j\}_{j=1}^n$ and the eigenvectors $\{\psi_j\}_{j=1}^n$ obey $|\langle\delta_0, \psi_j\rangle|^2 = a_j \neq 0$. The unitary invariants of the pair (U, δ_0) are the spectral measures $\sum_{j=1}^n a_j\delta_{\lambda_j}$ where $\{\lambda_j\}_{j=1}^n$ are arbitrary distinct points and the $a_j > 0$ have the single restriction $\sum_{j=1}^n a_j = 1$. Thus, the number of real parameters is $n + (n-1) = 2n - 1$. The number of free parameters in an $n \times n$ finite CMV matrix is $n - 1$ complex numbers in $\mathbb{D}$ and one in $\partial\mathbb{D}$, that is, $2(n-1) + 1 = 2n - 1$. This suggests that:

Theorem 3.5. *There is a one–one correspondence between unitary equivalence classes of $n \times n$ unitary matrices with a cyclic vector and finite CMV matrices in that each equivalence class contains one CMV matrix* (*fixed by* $\delta_0 = (1, 0, \ldots, 0)^{\mathrm{t}}$) *and two CMV matrices with distinct parameters are not unitarily equivalent by a unitary fixing* $(1, 0, \ldots, 0)^{\mathrm{t}}$.

The proof is identical to the proof of Theorem 3.4 except that A nonunitary is replaced by A unitary so $|\alpha_{n-1}| = 1$. As noted in the discussion after Lemma 3.3, this approach is close to that in Watkins [82]. This theorem is related to results in Ammar–Gragg–Reichel [5] and Killip–Nenciu [51]. The latter talk about matrices with CMV shape having the CMV form.

Instead of the cutoff CMV matrix, $\pi_n M_z \pi_n$, one can look at $\widehat{\pi}_n M_z \widehat{\pi}_n$ where $\widehat{\pi}_n$ is a not necessary self-adjoint projection. CMV [14] have shown that finite CMV matrices have this form and that they are the only normal operators of this form.

Two-sided CMV matrices: In a sense, CMV matrices are two-sided. For example, if $\alpha_n \equiv 0$, $\mathscr{C}$ is unitarily equivalent to a two-sided shift since $\mathscr{C}^k\delta_0 = \delta_{2k-1}$ and $\mathscr{C}^{-k}\delta_0 = \delta_{2k}$. However, as structures, the matrix is semi-infinite and there is a cyclic vector which is often not true for two-sided matrices. Thus, there is an extension to "two-sided" examples.

Let $\{\alpha_n\}_{n=-\infty}^{\infty}$ be a two-sided sequence of numbers in $\overline{\mathbb{D}}$. Let $\mathscr{H} = \ell^2(\mathbb{Z})$, that is, two-sided sequences $\{u_n\}_{n=-\infty}^{\infty}$ with $\sum_{n=-\infty}^{\infty} |u_n|^2 < \infty$. Let $\Theta_j(\beta)$ be $\Theta(\beta)$ acting on the two indices j and $j+1$. Define

$$\mathscr{E}(\{\alpha_j\}_{j=-\infty}^{\infty}) = \widetilde{\mathscr{L}}(\{\alpha_j\}_{j=-\infty}^{\infty})\widetilde{\mathscr{M}}(\{\alpha_j\}_{j=-\infty}^{\infty}), \tag{3.18}$$

where

$$\widetilde{\mathcal{M}} = \bigoplus_{j=-\infty}^{\infty} \Theta_{2j-1}(\alpha_{2j-1}),$$

$$\widetilde{\mathcal{L}} = \bigoplus_{j=-\infty}^{\infty} \Theta_{2j}(\alpha_{2j}).$$

$\mathcal{E}$ is called the extended CMV matrix.

The extended CMV matrix was introduced in [69]. Earlier, Bourget et al. [10] had considered some doubly infinite five-diagonal matrices which factor into a product of two direct sums of 2×2 matrices, but the 2×2 blocks were general unitaries rather than Θ's.

While $\mathcal{E}$ is natural and important for the periodic case, we will also see that it arises in the theory of essential spectrum of $\mathcal{C}$ (see Section 8).

One reason for the name "extended CMV matrix" is:

Proposition 3.6. *If $\alpha_{-1} = -1$, then $\mathcal{E}$ is a direct sum on $\ell^2(-\infty, -1] \oplus \ell^2[0, \infty)$ and $\mathcal{E} \restriction \ell^2[0, \infty)$* is the CMV matrix $\mathcal{C}(\{\alpha_j\}_{j=0}^{\infty})$. Moreover, $\mathcal{E} \restriction \ell^2(-\infty, -1]$ is unitarily equivalent to $\mathcal{C}(\{\bar{\alpha}_{-j-2}\}_{j=0}^{\infty})$.

Remark. $\ell^2[0, \infty)$ means those $u \in \ell^2(\mathbb{Z})$ with $u_n = 0$ if $n < 0$ and $\ell^2(-\infty, -1]$ those with $u_n = 0$ if $n > -1$.

Proof. $\Theta(-1) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$, so both $\widetilde{\mathcal{L}}$ and $\widetilde{\mathcal{M}}$ leave $\ell^2[0, \infty)$ and $\ell^2(-\infty, -1]$ invariant. Thus, $\mathcal{E}$ does.

$\widetilde{\mathcal{M}} \restriction \ell^2[0, \infty) = \mathcal{M}$ and $\widetilde{\mathcal{L}} \restriction \ell^2[0, \infty) = \mathcal{L}$, so $\mathcal{E} \restriction \ell^2[0, \infty)$ is $\mathcal{C}(\{\alpha_j\}_{j=0}^{\infty})$.

For the restriction to $\ell^2(-\infty, -1]$, note first that $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Theta(\alpha) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = \Theta(-\bar{\alpha})$. Thus, by labeling the basis backwards, $\mathcal{E}$ is unitarily equivalent to something that looks very much like $\mathcal{C}(\{-\bar{\alpha}_{-j-2}\}_{j=0}^{\infty})$ except $\mathcal{M}$ starts with -1, not 1. By the discussion in Section 5, there is a unitary that flips the spin of this -1 and all the α_j's. □

Changing α_{-1} from its value to $\alpha_{-1} = -1$ is a perturbation of rank at most two, so by the Kato–Rosenblum theorem [65], the a.c. spectrum of $\mathcal{E}$ is that of a direct sum of two $\mathcal{C}$'s. Since these a.c. spectra are only restricted by simplicity, we see that the a.c. spectrum of $\mathcal{E}$ has multiplicity at most 2, but is otherwise arbitrary: it can be partially multiplicity 0, partially 1, and partially 2. In particular, $\mathcal{E}$ may not have a cyclic vector.

It is a theorem of Simon [67] that the singular spectrum of $\mathcal{E}$ is simple. This is an analog of a theorem of Kac [47,48] and Gilbert [37,38] for Schrödinger operators.

Periodic CMV matrices: If $\{\alpha_j\}_{j=0}^{\infty}$ is a sequence of Verblunsky coefficients with

$$\alpha_{j+p} = \alpha_j \tag{3.19}$$

for $j \geqslant 0$, p fixed, and $\geqslant 1$, then α_j has a unique extension to $j \in \mathbb{Z}$ obeying (3.19). The corresponding $\mathcal{E}$ is called a *periodic CMV matrix*. The theory is simpler if p is even, which we henceforth assume. As explained in [70], there are several ways to analyze odd p once one has understood even p.

Associated to $\{\alpha_j\}_{j=0}^{p-1}$ is a natural Laurent polynomial, called the discriminant, $\Delta(z; \{\alpha_j\}_{j=0}^{p-1})$,

$$\Delta(z) = z^{-p/2}\,\mathrm{Tr}(A(\alpha_{p-1}, z)A(\alpha_{p-2}, z) \cdots A(\alpha_0, z)), \tag{3.20}$$

where

$$A(\alpha, z) = \rho^{-1} \begin{pmatrix} z & -\bar{\alpha} \\ -z\alpha & 1 \end{pmatrix}. \tag{3.21}$$

This is analyzed in [70, Section 11.1]. $\Delta(z)$ is real on $\partial\mathbb{D}$ and has positive leading coefficient. This means $\Delta(z)$ has p real parameters. This suggests the map from $\{\alpha_j\}_{j=0}^{p}$ (of real dimension $2p$) to Δ is many to 1, with inverse images generically of dimension p ($=2p - p$). This is in fact true: the inverse images are tori of dimension $d \leqslant p$ (we will see what d is in a moment). They are called *isospectral tori*.

For fixed $\{\alpha_j\}_{j=0}^{p-1}$, $\Delta^{-1}([-2,2])$ (which is the spectrum of $\mathcal{E}$) lies in $\partial\mathbb{D}$ and is naturally p closed intervals whose endpoints are $\Delta^{-1}(\{-2,2\})$. Generically (in α), the intervals are disjoint, that is, their complement (called the gaps) is p nonempty open intervals. In general, the number of open intervals in the gaps is d, the dimension of the isospectral torus.

Floquet CMV matrices: If $T: \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ by $(Tu)_n = u_{n+p}$ and p is even, and if $\alpha_n = \alpha_{n+p}$, then $T\widetilde{\mathcal{M}}T^{-1} = \widetilde{\mathcal{M}}$ and $T\tilde{\mathcal{L}}T^{-1} = \tilde{\mathcal{L}}$, so

$$T\mathcal{E}T^{-1} = \mathcal{E}. \tag{3.22}$$

(We will not consider odd p in detail, but we note in that case, $T\widetilde{\mathcal{M}}T^{-1} = \tilde{\mathcal{L}}$ and $T\tilde{\mathcal{L}}T^{-1} = \widetilde{\mathcal{M}}$ so, since $\widetilde{\mathcal{M}}^{\mathrm{t}} = \widetilde{\mathcal{M}}$ and $\tilde{\mathcal{L}}^{\mathrm{t}} = \tilde{\mathcal{L}}$ (on account of $\Theta^{\mathrm{t}} = \Theta$ where t is transpose), we have that $T\mathcal{E}T^{-1} = \mathcal{E}^{\mathrm{t}}$.)

Since T and $\mathcal{E}$ commute, they can be "simultaneously" diagonalized, in this case represented on a direct integral representation. One way of making this explicit is to define, for each $\beta \in \partial\mathbb{D}$, the space ℓ^∞_β, the sequences $\{u_n\}_{n=-\infty}^{\infty}$ obeying $u_{n+p} = \beta u_n$. This is clearly a space of dimension p since $\{u_n\}_{n=-\infty}^{\infty}$ mapping to $\{u_n\}_{n=0}^{p-1}$ (i.e., restriction) maps ℓ^∞_β to $\mathbb{C}^p$.

By (3.22), $\mathcal{E}$, which maps bounded sequences to bounded sequences, maps ℓ^∞_β to ℓ^∞_β, and so defines a finite-dimensional operator $\mathcal{E}_p(\beta)$ under the explicit relation of ℓ^∞_β mentioned above. One sees

$$\mathcal{E}_p(\beta) = \mathcal{L}_p\mathcal{M}_p(\beta), \tag{3.23}$$

where

$$\mathcal{L}_p = \Theta_0(\alpha_0) \oplus \cdots \oplus \Theta_{p-2}(\alpha_{p-2}), \tag{3.24}$$

$$\mathcal{M}_p(\theta) = \Theta_1(\alpha) \oplus \cdots \oplus \Theta_{p-3}(\alpha_{p-3}) \oplus \Theta^{(\beta)}_{p-1}(\alpha_{p-1}), \tag{3.25}$$

where $\Theta^{(\beta)}_{p-1}(\alpha)$ acts on δ_{p-1} and δ_0, and in that (ordered) basis has the form

$$\begin{pmatrix} \bar{\alpha} & \rho\beta \\ \rho\bar{\beta} & -\alpha \end{pmatrix}. \tag{3.26}$$

$\mathcal{E}_p(\beta)$ is called the *Floquet CMV matrix*. To make precise the connection to $\mathcal{E}$, we define the unitary Fourier transform $\mathcal{F}: \ell^2(\mathbb{Z}) \to L^2(\partial\mathbb{D}, \frac{\mathrm{d}\theta}{2\pi}; \mathbb{C}^p)$, the set of L^2 functions on $\partial\mathbb{D}$ with values in $\mathbb{C}^p$ by

$$(\mathcal{F}u)_k(\beta) = \sum_{n=-\infty}^{\infty} \beta^{-n} u_{k+np}. \tag{3.27}$$

Then

$$(\mathcal{F}\mathcal{E}\mathcal{F}^{-1}g)(\beta) = \mathcal{E}_p(\beta)g(\beta). \tag{3.28}$$

(For details, see [70, Section 11.2].)

Finally, we note a general relation of the eigenvalues of $\mathcal{E}_p(\beta)$ and the discriminant, $\Delta(z)$, of (3.19). For $z_0 \in \partial\mathbb{D}$ is an eigenvalue of $\mathcal{E}_p(\beta)$ if and only if there is $(u_1, u_0)^{\mathrm{t}}$ so that after a p-step transfer, we get $\beta(u_1, u_0)^{\mathrm{t}}$, that is, if and only if $z_0^{p/2}\beta$ is an eigenvalue of $T_p(z_0)$. This is true if and only if $z_0^{-p/2}T_p(z_0)$ has eigenvalues β and β^{-1} if and only if $\Delta(z_0) = \beta + \beta^{-1}$. It follows that

$$\det(z - \mathcal{E}_p(\beta)) = \left(\prod_{j=0}^{p-1} \rho_j\right) [z^{p/2}[\Delta(z) - \beta - \beta^{-1}]] \tag{3.29}$$

for both sides are monic polynomials of degree p and they have the same zeros.

4. CMV matrices for matrix-valued measures

Because of applications to perturbations of periodic Jacobi and CMV matrices [16], interest in matrix-valued measures (say, $k \times k$ matrices) has increased. Here we will provide the CMV basis and CMV matrices in this matrix-valued situation; these results are new here. Since adjoints of finite-dimensional matrices enter but we want to use * for Szegő reversed polynomials, in this section we use † for matrix adjoint.

