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Weyl–Titchmarsh theory for CMV operators associated with orthogonal polynomials on the unit circle☆

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Dedicated with great pleasure to Barry Simon on the occasion of his 60th birthday

Abstract

We provide a detailed treatment of Weyl–Titchmarsh theory for half-lattice and full-lattice CMV operators and discuss their systems of orthonormal Laurent polynomials on the unit circle, spectral functions, variants of Weyl–Titchmarsh functions, and Green's functions. In particular, we discuss the corresponding spectral representations of half-lattice and full-lattice CMV operators.

MSC: primary 34B20; 47A10; 47B36; secondary 34L40

1. Introduction

The aim of this paper is to develop Weyl–Titchmarsh theory for a special class of unitary doubly infinite five-diagonal matrices. The corresponding unitary semi-infinite five-diagonal matrices were recently introduced by Cantero, Moral, and Velázquez (CMV) [8] in 2003. In [33, Sects. 4.5, 10.5], Simon introduced the corresponding notion of unitary doubly infinite five-diagonal matrices and coined the term "extended" CMV matrices. To simplify notations we will often just speak of CMV operators whether or not they are half-lattice or full-lattice operators indexed by $\mathbb{N}$ or $\mathbb{Z}$, respectively.

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CMV operators on $\mathbb{Z}$ are intimately related to a completely integrable version of the defocusing nonlinear Schrödinger equation (continuous in time but discrete in space), a special case of the Ablowitz–Ladik system. Relevant references in this context are, for instance, [1,2,11,18,27–29], and the literature cited therein. A recent application to a Borg-type theorem (an inverse spectral result), which motivated us to write this paper, appeared in [20]. For more details we refer to Theorem 1.1 at the end of this introduction.

We denote by $\mathbb{D}$ the open unit disk in $\mathbb{C}$ and let α be a sequence of complex numbers in $\mathbb{D}$, $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}$. The unitary CMV operator U on $\ell^2(\mathbb{Z})$ then can be written as a special five-diagonal doubly infinite matrix in the standard basis of $\ell^2(\mathbb{Z})$ according to [33, Sects. 4.5, 10.5]) as

$$U = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots & \ddots & & & & \\ & 0 & -\alpha_0\rho_{-1} & -\overline{\alpha_{-1}}\alpha_0 & -\alpha_1\rho_0 & \rho_0\rho_1 & & \mathbf{0} & \\ & & \rho_{-1}\rho_0 & \overline{\alpha_{-1}}\rho_0 & -\overline{\alpha_0}\alpha_1 & \overline{\alpha_0}\rho_1 & 0 & & \\ & & & 0 & -\alpha_2\rho_1 & -\overline{\alpha_1}\alpha_2 & -\alpha_3\rho_2 & \rho_2\rho_3 & \\ & & \mathbf{0} & & \rho_1\rho_2 & \overline{\alpha_1}\rho_2 & -\overline{\alpha_2}\alpha_3 & \overline{\alpha_2}\rho_3 & 0 \\ & & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{1.1}$$

Here the sequence of positive real numbers $\{\rho_k\}_{k\in\mathbb{Z}}$ is defined by

$$\rho_k = \sqrt{1-|\alpha_k|^2}, \quad k \in \mathbb{Z} \tag{1.2}$$

and terms of the form $-\overline{\alpha_k}\alpha_{k+1}$, $k \in \mathbb{Z}$, represent the diagonal entries in the infinite matrix (1.1). For the corresponding half-lattice CMV operators $U_{+,k_0}^{(s)}$, $s \in [0, 2\pi)$ in $\ell^2([k_0,\infty)\cap\mathbb{Z})$ we refer to (2.29).

The relevance of this unitary operator U on $\ell^2(\mathbb{Z})$, more precisely, the relevance of the corresponding half-lattice CMV operator $U_{+,0}$ in $\ell^2(\mathbb{N}_0)$ (cf. (2.31)) is derived from its intimate relationship with the trigonometric moment problem and hence with finite measures on the unit circle $\partial\mathbb{D}$. (Here $\mathbb{N}_0 = \mathbb{N} \cup \{0\}$.) Let $\{\alpha_k\}_{k\in\mathbb{N}} \subset \mathbb{D}$ and define the transfer matrix

$$S(\zeta,k) = \begin{pmatrix} \zeta & \alpha_k \\ \overline{\alpha_k}\zeta & 1 \end{pmatrix}, \quad \zeta \in \partial\mathbb{D},\ k \in \mathbb{N} \tag{1.3}$$

with spectral parameter $\zeta \in \partial\mathbb{D}$. Consider the system of difference equations

$$\begin{pmatrix} \varphi_+(\zeta,k) \\ \varphi_+^*(\zeta,k) \end{pmatrix} = S(\zeta,k) \begin{pmatrix} \varphi_+(\zeta,k-1) \\ \varphi_+^*(\zeta,k-1) \end{pmatrix}, \quad \zeta \in \partial\mathbb{D},\ k \in \mathbb{N} \tag{1.4}$$

with initial condition

$$\begin{pmatrix} \varphi_+(\zeta,0) \\ \varphi_+^*(\zeta,0) \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \zeta \in \partial\mathbb{D}. \tag{1.5}$$