Measures which are nontrivial in a suitable sense are described by a sequence $\{\alpha_j\}_{j=0}^\infty$ of Verblunsky coefficients that are $k \times k$ matrices with $\|\alpha_j\| < 1$.

To jump to the punch line, we will see that $\mathscr{C}$ still has an $\mathscr{L}\mathscr{M}$ factorization, where $\Theta(\alpha)$ is the $2k \times 2k$ matrix

$$\Theta(\alpha) = \begin{pmatrix} \alpha^\dagger & \rho^{\mathrm{L}} \\ \rho^{\mathrm{R}} & -\alpha \end{pmatrix}, \tag{4.1}$$

where

$$\rho^{\mathrm{L}} = (1 - \alpha^\dagger \alpha)^{1/2}, \quad \rho^{\mathrm{R}} = (1 - \alpha\alpha^\dagger)^{1/2}. \tag{4.2}$$

It is an interesting calculation to check that Θ is unitary, that is,

$$\begin{pmatrix} \alpha & \rho^{\mathrm{R}} \\ \rho^{\mathrm{L}} & -\alpha^\dagger \end{pmatrix} \begin{pmatrix} \alpha^\dagger & \rho^{\mathrm{L}} \\ \rho^{\mathrm{R}} & -\alpha \end{pmatrix} = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & \mathbf{1} \end{pmatrix}. \tag{4.3}$$

That $\alpha\alpha^\dagger + (\rho^{\mathrm{R}})^2 = 1 = (\rho^{\mathrm{L}})^2 + \alpha^\dagger\alpha$ follows from (4.2). That $\alpha\rho^{\mathrm{L}} - \rho^{\mathrm{R}}\alpha = \rho^{\mathrm{L}}\alpha^\dagger - \alpha^\dagger\rho^{\mathrm{R}} = 0$ follows by expanding the square roots in (4.2) in a Taylor series and using $\alpha(\alpha^\dagger\alpha)^m = (\alpha\alpha^\dagger)^m\alpha$.

To describe the model specifically, we have a $k \times k$ matrix-valued (normalized, positive) measure which can be described as follows: $\mathrm{d}\mu_t(\theta)$ is a positive scalar measure on $\partial\mathbb{D}$ and for a.e. $(\mathrm{d}\mu_t(\theta))$ a matrix $A(\theta)$ obeying

$$A(\theta) \geqslant 0, \quad \mathrm{Tr}(A(\theta)) = 1. \tag{4.4}$$

We write $\mathrm{d}\mu(\theta) = A(\theta)\,\mathrm{d}\mu_t(\theta)$. We assume $\mathrm{d}\mu$ is normalized in the sense that $\int A(\theta)\,\mathrm{d}\mu_t = \mathbf{1}$. We will consider $\mathscr{H}_{\mathrm{R}}$ to be the $k \times k$ matrix-valued functions, f, on $\partial\mathbb{D}$ with

$$\int \mathrm{Tr}(f(\theta)^\dagger A(\theta) f(\theta))\,\mathrm{d}\mu_t(\theta) < \infty. \tag{4.5}$$

The measure $\mathrm{d}\mu$ is called nontrivial if

$$\dim[\mathrm{span}\{B_\ell z^\ell\}_{\ell=0}^{n-1}] = nk^2 \tag{4.6}$$

for each n. Equivalently, for each n and $\{B_\ell\}_{\ell=0}^{n-1}$ in $\mathscr{L}(\mathbb{C}^k)$, we have $\sum_{\ell=0}^{n-1} B_\ell z^\ell = 0$ in $\mathscr{H}_{\mathrm{R}}$ implies $B_0 = B_1 = \cdots = B_{n-1} = 0$. Also equivalent is that $\langle\varphi, A(\theta)\varphi\rangle\,\mathrm{d}\mu_t(\theta)$ is nontrivial for each $\varphi \in \mathbb{C}^k \setminus \{0\}$.

Similarly, we define $\mathscr{H}_{\mathrm{L}}$ to be f's with

$$\int \mathrm{Tr}(f(\theta) A(\theta) f^\dagger(\theta))\,\mathrm{d}\mu_t(\theta) < \infty. \tag{4.7}$$

It is easy to see that nontriviality implies (4.6) holds also in $\mathscr{H}_{\mathrm{L}}$.

We define two "inner products," sesquilinear forms from $\mathscr{H}_{\mathrm{R}}$ and $\mathscr{H}_{\mathrm{L}}$ to $\mathscr{L}(\mathbb{C}^k)$, the $k \times k$ matrices:

$$\langle\langle f, g\rangle\rangle_{\mathrm{R}} = \int f^\dagger(\theta)\,\mathrm{d}\mu(\theta) g(\theta), \tag{4.8}$$

$$\langle\langle f, g\rangle\rangle_{\mathrm{L}} = \int g(\theta)\,\mathrm{d}\mu(\theta) f^\dagger(\theta). \tag{4.9}$$

The right side of (4.8) is shorthand for

$$\int f^\dagger(\theta) A(\theta) g(\theta)\,\mathrm{d}\mu_t(\theta)$$

so the LHS of (4.5) is $\mathrm{Tr}(\langle\langle f, g\rangle\rangle_{\mathrm{R}})$. The symbols L, R (for left and right) come from

$$\langle\langle f, gB\rangle\rangle_{\mathrm{R}} = \langle\langle f, g\rangle\rangle B \tag{4.10}$$

$$\langle\langle f, Bg\rangle\rangle_{\mathrm{L}} = B\langle\langle f, g\rangle\rangle \tag{4.11}$$

for constant $k \times k$ matrices, B.

The normalized matrix OPUC, $\varphi_n^{\mathrm{R}}, \varphi_n^{\mathrm{L}}$, are polynomials in z of degree n with matrix coefficients with

$$\langle\langle \varphi_n^{\mathrm{R}}, \varphi_m^{\mathrm{R}}\rangle\rangle_{\mathrm{R}} = \delta_{nm}\mathbf{1}, \quad \langle\langle \varphi_n^{\mathrm{L}}, \varphi_m^{\mathrm{L}}\rangle\rangle_{\mathrm{R}} = \delta_{nm}\mathbf{1}. \tag{4.12}$$

This determines φ uniquely up to a unitary right (resp., left) prefactor. We will pick this prefactor by demanding

$$\varphi_n^{\mathrm{R,L}}(z) = \kappa_n^{\mathrm{R,L}} z^n + \text{lower order}, \tag{4.13}$$

$$\kappa_{n+1}^{\mathrm{L}}(\kappa_n^{\mathrm{L}})^{-1} > 0, \quad (\kappa_n^{\mathrm{R}})^{-1}\kappa_{n+1}^{\mathrm{R}} > 0. \tag{4.14}$$

With this choice of normalization, one has a sequence of $k \times k$ matrices, $\{\alpha_n\}_{n=0}^{\infty}$, and the recursion relations

$$z\varphi_n^{\mathrm{L}} = \rho_n^{\mathrm{L}}\varphi_{n+1}^{\mathrm{L}} + \alpha_n^{\dagger}(\varphi_n^{\mathrm{R}})^*, \tag{4.15}$$

$$z\varphi_n^{\mathrm{R}} = \varphi_{n+1}^{\mathrm{R}}\rho_n^{\mathrm{R}} + (\varphi_n^{\mathrm{L}})^*\alpha_n^{\dagger}, \tag{4.16}$$

$$(\varphi_n^{\mathrm{L}})^* = (\varphi_{n+1}^{\mathrm{L}})^*\rho_n^{\mathrm{L}} + z\varphi_n^{\mathrm{R}}\alpha_n, \tag{4.17}$$

$$(\varphi_n^{\mathrm{R}})^* = \rho_n^{\mathrm{R}}\varphi_{n+1}^* + \alpha_n z\varphi_n^{\mathrm{L}}, \tag{4.18}$$

where $\rho_n^{\mathrm{R}}, \rho_n^{\mathrm{L}}$ are given by (4.2) and $P_n^*(z) = z^n P_n(1/\bar{z})^{\dagger}$. For construction of $\varphi_n^{\mathrm{L,R}}$ and proof of (4.15)–(4.18), see [7] or [69, Section 2.13] following Delsarte et al. [17] and Geronimo [29].

It will help to also have the following, which can be derived from (4.15)–(4.18):

$$\varphi_{n+1}^{\mathrm{L}} = \rho_n^{\mathrm{L}} z\varphi_n^{\mathrm{L}} - \alpha_n^{\dagger}(\varphi_{n+1}^{\mathrm{R}})^*, \tag{4.19}$$

$$(\varphi_{n+1}^{\mathrm{R}})^* = \rho_n^{\mathrm{R}}(\varphi_n^{\mathrm{R}})^* - \alpha_n\varphi_{n+1}^{\mathrm{L}}. \tag{4.20}$$

Following (2.19) and (2.20), we define the CMV and alternate CMV basis by

$$\chi_{2k}(z) = z^{-k}(\varphi_{2k}^{\mathrm{R}}(z))^*, \quad \chi_{2k-1}(z) = z^{-k+1}\varphi_{2k-1}^{\mathrm{L}}(z), \tag{4.21}$$

$$x_{2k}(z) = z^{-k}\varphi_{2k}^{\mathrm{L}}(z), \quad x_{2k-1}(z) = z^{-k}(\varphi_{2k-1}^{\mathrm{R}}(z))^*. \tag{4.22}$$

Proposition 4.1. *$\{\chi_\ell(z)\}_{\ell=0}^{\infty}$ and $\{x_\ell(z)\}_{\ell=0}^{\infty}$ are $\langle\langle\cdot,\cdot\rangle\rangle_{\mathrm{L}}$ orthonormal, that is,*

$$\langle\langle \chi_\ell, \chi_m\rangle\rangle_{\mathrm{L}} = \delta_{\ell m}, \quad \langle\langle x_\ell, x_m\rangle\rangle_{\mathrm{L}} = \delta_{\ell m}. \tag{4.23}$$

Moreover, χ_ℓ is in the module span of the first ℓ of $1, z, z^{-1}, \ldots$ and x_ℓ of $1, z^{-1}, z, \ldots$.

Remark. By module span of $\{f_j(z)\}_{j=1}^m$ of scalar functions, f, we mean elements in $\mathscr{H}_{\mathrm{L}}$ of the form $\sum_{j=1}^m B_j f_j(z)$ where $B_1, B_2, \ldots$ are fixed $k \times k$ matrices.

Proof. Eq. (4.23) for $\ell = m$ holds by (4.12) and (4.21), (4.22) if we note that

$$\langle\langle P_n^*, Q_n^*\rangle\rangle_{\mathrm{L}} = \langle\langle Q_n, P_n\rangle\rangle_{\mathrm{R}}. \tag{4.24}$$

It is obvious from the definition of χ_ℓ and x_ℓ that they lie in the proper span. To get (4.23) for $\ell < m$, we need to know that χ_ℓ is orthogonal to the first $\ell - 1$ of $1, z, z^{-1}, \ldots$ and x_ℓ to the first $\ell - 1$ of $1, z, z^{-1}, \ldots$. For cases where χ_ℓ or x_ℓ is given by φ^{L}, this follows from $\langle\langle z^k, \varphi_\ell^{\mathrm{L}}\rangle\rangle = 0$ for $0 \leqslant k < \ell$ and when it is a $(\varphi_\ell^{\mathrm{R}})^*$ from (4.24) which says

$$\langle\langle z^k, (\varphi_\ell^{\mathrm{R}})^*\rangle\rangle_{\mathrm{L}} = \langle\langle \varphi_\ell^{\mathrm{R}}, z^{\ell-k}\rangle\rangle = 0$$

for $0 \leqslant \ell - k < \ell$. $\square$

By a (left-) module basis for $\mathscr{H}_{\mathrm{L}}$, we mean a sequence $\{f_j\}_{j=0}^{\infty}$ orthonormal in $\langle\langle\cdot,\cdot\rangle\rangle_{\mathrm{L}}$, that is, $\langle\langle f_j, f_\ell\rangle\rangle_{\mathscr{L}} = \delta_{j\ell}$ so that as $\{B_j\}_{j=0}^{N}$ runs through all N-tuples of $k\times k$ matrices, $\sum_{j=0}^{N} B_j f_j$ is a sequence of subspaces whose union is dense in $\mathscr{H}_{\mathrm{L}}$. For any such basis, any $\eta\in\mathscr{H}_{\mathrm{L}}$ has a unique convergent expansion,

$$\eta = \sum\nolimits_{j=0}^{\infty} \langle\langle f_j, \eta\rangle\rangle f_j. \tag{4.25}$$

$\{\chi_j\}_{j=0}^{\infty}$ and $\{x_j\}_{j=0}^{\infty}$ are both module bases. That means, if $\mathscr{C}_{j\ell}$ is defined by

$$\mathscr{C}_{j\ell} = \langle \chi_j, z\chi_\ell\rangle \tag{4.26}$$

then the matrix, obtained by using the $k\times j$ blocks, $\mathscr{C}_{j\ell}$, is unitary. Moreover,

$$\mathscr{C}_{j\ell} = \sum_m \mathscr{L}_{jm}\mathscr{M}_{m\ell}, \tag{4.27}$$

where

$$\mathscr{L}_{j\ell} = \langle \chi_j, z x_\ell\rangle, \quad \mathscr{M}_{j\ell} = \langle x_j, \chi_\ell\rangle. \tag{4.28}$$

In (4.19), set $n=2k-1$ and multiply by z^{-k} to get

$$x_{2k} = -\alpha_n^\dagger \chi_{2k} + \rho_n^{\mathrm{L}}\chi_{2k-1}, \tag{4.29}$$

where a bottom row of Θ is clear. In this way, using (4.15), (4.18), (4.19), and (4.20), one obtains:

Theorem 4.2. *With $\Theta_j(\alpha)$ given by* (4.1) *acting on $\mathbb{C}^{2k}$ corresponding to δ_j, δ_{j+1}, we have*

$$\mathscr{M} = \mathbf{1}_{1\times 1} \oplus \Theta_1(\alpha_1) \oplus \Theta_3(\alpha_3) \oplus \cdots,$$
$$\mathscr{L} = \Theta_0(\alpha_0) \oplus \Theta_2(\alpha_2) \oplus \Theta_4(\alpha_4) \oplus \cdots.$$

The analog of (2.29) is

$$\mathscr{C} = \begin{pmatrix} \alpha_0^\dagger & \rho_0^{\mathrm{L}}\alpha_1^\dagger & \rho_0^{\mathrm{L}}\rho_1^{\mathrm{L}} & 0 & 0 & \ldots \\ \rho_0^{\mathrm{R}} & -\alpha_0\alpha_1^\dagger & -\alpha_0\rho_1^{\mathrm{L}} & 0 & 0 & \ldots \\ 0 & \rho_1^{\mathrm{R}}\alpha_2^\dagger & -\alpha_1\alpha_2^\dagger & \rho_2^{\mathrm{L}}\alpha_3^\dagger & \rho_2^{\mathrm{L}}\rho_3^{\mathrm{L}} & \ldots \\ 0 & \rho_1^{\mathrm{R}}\rho_2^{\mathrm{R}} & -\alpha_1\rho_2^{\mathrm{R}} & -\alpha_2\alpha_3^\dagger & -\alpha_2\rho_3^{\mathrm{L}} & \ldots \\ 0 & 0 & 0 & \rho_3^{\mathrm{R}}\alpha_4^\dagger & -\alpha_3\alpha_4^\dagger & \end{pmatrix}. \tag{4.30}$$

We note for later purposes that for this matrix case, the GGT matrix, which we will discuss in Section 10, has the form

$$\mathscr{G}_{k\ell} = \begin{cases} -\alpha_{k-1}\rho_k^{\mathrm{L}}\rho_{k+1}^{\mathrm{L}}\cdots\rho_{\ell-1}^{\mathrm{L}}\alpha_\ell^\dagger, & 0\leqslant k\leqslant \ell, \\ \rho_\ell^{\mathrm{R}}, & k=\ell+2, \\ 0, & k\geqslant \ell+2, \end{cases} \tag{4.31}$$

that is,

$$\mathscr{G} = \begin{pmatrix} \alpha_0^\dagger & \rho_0^{\mathrm{L}}\alpha_1^\dagger & \rho_0^{\mathrm{L}}\rho_1^{\mathrm{L}}\alpha_2^\dagger & \rho_0^{\mathrm{L}}\rho_1^{\mathrm{L}}\rho_2^{\mathrm{L}}\alpha_3^\dagger \\ \rho_0^{\mathrm{R}} & -\alpha_0\alpha_1^\dagger & -\alpha_0\rho_1^{\mathrm{L}}\alpha_2^\dagger & -\alpha_0\rho_1^{\mathrm{L}}\rho_2^{\mathrm{L}}\alpha_3^\dagger \\ 0 & \rho_1^{\mathrm{R}} & -\alpha_1\alpha_2^\dagger & -\alpha_1\rho_2^{\mathrm{L}}\alpha_3^\dagger \\ \ldots & \ldots & \ldots & \ldots \end{pmatrix}. \tag{4.32}$$

5. Rank one covariances

For self-adjoint matrices, the most elementary rank one perturbations are diagonal, that is, $J\mapsto J+\lambda(\delta_n,\cdot)\delta_n$, where δ_n is the vector with 1 in position n and 0 elsewhere. The impact of such a change on Jacobi parameters is trivial:

$a_m \to a_m$, $b_m \to b_m + \lambda\delta_{nm}$ (if we label vectors in the self-adjoint case starting at $n = 1$). One of our goals is to find the analog for CMV matrices, where we will see that the impact on Verblunsky coefficients is more subtle.

We will also address a related issue: in the spectral theory of OPUC, the family of measures, $d\mu_\lambda$ with $\alpha_n(d\mu_\lambda) = \lambda\alpha_n$ for a fixed $\{\alpha_n\}_{n=0}^{\infty}$, called an Aleksandrov family, plays an important role analogous to a change of boundary condition in ODE's. If φ_n are the normalized OPUC, the GGT matrix,

$$\mathcal{G}_{k\ell}(\{\alpha_n\}_{n=0}^{\infty}) = \langle \varphi_k, z\varphi_\ell \rangle \tag{5.1}$$

has the property that $\mathcal{G}(\{\lambda\alpha_n\}_{n=0}^{\infty}) - \mathcal{G}(\{\alpha_n\}_{n=0}^{\infty})$ is rank one (see [69, p. 259]). But for the CMV basis, $\mathcal{C}(\{\lambda\alpha_n\}_{n=0}^{\infty}) - \mathcal{C}(\{\alpha_n\}_{n=0}^{\infty})$ is easily seen to be infinite rank (if the α's are not mainly 0). However, we will see here that for a suitable U_λ (depending on λ but not on α!), $U_\lambda \mathcal{C}(\{\lambda\alpha_n\}_{n=0}^{\infty})U_\lambda^{-1} - \mathcal{C}(\{\alpha_n\}_{n=0}^{\infty})$ is rank one.

We need to begin by figuring out what are natural rank one perturbations. The key realization is that the proper format is multiplicative: let P be a rank one projection and $W_\theta = e^{i\theta P} = (\mathbf{1} - P) + e^{i\theta}P$. Then $W_\theta - \mathbf{1} = (e^{i\theta} - 1)P$ is rank one, and for any U, UW_θ is a rank one perturbation of U. It will be convenient to parametrize by $\lambda = e^{i\theta} \in \partial\mathbb{D}$. Thus, we define

$$W^{(m)}(\lambda) = \mathbf{1} + (e^{i\theta} - 1)(\delta_m, \cdot\, \delta_m) \tag{5.2}$$

and given any CMV matrix $\mathcal{C}$, we let

$$\mathcal{C}^m(\lambda) = \mathcal{C}W^{(m)}(\lambda). \tag{5.3}$$

We will use $\mathcal{C}^m(\lambda; \{\alpha_k\})$ where we want to make the α-dependence explicit. Notice that

$$\mathcal{C}^m_{\ell k}(\lambda) = \begin{cases} \mathcal{C}_{\ell k} & \text{if } k \neq m, \\ \lambda\mathcal{C}_{\ell k} & \text{if } k = m, \end{cases} \tag{5.4}$$

that is, we multiply column m by λ.

Part of the result we are heading towards is that

$$\alpha_\ell(\mathcal{C}^m(\lambda)) = \begin{cases} \alpha_\ell(\mathcal{C}) & \ell < m, \\ \lambda^{-1}\alpha_\ell(\mathcal{C}) & \ell \geqslant m, \end{cases} \tag{5.5}$$

In particular, $\mathcal{C}^0(\bar{\lambda})$ realizes the fact that $\mathcal{C}(\{\lambda\alpha_k\}_{k=0}^{\infty})$ is unitarily equivalent to a rank one perturbation of $\mathcal{C}(\{\alpha_k\}_{k=0}^{\infty})$. Eq. (5.5) for the important case $m = 0$ is due to Simon [69, Theorem 4.2.9] and for the general case to Simon [72]. We will sketch the various proofs.

While we will eventually provide explicit unitaries that show $\mathcal{C}^m(\lambda; \{\alpha_j\}_{j=0}^{\infty})$ is unitarily equivalent to $\mathcal{C}$ (right side of (5.5)), we begin with a direct proof of (5.5) in case $m = 0$.

Theorem 5.1. $\mathcal{C}^{m=0}(\lambda; \{\alpha_j\}_{j=0}^{\infty})$ *has Verblunsky coefficients* $\{\lambda^{-1}\alpha_j\}_{j=0}^{\infty}$.

Remark. If $\mathcal{M}^{(\lambda)} = \lambda\mathbf{1} \oplus \Theta(\alpha_1) \oplus \Theta(\alpha_3) \oplus \cdots$, that is, the 1 in the upper left corner is replaced by λ, then $\mathcal{L}\mathcal{M}^{(\lambda)} = \mathcal{C}W^{(0)}(\lambda)$.

Sketch proof (*See [69, Theorems 4.2.9, Subsection 1.4.16]*). By definition,

$$\mathcal{C}^{m=0}_\lambda - \mathcal{C} = (\lambda - 1)\mathcal{C}P_0, \tag{5.6}$$

where $P_0 = \langle \delta_0, \cdot \rangle \delta_0$. Define, for $z \in \mathbb{D}$, F_λ and the f_λ by

$$F_\lambda(z) = \langle \delta_0, (\mathcal{C}^{m=0}_\lambda - z)(C^{m=0}_\lambda + z)^{-1}\delta_0 \rangle \tag{5.7}$$

$$= \frac{1 + zf_\lambda(z)}{1 - zf_\lambda(z)}. \tag{5.8}$$

Using the second resolvent formula and (5.6) implies (see [69, Subsection 1.4.16]) that

$$f_\lambda(z) = \lambda^{-1} f(z). \tag{5.9}$$

The Schur algorithm and Geronimus theorem (see [69, Chapter 3]) then imply (5.5) for $m = 0$. □

For discussion of the movement of eigenvalues under the perturbations of Theorem 5.1, see [6,13,25,69, Theorem 3.2.17].

The key to an explicit unitary equivalence is the following. Let

$$v(\lambda) = \begin{pmatrix} 1 & 0 \\ 0 & \lambda \end{pmatrix}, \quad \tilde{v}(\lambda) = \begin{pmatrix} \lambda & 0 \\ 0 & 1 \end{pmatrix}. \tag{5.10}$$

Then, by a simple calculation,

$$v(\lambda)\Theta(\lambda^{-1}\alpha)v(\lambda) = \lambda\Theta(\alpha), \tag{5.11}$$
$$\tilde{v}(\lambda)^{-1}\Theta(\lambda^{-1}\alpha)\tilde{v}(\lambda)^{-1} = \lambda^{-1}\Theta(\alpha). \tag{5.12}$$

Note that (5.11) does not use $v(\lambda)$ and $v(\lambda)^{-1}$ but $v(\lambda)$ in both places. Similarly, (5.12) has $\tilde{v}(\lambda)^{-1}$ in both places. In the full calculation, one does not use

$$U\mathscr{L}\mathscr{M}U^{-1} = (U\mathscr{L}U^{-1})(U\mathscr{M}U^{-1})$$

but rather

$$U\mathscr{L}\mathscr{M}U^{-1} = (U\mathscr{L}U)(U^{-1}\mathscr{M}U^{-1}). \tag{5.13}$$

We need a notation for diagonal matrices. $D(1^{2k}(1\lambda)^{\infty})$ indicates the diagonal matrix with entries 1 $2k$ times, then alternating 1's and λ's. Thus,

$$W^{(m)}(\lambda) = D(1^m\lambda 1^{\infty}). \tag{5.14}$$

Using (5.11)–(5.14), a direct calculation (see [72, Section 5]) shows:

Theorem 5.2. *For* $n = 0, 1, 2, \ldots,$ *define*

$$U_{2k-1} = D(1^{2k}(1\lambda)^{\infty}), \tag{5.15}$$
$$U_{2k} = D(\lambda^{2k}(1\lambda)^{\infty}), \tag{5.16}$$
$$T_{n,\lambda}(\{\alpha_j\}_{j=0}^{\infty}) = \beta_j, \tag{5.17}$$

where

$$\beta_j = \begin{cases} \alpha_j & j < n, \\ \lambda\alpha_j & j \geqslant n. \end{cases} \tag{5.18}$$

Then

$$U_n\mathscr{C}(T_{n,\lambda^{-1}}(\{\alpha_j\}_{j=0}^{\infty}))U_n^{-1} = \mathscr{C}(\{\alpha_j\}_{j=0}^{\infty})W^{(n)}(\lambda). \tag{5.19}$$

In particular, (5.5) *holds*.

Remark 1. It is important that δ_0 is an eigenvector of U_n since Verblunsky coefficients involve a unitary and a cyclic vector. Eq. (5.19) also shows that $\mathscr{C}W^{(n)}(\lambda)$ has δ_0 as a cyclic vector.

2. One can also ask about Verblunsky coefficients of $W^{(n)}(\lambda)\mathscr{C}(\{\alpha_j\}_{j=0}^{\infty})$. Since Verblunsky coefficients are invariant under unitaries that have δ_0 as an eigenvector and

$$W^{(n)}\mathscr{C} = W^{(n)}\mathscr{C}W^{(n)}(W^{(n)})^{-1}$$

the Verblunsky coefficients of $\mathscr{C}W^{(n)}$ and $W^{(n)}\mathscr{C}$ are the same.

Eqs. (5.11)–(5.13) imply a result about extended CMV matrices. For $\lambda \in \partial\mathbb{D}$, let $\widetilde{W}(\lambda)$ be the two-sided diagonal matrix with $d_{2j} = 1$, $d_{2j+1} = \lambda$. Then:

Theorem 5.3. *Let* $\lambda \in \partial\mathbb{D}$. *Then* $\widetilde{W}(\lambda)\mathscr{E}(\{\alpha_n\}_{n=-\infty}^{\infty})\widetilde{W}(\lambda)^{-1} = \mathscr{E}(\{\lambda\alpha_n\}_{n=-\infty}^{\infty})$.

Remark. In particular, spectral properties of $\mathscr{E}(\{\alpha_n\}_{n=-\infty}^{\infty})$ and $\mathscr{E}(\{\lambda\alpha_n\}_{n=-\infty}^{\infty})$ are identical and $\alpha_n \to \lambda\alpha_n$ preserves isospectral tori in the periodic case.

6. Resolvents of CMV matrices

In this section, we will present formulae for the resolvent of $\mathcal{C}$ analogous to the Green's function formula for Jacobi matrices (see [69, Theorem 4.4.3]). These formulae appeared first in [69, Section 4.4]. Similar formulae for GGT matrices appeared earlier in Geronimo–Teplyaev [33] (see also [31,32]).

Clearly, we need an analog of Jost solutions. For OPUC, these were found by Golinskii–Nevai [41] who proved:

Theorem 6.1. *Fix $z \in \mathbb{D}$. Let φ_n be the normalized OPUC for a probability measure $\mathrm{d}\mu$ on $\partial\mathbb{D}$, and ψ_n the normalized OPUC for Verblunsky coefficients $-\alpha_n(\mathrm{d}\mu)$ (so-called second kind polynomials). Then*

$$\sum_{n=0}^{\infty} |\psi_n(z) + F(z)\varphi_n(z)|^2 + |\psi_n^*(z) - F(z)\varphi_n^*(z)|^2 < \infty, \tag{6.1}$$

where F is the Carathéodory function:

$$F(z) \equiv \int \frac{\mathrm{e}^{\mathrm{i}\theta} + z}{\mathrm{e}^{\mathrm{i}\theta} - z}\,\mathrm{d}\mu(\theta). \tag{6.2}$$

Remark 1. This is an analog of Weyl's formula; see [69, (1.2.53)].
2. See [41] or [69, Section 3.2] for a proof.

With this in mind, we define

$$y_n = \begin{cases} z^{-\ell}\psi_{2\ell} & n = 2\ell, \\ -z^{-\ell}\psi_{2\ell-1}^* & n = 2\ell - 1, \end{cases} \tag{6.3}$$

$$\Upsilon_n = \begin{cases} -z^{-\ell}\psi_{2\ell}^* & n = 2\ell, \\ z^{-\ell+1}\psi_{2\ell-1} & n = 2\ell - 1, \end{cases} \tag{6.4}$$

$$p_n = y_n + F(z)x_n, \tag{6.5}$$

$$\pi_n = \Upsilon_n + F(z)\chi_n. \tag{6.6}$$

Then Theorem 4.4.1 of [69] says:

Theorem 6.2. *We have that for $z \in \mathbb{D}$,*

$$[(\mathcal{C} - z)^{-1}]_{k\ell} = \begin{cases} (2z)^{-1}\chi_\ell(z)p_k(z), & k > \ell \text{ or } k = \ell = 2n - 1, \\ (2z)^{-1}\pi_\ell(z)x_k(z), & \ell > k \text{ or } k = \ell = 2n. \end{cases} \tag{6.7}$$

As a special case, since $\delta_n = \chi_n(\mathcal{C})\delta_0$ and $|\chi_n(\mathrm{e}^{\mathrm{i}\theta})| = |\varphi_n(\mathrm{e}^{\mathrm{i}\theta})|$, we obtain from a spectral representation

$$\int \frac{|\varphi_n(\mathrm{e}^{\mathrm{i}\theta})|^2}{\mathrm{e}^{\mathrm{i}\theta} - z}\,\mathrm{d}\mu(\theta) = (2z^{n+1})^{-1}\varphi_n(z)[-\psi_n^*(z) + F(z)\varphi_n^*(z)]. \tag{6.8}$$

As shown in remarks to [70, Theorem 9.2.4], this is equivalent to a formula of Khrushchev [49] for $\int \frac{\mathrm{e}^{\mathrm{i}\theta}+z}{\mathrm{e}^{\mathrm{i}\theta}-z}|\varphi_n(\mathrm{e}^{\mathrm{i}\theta})|^2\,\mathrm{d}\mu(\theta)$. For an application of Theorem 6.2, see Stoiciu [74].

7. $\mathcal{I}^p$ perturbations

In this section, we give some elementary estimates of Golinskii–Simon [42] on the $\mathcal{I}^p$ norm of $\mathcal{C}(\{\alpha_n\}_{n=0}^\infty) - \mathcal{C}(\{\beta_n\}_{n=0}^\infty)$. (For definition and background on Schatten p-classes, see Gohberg–Krein [39] and Simon [71].)

In this section, we will use these estimates to write the Szegő function in terms of Fredholm determinants of the CMV matrices and to discuss scattering theory. Further applications appear in Section 9.

A diagonal matrix, A, has $\mathscr{I}_p$ norm $(\sum_j |a_{jj}|^p)^{1/p}$) and $\|A\|_p$ is invariant under multiplication by a unitary. So if A has only a nonvanishing kth principal diagonal, A has $\mathscr{I}_p$ norm $(\sum_j |a_{j\,j+k}|^p)^{1/p}$. Since $(a^{1/p}+b^{1/p}+c^{1/p}) \leqslant (a+b+c)^{1/p}3^{1-1/p}$ (by Hölder's inequality), we see for tridiagonal matrices that

$$\|A-B\|_p \leqslant 3^{1-1/p}\left(\sum_{i,j}|a_{ij}-b_{ij}|^p\right)^{1/p}. \tag{7.1}$$

This lets us estimate $\|\mathscr{L}(\{\alpha_n\}_{n=0}^\infty) - \mathscr{L}(\{\beta_n\}_{n=0}^\infty)\|_p$, and similarly for $\mathscr{M}$. Using unitarity of $\mathscr{L}$ and $\mathscr{M}$, $\|\mathscr{L}\mathscr{M} - \mathscr{L}'\mathscr{M}'\|_p \leqslant \|(\mathscr{L}-\mathscr{L}')\mathscr{M}\|_p + \|\mathscr{L}'(\mathscr{M}-\mathscr{M}')\|_p \leqslant \|\mathscr{L}-\mathscr{L}'\|_p + \|\mathscr{M}-\mathscr{M}'\|_p$. So using $(a^{1/p}+b^{1/p}) \leqslant 2^{1-1/p}(a+b)^{1/p}$, we find:

Theorem 7.1 (*Simon [69, Theorem 4.3.2]*). *Let $\{\alpha_n\}_{n=0}^\infty$, $\{\beta_n\}_{n=0}^\infty$ be two sequences in $\overline{\mathbb{D}}^\infty$ and let $\rho_n = (1-|\alpha_n|^2)^{1/2}$, $\sigma_n = (1-|\beta_n|^2)^{1/2}$. Then*

$$\|\mathscr{C}(\{\alpha_n\}_{n=0}^\infty) - \mathscr{C}(\{\beta_n\}_{n=0}^\infty)\|_p \leqslant 6^{1-1/p}\left(\sum_{n=0}^\infty |\alpha_n-\beta_n|^p + |\rho_n-\sigma_n|^p\right)^{1/p}. \tag{7.2}$$

Remark. Eq. [69] has the constants 2 for $1 \leqslant p \leqslant 2$ and $2\cdot 3^{1-1/2p}$ for $2 \leqslant p \leqslant \infty$, but the proof there actually shows $2^{1-1/p}$ and $2^{1-1/p}\,3^{1-1/2p}$. This improves the constant in (7.2).

To rephrase in terms of $|\alpha_n - \beta_n|$ only, we first note that

$$\sup_{|z|\leqslant R}\left|\frac{\mathrm{d}}{\mathrm{d}z}(1-|z|^2)^{1/2}\right| \leqslant (1-R^2)^{-1/2}$$

and $||z|-|w|| \leqslant |z-w|$ to see that

$$\sup_{|z|,|w|\leqslant R} |(1-|z|^2)^{1/2} - (1-|w|^2)^{1/2}| \leqslant (1-R^2)^{-1/2}|z-w|. \tag{7.3}$$

We need to note that $|\sqrt{a}-\sqrt{b}\,| \leqslant \sqrt{|a-b|}$ and $||\alpha|^2-|\beta|^2| \leqslant 2|\alpha-\beta|$, so

$$|(1-|z|^2)^{1/2} - (1-|w|^2)^{1/2}| \leqslant \sqrt{2}\,|z-w|^{1/2}. \tag{7.4}$$

Thus,

Theorem 7.2. *Let $\{\alpha_n\}_{n=0}^\infty$ and $\{\beta_n\}_{n=0}^\infty$ be two sequences in $\overline{\mathbb{D}}^\infty$ and let $\rho_n = (1-|\alpha_n|^2)^{1/2}$, $\sigma_n = (1-|\beta_n|^2)^{1/2}$. Then*

(a) If $\sup_n|\alpha_n| \leqslant R < 1$ *and* $\sup_n|\beta_n| \leqslant R$, *then*

$$\|\mathscr{C}(\{\alpha_n\}_{n=0}^\infty) - \mathscr{C}(\{\beta_n\}_{n=0}^\infty)\|_p \leqslant 6^{1-1/p}[1+(1-R^2)^{-p/2}]^{1/p}\left(\sum_{n=0}^\infty |\alpha_n-\beta_n|^p\right)^{1/p}. \tag{7.5}$$

(b) *In general, for $1 \leqslant p \leqslant \infty$,*

$$\|\mathscr{C}(\{\alpha_n\}_{n=0}^\infty) - \mathscr{C}(\{\beta_n\}_{n=0}^\infty)\|_p \leqslant 6^{1-1/p}\left(\sum_{n=0}^\infty |\alpha_n-\beta_n|^p + 2^{p/2}|\alpha_n-\beta_n|^{p/2}\right)^{1/p}. \tag{7.6}$$

One thing made possible by CMV matrices is scattering theory because all CMV matrices act on the same space ($\ell^2(\{0,1,2,\ldots\})$). This is an important tool made possible by the CMV matrix. Thus,

Theorem 7.3. *Suppose* $\sup_n |\alpha_n| \leqslant R \leqslant 1$, $\sup_n |\beta_n| \leqslant R < 1$, *and*

$$\sum_{n=0}^{\infty} |\alpha_n - \beta_n| < \infty. \tag{7.7}$$

Then, if $P_{\mathrm{ac}}(\cdot)$ *is the projection onto the absolutely continuous subspace of an operator and* $\mathcal{C} = \mathcal{C}(\{\alpha_n\}_{n=0}^{\infty})$, $\widetilde{\mathcal{C}} = \mathcal{C}(\{\beta_n\}_{n=0}^{\infty})$, *then*

$$\lim_{n\to\pm\infty} \mathcal{C}^n \widetilde{\mathcal{C}}^{-n} P_{\mathrm{ac}}(\widetilde{\mathcal{C}})$$

exists and is a partial isometry with range $P_{\mathrm{ac}}(\mathcal{C})$. *In particular,* $\mathcal{C} \restriction P_{\mathrm{ac}}(\mathcal{C})$ *and* $\widetilde{\mathcal{C}} \restriction P_{\mathrm{ac}}(\widetilde{\mathcal{C}})$ *are unitarily equivalent.*

Remark 1. This follows from the fact that $\mathcal{C} - \widetilde{\mathcal{C}}$ is trace class and from the Kato–Birman theorem [65].

2. If $\{\alpha_n\}_{n=0}^{\infty}$ corresponds to

$$\mathrm{d}\mu = f(\theta)\,\frac{\mathrm{d}\theta}{2\pi} + \mathrm{d}\mu_\delta \tag{7.8}$$

and $\{\beta_n\}_{n=0}^{\infty}$ corresponds to

$$\mathrm{d}\nu = g(\theta)\,\frac{\mathrm{d}\theta}{2\pi} + \mathrm{d}\nu_\delta \tag{7.9}$$

then this theorem implies that up to sets of $\mathrm{d}\theta$-measure 0,

$$\{\theta \,|\, f(\theta) \neq 0\} = \{\theta \,|\, g(\theta) \neq 0\} \tag{7.10}$$

(also see Theorem 9.3).

3. For the case $\beta_n \equiv 0$, this holds if only $\sum_{n=0}^{\infty} |\alpha_n|^2 < \infty$; see [70, Section 10.7].

Finally, following Simon [69, Section 4.2], we want to state the connection of $\mathcal{C}$ to the Szegő function, defined for $|z| < 1$ by

$$D(z) = \lim_{n\to\infty} \varphi_n^*(z)^{-1} \tag{7.11}$$

which exists and is nonzero if (and only if)

$$\sum_{j=0}^{\infty} |\alpha_j|^2 < \infty \tag{7.12}$$

(see [69, Section 2.4]). We will let $\mathcal{C}_0$ be the free CMV matrix corresponding to $\mathrm{d}\mu = \frac{\mathrm{d}\theta}{2\pi}$; equivalently, $\alpha_n \equiv 0$.

Theorem 7.4. *Suppose*

$$\sum_{n=0}^{\infty} |\alpha_n| < \infty. \tag{7.13}$$

Then $\mathcal{C} - \mathcal{C}_0$ *is trace class and*

$$D(z)^{-1} D(0) = \det\left(\frac{1 - z\bar{\mathcal{C}}}{1 - z\bar{\mathcal{C}}_0}\right). \tag{7.14}$$

If (7.12) *holds, then* $\mathcal{C} - \mathcal{C}_0$ *is Hilbert–Schmidt, and*

$$D(z)^{-1} D(0) = \det\nolimits_2\left(\frac{1 - z\bar{\mathcal{C}}}{1 - z\bar{\mathcal{C}}_0}\right) \mathrm{e}^{-zw_1}, \tag{7.15}$$

where

$$w_1 = \alpha_0 - \sum_{j=1}^{\infty} \alpha_j \bar{\alpha}_{j-1}. \tag{7.16}$$

Remarks. 1. Alas, [69, (4.2.53)] has a sign error: it is e^{-zw_1} as we have here, not e^{zw_1} as appears there!

2. By $\det\left(\frac{1-z\bar{\mathscr{C}}}{1-z\bar{\mathscr{C}}_0}\right)$, we mean $\det((1-z\bar{\mathscr{C}})(1-z\bar{\mathscr{C}}_0)^{-1})$. Since

$$(1-z\bar{\mathscr{C}})(1-z\bar{\mathscr{C}}_0)^{-1} = 1 - z(\bar{\mathscr{C}} - \bar{\mathscr{C}}_0)(1-z\bar{\mathscr{C}}_0)^{-1}$$

we see that this is 1+ trace class (resp., Hilbert–Schmidt) if $\mathscr{C} - \mathscr{C}_0$ is trace class (resp., Hilbert–Schmidt).

3. For a proof, see [69, Section 4.2, Theorem 4.2.14].

4. $\bar{\mathscr{C}}$ is the complex conjugate of $\mathscr{C}$, that is, $(\bar{\mathscr{C}})_{ij} = \overline{(\mathscr{C}_{ij})}$.

5. $\det(\cdot)$ is defined on operators of the form $1 + A$ with A trace class, and then $\det_2$ on $1 + A$ with A Hilbert–Schmidt by

$$\det(1 + A) = \det_2((1 + A)e^{-A}). \tag{7.17}$$

When A is trace class,

$$\det(1 + A) = \det_2(1 + A)e^{\mathrm{Tr}(A)}. \tag{7.18}$$

If (7.13) holds, $-zw_1 = \mathrm{Tr}((1-z\bar{\mathscr{C}})/(1-z\bar{\mathscr{C}}_0))$ and (7.14)/(7.15) are consistent by (7.18). See [39] or [71] for a discussion of $\det(\cdot)$ and $\det_2(\cdot)$.

6. The connection for one-dimensional Schrödinger operators of the Jost function and Fredholm determinants goes back to Jost–Pais [46]. For Jacobi matrices, under the name “perturbation determinant,” they were used in [52].

8. Essential spectra

The *discrete spectrum* of an operator is the set of isolated points of finite multiplicity. The complement of the discrete spectrum in the spectrum is called the *essential spectrum*. Since a CMV matrix has a cyclic vector, the essential spectrum is just the set of nonisolated points in the support of the spectral measure, $d\mu$, often called the *derived set* of $\mathrm{supp}(d\mu)$. Last–Simon [54] have a general result for the essential spectrum of a CMV matrix $\mathscr{C}(\{\alpha_n\}_{n=0}^{\infty})$.

Definition. A *right limit* of $\{\alpha_n\}_{n=0}^{\infty}$ is any two-sided sequence $\{\beta_n\}_{n=-\infty}^{\infty}$ in $\overline{\mathbb{D}}^{\mathbb{Z}}$ for which there exists $n_\ell \to \infty$ so $\lim_{\ell\to\infty} \alpha_{n_\ell + j} = \beta_j$ for each $j \in \mathbb{Z}$. $\mathscr{R}(\{\alpha_n\}_{n=0}^{\infty})$ is the set of right limits of $\{\alpha_n\}_{n=0}^{\infty}$.

Since $\overline{\mathbb{D}}^{\mathbb{Z}}$ is compact, $\mathscr{R}$ is nonempty. Indeed, if $\tilde{\beta}_0$ is any limit point of α_n, there is a right limit with $\beta_0 = \tilde{\beta}_0$.

Theorem 8.1 (*Last–Simon [54]*). *For any* $\{\alpha_n\}_{n=0}^{\infty} \in \overline{\mathbb{D}}^{\infty}$, *we have*

$$\sigma_{\mathrm{ess}}(\mathscr{C}(\{\alpha_n\}_{n=0}^{\infty})) = \overline{\bigcup_{\beta\in\mathscr{R}(\{\alpha_n\}_{n=0}^{\infty})} \sigma(\mathscr{E}(\{\beta_n\}_{n=0}^{\infty}))} \tag{8.1}$$

Remark 1. The proof [54] uses a Weyl trial sequence argument. The key is that because $\mathscr{C}$ has finite width, for any $\lambda_0 \in \sigma_{\mathrm{ess}}(\mathscr{C})$ and ε, there exist $L, n_j \to \infty$ and φ_j supported in $(n_j - L, n_j + L)$ with $\|\varphi_j\| = 1$ and

$$\limsup_{j\to\infty} \|(\mathscr{C} - \lambda_0)\varphi_j\| \leqslant \varepsilon. \tag{8.2}$$

2. Right limits of Verblunsky coefficients were considered earlier by Golinskii–Nevai [41], motivated by earlier work on Schrödinger operators in [53]. This work was in the context of a.c. spectrum (see [70, Theorem 10.9.11(ii)]).

3. Ref. [54] used the same methods to study Jacobi and Schrödinger operators. Earlier results of form (7.1) for Schrödinger operators (but not for CMV matrices) are due to Georgescu–Iftimovici [28], Măntoiu [56], and Rabinovich

[63]. These rely on what I regard as elaborate machines (connected with C^*-algebras or with Fredholm operators) although, no doubt, their authors regard them as very natural.

One can combine this with Theorem 5.3 to obtain:

Theorem 8.2. *Let* $\{\alpha_j\}_{j=0}^\infty$ and $\{\beta_j\}_{j=0}^\infty$ *be two sequences of Verblunsky coefficients. Suppose there exist* $\lambda_j \in \partial\mathbb{D}$ *so that*

$$\text{(i)} \quad \beta_j\lambda_j - \alpha_j \to 0, \tag{8.3}$$

$$\text{(ii)} \quad \lambda_{j+1}\bar{\lambda}_j \to 1. \tag{8.4}$$

Then

$$\sigma_{\text{ess}}(\mathcal{C}(\{\alpha_j\}_{j=0}^\infty)) = \sigma_{\text{ess}}(\mathcal{C}(\{\beta_j\}_{j=0}^\infty)). \tag{8.5}$$

Proof. Let $\{\gamma_j\}_{j=-\infty}^\infty$ be a right limit of $\{\beta_j\}_{j=0}^\infty$. By passing to a subsequence, we can suppose $\lambda_{n_j} \to \lambda_\infty$ and $\beta_{n_j+k} \to \gamma_k$. Since $\lambda_{n_j+k}\lambda_{n_j}^{-1} \to 1$, we see that $\alpha_{n_j+k} \to \lambda_\infty\gamma_k$. By Theorem 5.3, $\sigma(\mathcal{E}(\{\gamma_k\}_{k=-\infty}^\infty)) = \sigma(\mathcal{E}(\{\lambda_\infty\gamma_k\}_{k=-\infty}^\infty))$. It follows (using symmetry) that (8.5) holds. $\square$

Remark. This proof is from [54], but the result appears earlier [69, Theorem 4.3.8], motivated by a special case of Barrios–López [9].

Example 8.3. (This is due to Golinskii [40]; the method of proof is due to [54]. See the discussion in [54] for earlier related results.) Suppose $|\alpha_n| \to 1$ as $n \to \infty$. Then $\sigma_{\text{ess}}(\mathcal{C}(\{\alpha_n\})_{n=0}^\infty)$ is the set of limit points of $\{-\bar{\alpha}_{j+1}\alpha_j\}_{j=0}^\infty$. For any limit point has $\mathcal{E}(\{\beta_j\}_{j=0}^\infty)$ diagonal (since $(1-|\beta_j|^2)^{1/2} \equiv 0$) with diagonal values $-\bar{\beta}_{j+1}\beta_j$, and by compactness, any limit point of $-\bar{\alpha}_{j+1}\alpha_j$ occurs as some $-\bar{\beta}_1\beta_0$. In particular, this (plus an extra argument) implies $\sigma_{\text{ess}}(\mathcal{E}) = \{\lambda_0\}$ if and only if $|\alpha_n| \to 1$ and $\bar{\alpha}_{n+1}\alpha_n \to -\lambda_0$. See [40,54] for a discussion of when $\sigma_{\text{ess}}(\mathcal{C})$ is a finite set.

It is well known (see [69, Example 1.6.12]; [70, Example 11.1.4]) that if $\alpha_n \equiv a \in \mathbb{D}$, then $\sigma_{\text{ess}}(\mathcal{C}) = \Delta_{|a|} = \{z \in \partial\mathbb{D} \mid |\arg z| \geqslant 2\arcsin(|a|)\}$, which increases as $|a|$ decreases. It follows:

Example 8.4 (*Last and Simon [54, Theorem 7.8]; one direction was proven in [14], which motivated [54, Theorem 7.8].*). Suppose

$$\frac{\alpha_{j+1}}{\alpha_j} \to 1 \quad \liminf |\alpha_j| = a. \tag{8.6}$$

Then

$$\sigma_{\text{ess}}(\mathcal{C}(\{\alpha_n\}_{n=0}^\infty)) = \Delta_a. \tag{8.7}$$

For $\frac{\alpha_{j+1}}{\alpha_j} \to 1$ implies that each limit is of the form $\beta_j \equiv b$ for some $b \in \mathbb{D}$, so

$$\sigma_{\text{ess}}(\mathcal{C}) = \bigcup_{b=\text{limits of } \alpha_j} \Delta_{|b|} = \Delta_a$$

since $\Delta_{|b|} \subseteq \Delta_a$ if $|b| \geqslant a$.

9. Spectral consequences

[69, Section 4.3] describes joint work of Golinskii–Simon [42] that uses CMV matrices to obtain spectral results that relate properties of $\{\alpha_n\}_{n=0}^\infty$ to the associated measures. Here, in brief, are some of their main results:

Theorem 9.1 ($\equiv$ *[69, Theorem 4.3.5]; subsumed in Theorem 8.2*). *If* $|\alpha_n - \beta_n| \to 0$, *then* $\sigma_{\text{ess}}(\mathcal{C}(\{\alpha_n\}_{n=0}^\infty)) = \sigma_{\text{ess}}(\mathcal{C}(\{\beta_n\}_{n=0}^\infty))$.

Remark. Of course, Theorem 9.1 also follows from Theorem 8.1.

Proof. By (7.6) and a limiting argument, $\mathscr{C}(\{\alpha_n\}_{n=0}^\infty)-\mathscr{C}(\{\beta_n\}_{n=0}^\infty)$ is compact. The result follows from Weyl's theorem on the invariance of essential spectrum under compact perturbation. □

Theorem 9.2 (≡ [69, Theorem 4.3.4]). *If* $\limsup |\alpha_n(\mathrm{d}\mu)|=1$, *then* $\mathrm{d}\mu$ *is purely singular*.

Remark 1. This result is called Rakhmanov's lemma, after [64]. The proof is motivated by earlier results for Jacobi matrices of Dombrowski [18] and Simon–Spencer [73].

Proof. Let $\widehat{\alpha}_n$ be defined by

$$\widehat{\alpha}_n=\begin{cases}1 & \text{if } \alpha_n=0,\\ \frac{\alpha_n}{|\alpha_n|} & \text{if } \alpha_n\neq 0.\end{cases}$$

Since $\limsup|\alpha_n|=1$, we can find a sequence $n_j\to\infty$, so

$$\sum_{j=0}^\infty |\alpha_{n_j}-\widehat{\alpha}_{n_j}|^{1/2}<\infty.$$

Let

$$\beta_n=\begin{cases}\widehat{\alpha}_n & \text{if } n=n_j \text{ for some } j,\\ \alpha_n & \text{otherwise.}\end{cases}$$

Then $\mathscr{C}(\{\beta_n\}_{n=0}^\infty)-\mathscr{C}(\{\alpha_n\}_{n=0}^\infty)$ is trace class by (7.6). By the Kato–Birman theorem [65],

$$\sigma_{\mathrm{ac}}(\mathscr{C}(\{\alpha_n\}_{n=0}^\infty))=\sigma_{\mathrm{ac}}(\mathscr{C}(\{\beta_n\}_{n=0}^\infty)).$$

Since $|\widehat{\alpha}_n|=1$, $\mathscr{C}(\{\beta_n\}_{n=0}^\infty)$ is a direct sum of finite matrices of size $n_{j+1}-n_j$, and so it has no a.c. spectrum. □

Theorem 9.3 (≡ [69, Theorem 4.3.6]). *If* $\{\alpha_n\}_{n=0}^\infty$ *and* $\{\beta_n\}_{n=0}^\infty$ *are the Verblunsky coefficients of* $\mathrm{d}\mu$ *and* $\mathrm{d}\nu$ *given by* (7.8) *and* (7.9), *and* (7.7) *holds*, *then* (7.10) *holds*.

Proof. If $\limsup|\alpha_n|<1$, then $\limsup|\beta_n|<1$, and by Theorem 7.3, (7.10) holds. If $\limsup|\alpha_n|=\limsup|\beta_n|=1$, then $\sigma_{\mathrm{ac}}(\mathscr{C}(\{\alpha_n\}_{n=0}^\infty))=\sigma_{\mathrm{ac}}(\mathscr{C}(\{\beta_n\}_{n=0}^\infty))=\emptyset$ by Theorem 9.2. □

10. The AGR factorization of GGT matrices

This section is primarily preparatory for the next and discusses GGT matrix representations (for [34,43,78]) associated to a measure on $\partial\mathbb{D}$:

$$\mathscr{G}_{k\ell}(\{\alpha_n\}_{n=0}^M)=\langle\varphi_k, z\varphi_\ell\rangle \tag{10.1}$$

and discussed in [69, Section 4.1]. If μ is nontrivial, M in (10.1) is ∞ and $\alpha_n\in\mathbb{D}$ for all n. If μ is supported on exactly N points, $M=N-1$ and $\alpha_0,\ldots,\alpha_{N-2}\in\mathbb{D}$, $\alpha_{N-1}\in\partial\mathbb{D}$. There is an explicit calculation (see [69, Proposition 1.5.9]):

$$\mathscr{G}_{k\ell}=\begin{cases}-\bar{\alpha}_\ell\alpha_{k-1}\prod_{m=k}^{\ell-1}\rho_m & 0\leqslant k\leqslant \ell,\\ \rho_\ell & k=\ell+1,\\ 0 & k\geqslant \ell+2.\end{cases} \tag{10.2}$$

We present a remarkable factorization of GGT matrices due to Ammar et al. [6], use it to provide a result about cosets in $\mathbb{U}(N)/\mathbb{U}(N-1)$, and then present an alternate proof of Theorems 9.2 and 9.3 using GGT rather than CMV matrices. For the special case of orthogonal matrices (all $\alpha_j\in(-1,1)$), AGR found this factorization earlier [5].

We defined $\Theta_j(\alpha)$ before (3.18) as a 2×2 matrix acting on the span of δ_j,δ_{j+1}. We define $\widetilde{\Theta}(\alpha_j)$ to be this matrix viewed as an operator on $\mathbb{C}^N$ by $\mathbf{1}_j\oplus\Theta_j(\alpha)\oplus\mathbf{1}_{N-j-2}$. $\widetilde{\widetilde{\Theta}}_{N-1}(\alpha)$ is the matrix $\mathbf{1}_{N-1}\oplus\bar{\alpha}$.

Theorem 10.1 (*AGR factorization*). *For any finite $N \times N$ GGT matrix*,

$$\mathscr{G}(\{\alpha\}_{n=0}^{N-1}) = \widetilde{\Theta}_0(\alpha_0)\dots\widetilde{\Theta}_{N-2}(\alpha_{N-2})\widetilde{\widetilde{\Theta}}_{N-1}(\alpha_{N-1}). \tag{10.3}$$

For $N = \infty$,

$$\mathscr{G}(\{\alpha_n\}_{n=0}^{\infty}) = \operatorname*{s-lim}_{M\to\infty} \widetilde{\Theta}_0(\alpha_0)\dots\widetilde{\Theta}_M(\alpha_M). \tag{10.4}$$

Remark 1. Eq. (10.4) follows from (10.3) by a simple limiting argument. We will only prove (10.3) below.

2. We will give three proofs which illustrate slightly different aspects of the formula.

3. As explained in Killip–Nenciu [50], the Householder algorithm lets one write any unitary as a product of $N-1$ reflections; in many ways, representation (10.4) is more useful.

Proof (*First Proof*). By a direct calculation using (10.2),

$$\mathscr{G}(\{\alpha_n\}_{n=0}^{N-1}) = \Theta_0(\alpha_0)[\mathbf{1}_{1\times 1} \oplus \mathscr{G}(\{\alpha_{n+1}\}_{n=0}^{N-2})] \tag{10.5}$$

(10.3) follows by induction.

Second Proof (*that of AGR* [6]). We will prove first that any unitary (upper) Hessenberg matrix H (i.e., $H_{k\ell} = 0$ if $k \geqslant \ell + 1$) with positive subdiagonal (i.e., $H_{\ell+1,\ell} > 0$ for all ℓ) has the form (10.3) for suitable $\alpha_0, \alpha_1, \dots, \alpha_{N-2} \in \mathbb{D}$ and $\alpha_{N-1} \in \partial\mathbb{D}$. The first column of H has the form $(\bar\alpha_0, \rho_0, 0, \dots, 0)^{\mathrm{t}}$ for some $\alpha_0 \in \mathbb{D}$. Then $\Theta_0(\alpha_0)^{-1}H$ is of the form $\mathbf{1}_{1\times 1} \oplus H^{(1)}$, where $H^{(1)}$ is a unitary $(N-1) \times (N-1)$ Hessenberg matrix with positive subdiagonal. By induction, H has the form (10.3). One proves that $\{\alpha_n\}_{n=0}^{N-1}$ are the Verblunsky coefficients of the GGT matrix, either by using (10.2) or by deriving recursion relations.

For the third proof, we need a lemma that is an expression of Szegő recursion.

Lemma 10.2. *We have that*

$$\langle \varphi_j^*, z\varphi_j \rangle = \bar\alpha_j, \tag{10.6}$$

$$\langle \varphi_{j+1}, z\varphi_j \rangle = \rho_j, \tag{10.7}$$

$$\langle \varphi_{j+1}, \varphi_{j+1}^* \rangle = -\bar\alpha_j, \tag{10.8}$$

$$\langle \varphi_j^*, \varphi_{j+1}^* \rangle = \rho_j. \tag{10.9}$$

Remark. This says that a certain change of basis on a two-dimensional space is $\Theta(\alpha_j)$.

Proof. $\varphi_{j+1} \perp \varphi_j^*$ since $\deg(\varphi_n^*) \leqslant j$. Moreover, by (2.5) and (2.12),

$$z\varphi_j = \rho_j\varphi_{j+1} + \bar\alpha_j\varphi_j^*,$$
$$\varphi_{j+1}^* = -\alpha_j\varphi_{j+1} + \rho_j\varphi_j,$$

from which (10.6)–(10.9) are immediate. □

(*Third Proof of Theorem 10.1*). This is an analog of the proof of $\mathscr{L}\mathscr{M}$ factorization in Section 2. There $\mathscr{C}$ is the matrix of overlap of the orthonormal bases $\{z\chi_\ell\}_{\ell=0}^{\infty}$ and $\{\chi_\ell\}_{\ell=0}^{\infty}$. The $\mathscr{L}\mathscr{M}$ factorization comes from inserting the basis $\{zx_\ell\}_{\ell=0}^{\infty}$. Here we have the bases

$$e^{(0)} = (z\varphi_0, \dots, z\varphi_{N-1}), \tag{10.10}$$

$$e^{(N)} = (\varphi_0, \dots, \varphi_{N-1}),$$

and $\mathscr{G}$ is an overlap matrix. We introduce $N-1$ intermediate bases:

$$
\begin{aligned}
&e^{(1)} = (z\varphi_0, \ldots, z\varphi_{N-2}, \varphi^*_{N-1}),\\
&e^{(2)} = (z\varphi_0, \ldots, z\varphi_{N-3}, \varphi^*_{N-2}, \varphi_{N-1}),\\
&\ldots\\
&e^{(j)} = (z\varphi_0, \ldots, z\varphi_{N-j-1}, \varphi^*_{N-j}, \varphi_{N-j+1}, \ldots, \varphi_{N-1}),\\
&\ldots
\end{aligned}
$$

where $e^{(N)}$ is given by (10.10) since $\varphi^*_0 = 1 = \varphi_0$.

Thus

$$
\begin{aligned}
\mathscr{G}_{k\ell} &= \langle e^{(N)}_k, e^{(0)}_\ell \rangle\\
&= \sum_{m_1 \ldots m_{N-1}} \langle e^{(N)}_k, e^{(N-1)}_{m_1} \rangle \cdots \langle e^{(N-j)}_{m_j}, e^{(N-j-1)}_{m_{j+1}} \rangle \cdots \langle e^{(1)}_{m_{N-1}}, e^{(0)}_\ell \rangle
\end{aligned} \tag{10.11}
$$

is a product of N matrices. $N-1$ have a change from $z\varphi_j, \varphi^*_{j+1}$ to φ^*_j, φ_j whose overlap matrix, by (10.6)–(10.9), is $\widetilde{\Theta}(\alpha_j)$ and the extreme right has a change from $z\varphi_{N-1}$ to φ^*_{N-1}, which is $\widetilde{\widetilde{\Theta}}(\alpha_{N-1})$ since in $L^2(\partial\mathbb{D})$,

$$
z\varphi_{N-1} - \bar{\alpha}_{N-1}\varphi^*_{N-1} = 0
$$

Thus, (10.11) is (10.3). □

As a first application, we want to show that each finite unitary has an $\mathscr{L}\mathscr{M}$ factorization without recourse to orthogonal polynomials. By taking limits, one obtains an $\mathscr{L}\mathscr{M}$ factorization in general. This calculation fleshes out an argument given in [5] in the orthogonal case by using induction to make the proof more transparent:

Theorem 10.3. *Let U be a unitary matrix on $\mathbb{C}^N$ with $(1, 0, \ldots 0)^{\mathrm{t}}$ as cyclic vector. Then there exists a unitary V on $\mathbb{C}^N$ with $V(1, 0, \ldots 0)^{\mathrm{t}} = (1, 0, \ldots, 0)^{\mathrm{t}}$ so that VUV^{-1} has an $\mathscr{L}\mathscr{M}$ factorization.*

Remark. By $\mathscr{L}\mathscr{M}$ factorization, we mean $\mathscr{L} = \widetilde{\Theta}(\alpha_0) \oplus \widetilde{\Theta}(\alpha_2) \oplus \cdots$ and $\mathscr{M} = \mathbf{1}_{1\times 1} \oplus \widetilde{\Theta}(\alpha_1) \oplus \widetilde{\Theta}(\alpha_3) \oplus \ldots$, with a $\widetilde{\widetilde{\Theta}}(\alpha_{N-1})$ at the end of $\mathscr{L}$ if N is odd and of $\mathscr{M}$ is N is even.

Proof. We use induction on N. $N=1$, which says $U = (\widetilde{\widetilde{\Theta}}(\alpha_0)(\mathbf{1})$, is trivial. By the GGT representation and AGR factorization, we can find W (with $W(1, 0, \ldots, 0)^{\mathrm{t}} = (1, 0, \ldots, 0)^{\mathrm{t}}$) so

$$
WUW^{-1} = \widetilde{\Theta}_0(\alpha_0)\widetilde{\Theta}_1(\alpha_1) \ldots \widetilde{\widetilde{\Theta}}_{N-1}(\alpha_{N-1}).
$$

Let

$$
U_1 = \widetilde{\Theta}_0(\alpha_1) \ldots \widetilde{\widetilde{\Theta}}_{N-2}(\alpha_{N-1}) \tag{10.12}
$$

on $\mathbb{C}^{N-1}$. By induction and adding $\mathbf{1}_{1\times 1} \oplus \cdots$ everywhere, we can find $\mathscr{L}_1$, $\mathscr{M}_1$, and V_1 so

$$
(1 \oplus V_1)WUW^{-1}(1 + V_1)^{-1} = \widetilde{\Theta}_0(\alpha_0)[\mathbf{1} \oplus \mathscr{L}_1][1 \oplus \mathscr{M}_1]. \tag{10.13}
$$

Define

$$
V = [1 \oplus \mathscr{M}_1][1 \oplus V_1]W
$$

(note V maps $(1\,0 \ldots 0)^{\mathrm{t}}$ to itself). We have

$$
VUV^{-1} = \{[1 \oplus \mathscr{M}_1]\widetilde{\Theta}_0(\alpha_0)\}\{[\mathbf{1} \oplus \mathscr{L}_1]\}
$$

which precisely has the form $\mathscr{L}\mathscr{M}$. □

As a second application, we want to provide an explicit map that will be critical in the next section. Fix $\delta_0 \in \mathbb{C}^n$ and $U \in \mathbb{U}(n)$, the $n \times n$ unitary matrices. Let $\mathbb{U}(n-1) = \{U \in U(n) | U\delta_0 = \delta_0\}$. The symbol $\mathbb{U}(n-1)$ is accurate since each such U defines and is defined by a unitary on $\{\delta_0\}^\perp \cong \mathbb{C}^{n-1}$. Let $\mathbb{SC}^{2n-1} = \mathbb{U}(n)/\mathbb{U}(n-1)$, the group theoretic quotient. By mapping

$$\pi: U \in \mathbb{U}(n) \to U\delta_0 \tag{10.14}$$

we see that $\mathbb{SC}^{2n-1} \cong \{z \in \mathbb{C}^n \,||z| = 1\}$, the sphere of real dimension $2n-1$. Here is the result we will need:

Theorem 10.4. *There exists continuous maps g_1 and g_2 defined on $\{z \in \mathbb{SC}^{2n-1} | z \neq \delta_0\}$ with g_1 mapping to $\mathbb{U}(n)$ and g_2 to $\mathbb{SC}^{2n-3} = \{z \in \mathbb{SC}^{2n-1} | \langle \delta_0, z\rangle = 0\}$ so that*

(i)

$$\pi[g_1(z)] = z. \tag{10.15}$$

(ii) $V(U) \equiv g_1(\pi(U))^{-1}U \in \mathbb{U}(n-1)$ *for all* $U \notin \mathbb{U}(n-1)$.
(iii) *If δ_0 is cyclic for U with Verblunsky coefficients $\alpha_j(U, \delta_0)$, then $g_2(\pi(U))$ is cyclic for $V(U)\restriction\mathbb{C}^{n-1}$ and*

$$\alpha_j(V(U), g_2(\pi(U))) = \alpha_{j+1}(U, \delta_0). \tag{10.16}$$

(iv)

$$\langle \delta_0, U\delta_0\rangle = \overline{\alpha_0(U, \delta_0)} \tag{10.17}$$

if δ_0 is cyclic for U.

Proof. If $z \neq \delta_0$, $a(z) = \overline{\langle \delta_0, z\rangle} \in \mathbb{D}$ and so

$$g_2(z) = \frac{z - \langle \delta_0, z\rangle\delta_0}{\|z - \langle \delta_0, z\rangle\delta_0\|}$$

is well defined and in $\mathbb{SC}^{2n-3}$. In particular, if $p(z) = (1 - a(z)^2)^{1/2} = \|z - \langle \delta_0, z\rangle\delta_0\|$, we have

$$z = p(z)g_2(z) + \overline{a(z)}\delta_0. \tag{10.18}$$

Define $g_1(z)$ by

$$g_1(z)w = \begin{cases} w & \text{if } w \perp \delta_0, g_2(z), \\ z & \text{if } w = \delta_0, \\ -a(z)g_2(z) + p(z)\delta_0 & \text{if } w = g_2(z) \end{cases}$$

and otherwise linear. Then $g_1(z)$ is unitary since $\Theta(a(z))$ is unitary. (i) is obvious from $g_1(z)\delta_0 = z$. (ii) is a restatement of (i). (iii) follows from the fact that $g_2(z)$ corresponds to δ_1 in a $\delta_j = \chi_j(z)$ basis and the AGR factorization. (iv) is a consequence of $z\varphi_0 - \bar{\alpha}_0\varphi_0^* = \varphi_1$, so $\langle \varphi_0, z\varphi_0\rangle = \bar{\alpha}_0\langle \varphi_0, \varphi_0^*\rangle = \bar{\alpha}_0$. □

We want to close this section by noting that the AGR factorization implies an estimate on the GGT matrices that is not obvious from (10.2). Indeed, in [69, Section 4.1], an unnecessary condition, $\liminf |\alpha_n| > 0$, is made because the estimate below is not obvious.

In essence, the AGR factorization plays the role for estimates of GGT matrices that the $\mathcal{LM}$ factorization does for CMV matrices. In some ways, it is more critical because CMV matrices are five-diagonal with matrix elements which are quadratic in α and ρ, so one can easily get estimates like (7.2) (but with a worse constant) without using the $\mathcal{LM}$ factorization. Since GGT matrices are not finite width and have matrix elements that are products of arbitrary orders, direct estimates from (10.2) are much harder.

Theorem 10.5. *Let $\{\alpha_n\}_{n=0}^\infty$ and $\{\beta_n\}_{n=0}^\infty$ be two sequences in $\overline{\mathbb{D}}^\infty$ and let $\sigma_n = (1 - |\beta_n|^2)^{1/2}$. Then*

$$\|\mathcal{G}(\{\alpha_n\}_{n=0}^\infty) - \mathcal{G}(\{\beta_n\}_{n=0}^\infty)\|_1 \leqslant 2\sum_{n=0}^\infty (|\alpha_n - \beta_n| + |\sigma_n - \rho_n|). \tag{10.19}$$

Proof. By (10.4) and standard trace class techniques [71], we need only prove for finite sequences that

$$\|\widetilde{\Theta}_0(\alpha_0)\ldots\widetilde{\Theta}_N(\alpha_N)-\widetilde{\Theta}_0(\beta_0)\ldots\Theta_N(\beta_N)\|_1\leqslant 2\sum_{n=0}^{N}(|\alpha_n-\beta_n|+|\sigma_n-\rho_n|). \tag{10.20}$$

Since $\|\widetilde{\Theta}_j(\alpha_j)-\widetilde{\Theta}_j(\beta_j)\|_1\leqslant 2(|\alpha_j-\beta_j|+|\sigma_j-\rho_j|)$, and $\|\widetilde{\Theta}(\alpha)\|=1$, writing the difference of products as a telescoping sum yields (10.20). □

Notice also that AGR factorization shows that if $|\alpha_j|=1$, $\mathscr{G}$ decouples. This fact and (10.19) provide an alternate proof of Rakhmanov's lemma (Theorem 9.2) by the same decoupling argument, but using $\mathscr{G}$ in place of $\mathscr{C}$. If $\sum_{n=0}^{\infty}|\alpha_n|^2=\infty$, one also gets a proof of Theorem 9.3, using $\mathscr{G}$ in place of $\mathscr{C}$ and (10.19). If $\sum_{n=0}^{\infty}|\alpha_n|^2<\infty$, one must use the extended GGT matrix, $\mathscr{F}$, of [69, Section 4.1] (see also [15]). It is easy to prove that if $\sum|\alpha_n|^2<\infty$ and $\sum|\alpha_n-\beta_n|<\infty$, then $\mathscr{F}(\{\alpha_n\}_{n=0}^{\infty})-\mathscr{F}(\{\beta_n\}_{n=0}^{\infty})$ is trace class since the difference of $\mathscr{F}$'s differs from the difference of $\mathscr{G}$'s by a rank one operator, which is always trace class!

11. CUE, Haar measure, and the Killip–Nenciu theorem

In [50], Killip and Nenciu proved the following result:

Theorem 11.1. *Let* $\mathrm{d}\mu$ *be a normalized Haar measure on* $\mathbb{U}(n)$, *the* $n\times n$ *unitary matrices. Then, for a.e.* U, $\delta_0=(1,0,\ldots,0)^{\mathrm{t}}$ *is cyclic, and the measure induced on* $\mathbb{D}^{n-1}\times\partial\mathbb{D}$ *by* $U\to\alpha_j(U_0,\delta_0)$ *is the product measure*:

$$\left\{\prod_{j=0}^{n-2}\left[\frac{n-j-1}{\pi}(1-|\alpha_j|^2)^{n-j-2}\,d^2\alpha_j\right]\right\}\frac{\mathrm{d}\theta(\alpha_{n-1})}{2\pi}, \tag{11.1}$$

where $\theta(\alpha_{n-1})$ *is defined by*

$$\alpha_{n-1}=\mathrm{e}^{\mathrm{i}\theta(\alpha_{n-1})} \tag{11.2}$$

and $d^2\alpha$ *is a two-dimensional Lebesgue measure on* $\mathbb{D}$.

Remark. By the "induced measure," we mean the measure $\mathrm{d}\nu$ on $\mathbb{D}^{n-1}\times\partial\mathbb{D}$ given by $\nu(B)=\mu(A^{-1}[B])$, where $A(U)=(\alpha_1(U),\ldots,\alpha_{n-1}(U))$.

This is really a result about Verblunsky coefficients, not CMV matrices, and both their proof and ours use the GGT, not the CMV, matrices. We provide this here because, first, Killip–Nenciu proved this result to provide a five-diagonal model for CUE (see below), and because the result was proven as part of the ferment stirred up by the CMV discovery. In this section, we will provide a partially new proof of Theorem 11.1 that is perhaps more natural from a group theoretic point of view, and then describe and sketch their somewhat shorter argument!

To understand where the factors in (11.1) come from:

Lemma 11.2. *Let* $\mathrm{d}\mu_{\mathbb{SC}^{2n-1}}$ *be the measure on the* $2n-1$ *real dimension manifold* $\{z\in\mathbb{C}^n\,|\,|z|=1\}$, *which is normalized and invariant under rotations. Map* $\mathbb{SC}^{2n-1}\xrightarrow{Q}\overline{\mathbb{D}}$ *by* $z\mapsto z_1$, *the first component, and let* $\mathrm{d}\nu$ *be the measure on* $\overline{\mathbb{D}}$ *given by* $\nu(B)=\mu_{\mathbb{SC}^{2n-1}}(Q^{-1}[B])$. *Then*

$$\mathrm{d}\nu(w)=\frac{n-1}{\pi}(1-|w|^2)^{n-2}\,d^2w. \tag{11.3}$$

Proof. Since $d^2w=\frac{1}{2}\,\mathrm{d}\theta\,\mathrm{d}|w|^2$,

$$\int_{\mathbb{D}}\mathrm{d}\nu(w)=\frac{2\pi(n-1)}{\pi}\,\frac{1}{2}\int_0^1(1-x)^{n-2}\,\mathrm{d}x=1$$

so $d\nu$ is normalized. Thus, we will not worry about constants. Using $x_1 + ix_2, x_3 + ix_4, \ldots$ for the n complex variables, the measure $\delta(1 - |x|^2)\, dx_1 \ldots dx_{2n}$ is

$$\frac{dx_1 \ldots dx_{2n-1}}{2(1 - \sum_{j=1}^{2n-1} x_j^2)^{1/2}}.$$

Integrating out $x_3, \ldots, x_{2n-1}$ for fixed x_1, x_2 with $\rho = (1 - |x_1|^2 - |x_2|^2)^{1/2}$, the measure is

$$\frac{1}{2} \int_{|y| \leqslant (1-\rho^2)^{1/2}} \frac{d^{2n-3} y}{(1 - \rho^2 - y^2)^{1/2}}.$$

Scaling $x = y/(1 - \rho^2)^{1/2}$, we find

$$\frac{1}{2}(1 - \rho^2)^{2n-4/2} \int_{|x| \leqslant 1} \frac{d^{2n-3} x}{(1 - x^2)^{1/2}}$$

so the measure is $C(1 - w^2)^{n-2}\, d^2 w$, proving (11.3). □

Theorem 11.4 must be well known to experts on homogeneous spaces.

Lemma 11.3. *Let* $d\nu_1, d\nu_2$ *be two probability measures on compact spaces X and Y, and let* $d\nu$ *be a probability measure on* $X \times Y$. *Suppose*

(i) $\pi_1^*(d\nu) = d\nu_1$, *that is, if* $\pi_1(x, y) = x$, *then* $\nu_1(B) = \nu(\pi_1^{-1}[B])$.
(ii) *For any continuous f on X,* $\int_X f\, d\nu = C_f\, d\nu_2$, *that is,*

$$\int f(x)g(y)\, d\nu = C_f \int g(y)\, d\nu_2 \tag{11.4}$$

for all continuous g on Y.
(ii) *Then* $d\nu = d\nu_1 \otimes d\nu_2$.

Proof. Taking $g = 1$ in (11.4),

$$C_f = \int f(x)\, d\nu = \int f(x)\, d\nu_1(x)$$

by (i). Thus,

$$\int f(x)g(y)\, d\nu = \left(\int f(x) d\nu_1(x)\right)\left(\int g(y)\, d\nu_2(y)\right)$$

so $d\nu = d\nu_1 \otimes d\nu_2$ integrated on product functions which are total in $C(X \times Y)$. □

Theorem 11.4. *Let G be a compact group and H a closed subgroup. Let* $d\nu_G, d\nu_H$ *be normalized Haar measures and* $\pi: G \to G/H$. *Let* $d\nu_{G/H}$ *be the measure induced by* $d\nu_G$ *on* G/H, *that is,*

$$\nu_{G/H}(B) = \nu_G(\pi^{-1}[B]).$$

Let $\mathcal{O}$ *be an open set in* G/H *and* $f: \mathcal{O} \to G$ *a continuous cross-section, that is,* $\pi[f(x)] = x$ *for all* $x \in \mathcal{O}$. *Coordinatize* $\pi^{-1}[\mathcal{O}]$ *by* $\mathcal{O} \times H$ *via*

$$(x, h) \mapsto f(x)h. \tag{11.5}$$

Then, on $\pi^{-1}[\mathcal{O}]$,

$$d\nu_G(x, h) = d\nu_{G/H}(x)\, d\nu_H(h). \tag{11.6}$$

Proof. The existence of a cross-section implies that under the coordinates (11.5), $\pi^{-1}[\mathcal{O}] \cong \mathcal{O} \times H$. Clearly, $\pi_1^*(\mathrm{d}\mu_G) = \mathrm{d}\mu_{G/H} \restriction \mathcal{O}$, by construction of $\mathrm{d}\mu_{G/H}$. On the other hand, $\int_{\mathcal{O}} f\, \mathrm{d}\mu_{G/H}$ is a measure on H invariant under right multiplication by any $h \in H$, so this is $C_f\, \mathrm{d}\mu_H$. Therefore, Lemma11.3 applies and (11.6) holds. □

Proof of Theorem 11.1. We use induction on n. $n = 1$, that is, that for $\mathbb{U}(1)$, $U = (\mathrm{e}^{\mathrm{i}\theta_0})$ has Haar measure $\frac{\mathrm{d}\theta_0}{2\pi}$, is immediate.

Note that $U \in \mathbb{U}(n)$ has δ_0 as a cyclic vector if and only if U has simple spectrum, and for each eigenvector φ_k of U, we have $\langle \varphi_k, \delta_0 \rangle \neq 0$. As is well known, $\{U | U$ has a degenerate eigenvalue$\}$ has codimension 3 and so zero Haar measure. Similarly, $\langle \varphi_k, \delta_0 \rangle = 0$ on a set of codimension 2 and so zero Haar measure. Thus, $\mathscr{C}_n = \{E | \delta_0$ is cyclic for $U\}$ has full Haar measure.

Let $\mathcal{O} = \{\eta \in \mathbb{SC}^{2n-1} | \eta \neq \delta_0\}$. Then $f(x) = g_1(z)$ given in Theorem 10.4 is a cross-section, and so $\mathrm{d}\mu_{\mathbb{U}(n)} = \mathrm{d}\mu_{\mathbb{SC}^{2n-1}} \otimes \mathrm{d}\mu_{\mathbb{U}(n-1)}$ by Theorem 11.4.

By Theorem 10.4, $g_1^{-1}(\pi_1[\mathscr{C}_n])$ is $(z, V(U))$ and $V(U)$ has Verblunsky coefficients $\{\alpha_{j+1}(U)\}_{j=0}^{n-2}$. Thus, by induction, $\mathrm{d}\mu_{\mathbb{U}(n-1)}$ on these α's is the product (11.6) without the α_0 factor.

By (10.18) and Lemma 11.3, the α_0 distribution generated by $\mathrm{d}\mu_{\mathbb{SC}^{2n-1}}$ is the α_0 factor in (11.1). □

The proof in [50] differs in two ways: first, in place of the AGR factorization, Killip–Nenciu use a (Householder) factorization as a phase factor times a product of reflections. Instead of using induction on symmetric spaces as we do, they use an alternate that would work with the AGR factorization also. Starting with $\varphi_0 = \delta_0$, we let $\psi_0 = U\varphi$. There is a unique vector, φ_1 (what we called $g_2(\pi(U))$ in Theorem 10.4), in the span of φ and ψ_0, so that $\langle \psi_0, \varphi_1 \rangle > 0$ and $\langle \varphi_1, \delta_0 \rangle = 0$. φ_1 is cyclic for $V(U)$ and so, by induction, we obtain $\psi_0, \psi_1, \ldots, \psi_{n-1}$ an ON basis with $|\langle \delta_j, \psi_j \rangle| < 1$. It is not hard to see that, via the AGR factorization, this sets up a one–one map of ON basis with $|\langle \delta_j, \psi_j \rangle| < 1$ and U's with δ_0 cyclic for U. Haar measure induces on the ψ's a measure as follows: ψ_0 is uniformly distributed on $\mathbb{SC}^{2n-1}$; ψ_1 uniformly on the copy of $\mathbb{SC}^{2n-3}$ of unit vectors orthogonal to ψ_1; $\psi_2$uniformly on $\mathbb{SC}^{2n-5}$, etc. Since $\langle \delta_j, \psi_j \rangle = \bar{\alpha}_j$, we obtain measure (11.1).

Since $\det(\widetilde{\Theta}_j(\alpha_j)) = -1$, $\det(\widetilde{\widetilde{\Theta}}_{N-1}(\alpha_{N-1})) = \bar{\alpha}_{N-1}$, we see

$$\det(\mathscr{G}(\{\alpha_n\}_{n=0}^{N-1})) = (-1)^{N-1}\bar{\alpha}_{N-1}.$$

Thus, $\mathbb{SU}(n) = \{U \in \mathbb{U}(n) | \det(U)\}$ is precisely these U with $\alpha_{N-1} = (-1)^{N-1}$. The same inductive argument thus proves:

Theorem 11.5. *Let* $\mathrm{d}\mu$ *be normalized Haar measure on* $\mathbb{SU}(n)$. *Then for a.e.* U, $\delta_0 = (1, 0, \ldots, 0)^{\mathrm{t}}$ *is cyclic and the measure induced on* $\mathbb{D}^{n-1}$ *by* $U \to \alpha_j(U, \delta_0)$ (*with* $\alpha_{n-1}(U, \delta_0) \equiv (-1)^{n-1}$) *is the product measure given by* (11.1) *with the final* $\mathrm{d}\theta$ *term dropped.*

$\mathbb{SO}[n]$ is the $n \times n$ real unitary matrices (i.e., orthogonal matrices). If δ_0 is cyclic, they have Verblunsky coefficients which are easily seen to lie in $(-1, 1)$. Conversely, it is easy to see that if $\alpha_j \in (-1, 1)$ for $j = 0, \ldots, n-2$, there is an orthogonal matrix with those α_j's. A similar analysis lets us compute the distribution on $(-1, 1)^{n-1}$ induced by Haar measure on $\mathbb{SO}[n]$. We need only replace Lemma 11.3 by

Lemma 11.6. *Let* $\mathrm{d}\eta_{n-1}$ *be the measure on the* $n-1$*-dimensional unit sphere in* $\mathbb{R}^n$. *The induced measure on* x_1 *is*

$$\frac{\Gamma(\frac{n}{2})(1 - |x_1|^2)^{(n-3)/2}\,\mathrm{d}x_1}{\sqrt{\pi}\Gamma(\frac{n-1}{2})}.$$

Proof. That the measure is $C(1 - |x_1|^2)^{(n-3/2)}\,\mathrm{d}x_1$ follows from the same calculation as in Lemma 11.3. The normalization is the inverse of the beta function $2^{2-n}\Gamma(n-1)/\Gamma(\frac{n-1}{2})$ which, as noted by [50] (there is a $(\ )^{-1}$ missing on the leftmost term in their (3.14)), can be written, using the duplication formula for beta functions, as $\Gamma(\frac{n}{2})/\sqrt{\pi}\,\Gamma(\frac{n-1}{2})$.

We thus have:

Theorem 11.7 (*Killip and Nenciu [50]*). *The measure on* $(-1,1)^{n-1}$ *induced by Haar measure on* $\mathbb{SO}[n]$ *mapped to the real Verblunsky coefficients is*

$$\frac{\Gamma(\frac{n}{2})}{\pi^{n/2}}\prod_{k=0}^{n-1}(1-\alpha_k^2)^{(n-k-3)/2}\,\mathrm{d}\alpha_k.$$

The CUE eigenvalue distribution [20–22] is the one for $U\in\mathbb{U}[n]$ induced by Haar measure. Weyl's integration formula (see, e.g., [66]) says that if $\lambda_1,\dots,\lambda_n$ with $\lambda_j=\mathrm{e}^{\mathrm{i}\theta_j}$ are the eigenvalues, this is $C\prod_{i<j}|\lambda_i-\lambda_j|^2\prod_{j=1}^{n}\frac{\mathrm{d}\theta_j}{2\pi}$. Theorem 11.1 says that CMV matrices with distribution of α's given by (11.1) has the same distribution, and so gives a model for CUE by five-diagonal matrices. Ref. [50] find a similar model for the "β-distributions" given by $C_\beta\prod_{i=j}|\lambda_i-\lambda_j|^\beta\frac{\mathrm{d}\theta_j}{2\pi}$; see also Forrester–Rains [25].

12. CMV and the AL flow

One of the great discoveries of the 1970s ([19,24,26,58,80] and dozens of other papers) is that lurking within one-dimensional Schrödinger operators and Jacobi matrices is a completely integrable system (resp., KdV and Toda flows), natural "invariant" tori, and a natural symplectic structure in which the Schrödinger operator or Jacobi matrix is the dynamical half of a Lax pair.

Such structures occur also for Verblunsky coefficients, and the dynamical half of the Lax pair is the CMV matrix. While the CMV part obviously requires CMV matrices, the other parts do not, and it is surprising that it was only in 2003–2004 that they were found. We will settle here for describing the two most basic structures, leaving further results to mentioning the followup papers: Geronimo–Gesztesy–Holden [30], Gesztesy–Zinchenko [36], Killip–Nenciu [51], Li [55], and Nenciu [61].

On $\mathbb{D}$, introduce the symplectic form given by the Poisson bracket (where, as usual, $\frac{\partial}{\partial z}$ and $\frac{\partial}{\partial \bar z}$ are $\frac12[\frac{\partial}{\partial x}\mp\mathrm{i}\frac{\partial}{\partial y}]$),

$$\{f,g\}=\mathrm{i}\rho^2\left[\frac{\partial f}{\partial\bar z}\frac{\partial g}{\partial z}-\frac{\partial f}{\partial z}\frac{\partial g}{\partial\bar z}\right]. \tag{12.1}$$

The ρ^2 is natural as we will see below. Extend this to $\mathbb{D}^p$ (coordinatized by $(\alpha_0,\dots,\alpha_{p-1})$ by

$$\{f,g\}=\mathrm{i}\sum_{j=0}^{p-1}\rho_j^2\left[\frac{\partial f}{\partial\bar\alpha_j}\frac{\partial g}{\partial\alpha_j}-\frac{\partial f}{\partial\alpha_j}\frac{\partial g}{\partial\bar\alpha_j}\right]. \tag{12.2}$$

Because of the ρ^2,

$$\left\{\prod_{j=0}^{p-1}\rho_j^2,g\right\}=-\prod_{j=0}^{p-1}\rho_j^2\left(\sum_{j=0}^{p+1}\frac{\partial g}{\partial\theta_j}\right)$$

and functions of $\rho_0\dots\rho_{p-1}$ generate simultaneous rotations of all phases. Nenciu–Simon [62] proved the following:

Theorem 12.1 (*Nenciu and Simon [62]*). *Let p be even and let* $\Delta(z,\{\alpha_j\}_{j=0}^{p-1})$ *be the discriminants* (*see* (3.20)) *for the periodic sequence with* $\alpha_{j+kp}=\alpha_j$ *for* $j=0,\dots,p-1$; $k=0,1,2,\dots$. *Then, with respect to the symplectic form* (12.2),

$$\{\Delta(w),\Delta(z)\}=0 \tag{12.3}$$

for all $w,z\in\mathbb{C}\backslash\{0\}$.

Note: See [55,51] for a discussion of symplectic forms on unitary matrices.

Since $\overline{\Delta(1/\bar{w})} = \Delta(w)$, and the leading coefficient is real, $\Delta(z)$ has p real coefficients, that is, $\Delta(z) = \sum_{j=-p/2}^{p/2} a_j z^j$ with $a_{-j} = \bar{a}_j$, then $a_{p/2}$, $\operatorname{Re} a_{p/2-1}$, $\operatorname{Im} a_{p/2-1}, \ldots, \operatorname{Re} a_1$, $\operatorname{Im} a_1$, a_0 are the p real functions of $\{\alpha_j\}_{j=0}^{p-1}$ which Poisson commute. They are independent at a.e. points (in α) and define invariant tori. Each one generates flows that are completely integrable. The simplest is

$$-\mathrm{i}\dot{\alpha}_j = \rho_j^2(\alpha_{j+1} + \alpha_{j-1}) \tag{12.4}$$

which has been known as a completely integrable system for a long time under the name "defocusing Ablowitz–Ladik flow" (after [1–3]).

Nenciu has proven a beautiful result:

Theorem 12.2 (*Nenciu [59–61]*). *The flows generated by the coefficients of Δ can be put into Lax pair form with the dynamical element being the Floquet CMV matrix.*

For details as well as extensions to some infinite CMV matrices, see the references above.

The flow generated by $\prod_{j=0}^{p-1} \rho_j^2$ realizes the $\alpha_j \to \lambda\alpha_j$ invariance of the isospectral tori. Flow (12.4) is generated by $\operatorname{Re}(a_1)$. The $\operatorname{Im}(a_k)$ generate flows that preserve the set of $\{\alpha_j\}_{j=0}^{p-1}$ where all α_j are real (as a set, not pointwise). The simplest of these, generated by $\operatorname{Im}(a_1)$, is

$$\dot{\alpha}_n = \rho_n^2(\alpha_{n+1} - \alpha_{n-1}) \tag{12.5}$$

called the Schur flow. Via the Geronimus relations of the next section, these generate a flow on Jacobi parameters that is essentially the Toda flow. For further discussion, see [4,23,27,59].

13. CMV matrices and the geronimus relations

In a celebrated paper, Szegő [76] found a connection between orthogonal polynomials for measures on $[-2, 2]$ (he had $[-1, 1]$; I use the scaling common in the Schrödinger operator community) and OPUC. Given a measure $\mathrm{d}\gamma$ on $[-2, 2]$, one defines the unique measure $\mathrm{d}\xi$ on $\partial\mathbb{D}$ which is invariant under $z \to \bar{z}$ and obeys

$$\int g(x)\,\mathrm{d}\gamma(x) = \int g(2\cos\theta)\,\mathrm{d}\xi(\theta). \tag{13.1}$$

What Szegő showed is that the orthonormal polynomials p_n for $\mathrm{d}\gamma$ and the OPUC for φ_n for $\mathrm{d}\xi$ are related by

$$p_n\left(z + \frac{1}{z}\right) = C_n z^{-n}(\varphi_{2n}(z) + \varphi_{2n}^*(z)). \tag{13.2}$$

The normalization constants C_n (see [70, (13.1.14)]) $\to 1$ as $n \to \infty$ if $\sum_{n=0}^{\infty} |\alpha_n|^2 < \infty$. Motivated by this, Geronimus [35] found a relation between the Verblunsky coefficients, α_n, for $\mathrm{d}\xi$ and the Jacobi parameters $\{a_n\}_{n=1}^{\infty}$, $\{b_n\}_{n=1}^{\infty}$ for $\mathrm{d}\gamma$ (see of [70, Theorem 13.1.7]):

$$a_{n+1}^2 = (1 - \alpha_{2n-1})(1 - \alpha_{2n}^2)(1 + \alpha_{2n+1}), \tag{13.3a}$$
$$b_{n+1} = (1 - \alpha_{2n-1})\alpha_{2n} - (1 + \alpha_{2n-1})\alpha_{2n-2}. \tag{13.3b}$$

In [50], Killip–Nenciu found a direct proof of (13.3) by finding a beautiful relation between CMV and some Jacobi matrices. We will sketch the idea, leaving the detailed calculations to [50] or the pedagogic presentation in [70, Section 13.2].

A measure is invariant under $z \to \bar{z}$ if and only if all $\{\alpha_n\}_{n=0}^{\infty}$ are real. $\Theta(\alpha)$ with α real is self-adjoint and unitary with determinant -1, hence eigenvalues ± 1, that is, a reflection on $\mathbb{C}^2$. Thus,

$$\alpha_n = \bar{\alpha}_n \quad \text{all } n \Rightarrow \mathscr{M}^2 = \mathscr{L}^2 = \mathbf{1}.$$

Since $\chi_n(z) = \overline{x_n(1/\bar{z})}$, we see that if μ is invariant and $(Mf)(z) = f(\bar{z})$, then

$$\langle \chi_j, M\chi_\ell \rangle = \mathscr{M}_{j\ell}.$$

$\mathcal{C}+\mathcal{C}^*$ is self-adjoint and maps $\{f \mid \mathcal{M}f=f\}$ to itself. Let us see in a natural basis that its restriction to this invariant subspace is a Jacobi matrix.

If α is real and

$$S(\alpha)=\frac{1}{\sqrt{2}}\begin{pmatrix}\sqrt{1-\alpha} & -\sqrt{1+\alpha}\\ \sqrt{1+\alpha} & \sqrt{1-\alpha}\end{pmatrix}$$

then

$$S(\alpha)\Theta(\alpha)S(\alpha)^{-1}=\begin{pmatrix}-1 & 0\\ 0 & 1\end{pmatrix}. \tag{13.4}$$

Define

$$\mathcal{S}=\mathbf{1}_{1\times 1}\oplus S(\alpha_1)\oplus S(\alpha_3)\oplus\cdots$$

so

$$\mathcal{S}\mathcal{M}\mathcal{S}^{-1}=\mathcal{R}=\begin{pmatrix}1 &&&& \\ & -1 &&& \\ && 1 && \\ &&& -1 & \\ &&&& \ddots\end{pmatrix}$$

and define

$$\mathcal{B}=\mathcal{S}\mathcal{L}\mathcal{S}^{-1}.$$

Then

$$\mathcal{S}(\mathcal{C}+\mathcal{C}^{-1})\mathcal{S}^{-1}=\mathcal{R}\mathcal{B}+\mathcal{B}\mathcal{R}$$

which commutes with $\mathcal{R}$.

$\mathcal{B}$ is seven-diagonal as a product of three tridiagonal matrices. Moreover, since $\mathcal{B}$ commutes with $\mathcal{R}$, its odd–even matrix elements vanish. It follows that

$$\mathcal{R}\mathcal{B}+\mathcal{B}\mathcal{R}=\mathcal{J}_{\mathrm{e}}\oplus\mathcal{J}_{\mathrm{o}},$$

where $\mathcal{J}_{\mathrm{e}}$ acts on $\{\delta_{2n}\}_{n=0}^{\infty}$ and $\mathcal{J}_{\mathrm{o}}$ on $\{\delta_{2n+1}\}_{n=0}^{\infty}$, and each is a Jacobi matrix. A calculation shows that the Jacobi parameters of $\mathcal{J}_{\mathrm{e}}$ are given by (13.3) and that the spectral measures are related by (13.1). One can also analyze $\mathcal{J}_{\mathrm{o}}$ which is related to another mapping of Szegő [76] and one gets two more Jacobi matrices by looking at $\mathcal{C}+\mathcal{C}^{-1}$ restricted to the spaces where $\mathcal{L}=1$ or $\mathcal{L}=-1$.

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