Then $\varphi_+(\,\cdot\,,k)$ are monic polynomials of degree k and

$$\varphi_+^*(\zeta,k) = \zeta^k\overline{\varphi_+(1/\overline{\zeta},k)}, \quad \zeta \in \partial\mathbb{D},\ k \in \mathbb{N}_0, \tag{1.6}$$

the reversed *-polynomial of $\varphi_+(\cdot,k)$, is at most of degree k. These polynomials were first introduced by Szegő in the 1920s in his work on the asymptotic distribution of eigenvalues of sections of Toeplitz forms [35,36] (see also [23, Chs. 1–4; 37, Ch. XI]). Szegő's point of departure was the trigonometric moment problem and hence the theory of orthogonal polynomials on the unit circle: Given a probability measure $d\sigma_+$ supported on an infinite set on the unit circle, find monic polynomials of degree k in $\zeta = e^{i\theta}$, $\theta \in [0, 2\pi]$, such that

$$\int_0^{2\pi} d\sigma_+(e^{i\theta})\, \overline{\varphi_+(e^{i\theta}, k)}\varphi_+(e^{i\theta}, k') = \gamma_k^{-2}\delta_{k,k'}, \quad k, k' \in \mathbb{N}_0, \tag{1.7}$$

where (cf. (1.2))

$$\gamma_k^2 = \begin{cases} 1, & k = 0, \\ \prod_{j=1}^k \rho_j^{-2}, & k \in \mathbb{N}. \end{cases} \tag{1.8}$$

One then also infers

$$\int_0^{2\pi} d\sigma_+(e^{i\theta})\, \overline{\varphi_+^*(e^{i\theta}, k)}\varphi_+^*(e^{i\theta}, k') = \gamma_{k''}^{-2}, \quad k'' = \max\{k, k'\},\ k, k' \in \mathbb{N}_0 \tag{1.9}$$

and obtains that $\varphi_+(\cdot, k)$ is orthogonal to $\{\zeta^j\}_{j=0,\dots,k-1}$ in $L^2(\partial\mathbb{D}; d\sigma_+)$ and $\varphi_+^*(\cdot, k)$ is orthogonal to $\{\zeta^j\}_{j=1,\dots,k}$ in $L^2(\partial\mathbb{D}; d\sigma_+)$. Additional comments in this context will be provided in Remark 2.9. For a detailed account of the relationship of $U_{+,0}$ with orthogonal polynomials on the unit circle we refer to the monumental two-volume treatise by Simon [33] (see also [32] and [34] for a description of some of the principal results in [33]) and the exhaustive bibliography therein. For classical results on orthogonal polynomials on the unit circle we refer, for instance, to [3,15–17,23,25,35–40]. More recent references relevant to the spectral theoretic content of this paper are [12–14,20,22,26,30,31].

We note that $S(\zeta, k)$ in (1.3) is not the transfer matrix that leads to the half-lattice CMV operator $U_{+,0}$ in $\ell^2(\mathbb{N}_0)$ (cf. (2.29)). After a suitable change of basis introduced by Cantero et al. [8], the transfer matrix $S(\zeta, k)$ turns into $T(\zeta, k)$ as defined in (2.18).

In Section 2, we provide an extensive treatment of Weyl–Titchmarsh theory for half-lattice CMV operators U_{+,k_0} on $\ell([k_0, \infty) \cap \mathbb{Z})$ and discuss various systems of orthonormal Laurent polynomials on the unit circle, the half-lattice spectral function of U_{+,k_0}, variants of half-lattice Weyl–Titchmarsh functions, and the Green's function of U_{+,k_0}. In particular, we discuss the spectral representation of U_{+,k_0}. While many of these results can be found in Simon's two-volume treatise [33], we survey some of this material here from an operator theoretic point of view, starting directly from the CMV operator. Section 3 then contains our new results on Weyl–Titchmarsh theory for full-lattice CMV operators U on $\ell^2(\mathbb{Z})$. Again we discuss systems of orthonormal Laurent polynomials on the unit circle, the 2×2 matrix-valued spectral and Weyl–Titchmarsh functions of U, its Green's matrix, and the spectral representation of U. Finally, Appendix A summarizes basic facts on Caratheodory and Schur functions relevant to this paper.

We conclude this introduction with citing a Borg-type (inverse spectral) result from our paper [20], which motivated us to write the present paper.

First we introduce our notation for closed arcs on the unit circle $\partial\mathbb{D}$,

$$\mathrm{Arc}\big(\big[e^{i\theta_1}, e^{i\theta_2}\big]\big) = \big\{e^{i\theta} \in \partial\mathbb{D} \,|\, \theta_1 \leqslant \theta \leqslant \theta_2\big\}, \quad \theta_1 \in [0, 2\pi),\ \theta_1 \leqslant \theta_2 \leqslant \theta_1 + 2\pi \tag{1.10}$$

and similarly for open arcs on $\partial\mathbb{D}$.

Theorem 1.1. *Let $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}$ be a reflectionless sequence of Verblunsky coefficients. Let U be the associated unitary CMV operator* (1.1) (*cf. also* (2.6)–(2.9)) *on $\ell^2(\mathbb{Z})$ and suppose that the spectrum of U consists of a connected arc of $\partial\mathbb{D}$,*

$$\sigma(U) = \mathrm{Arc}\big(\big[e^{i\theta_0}, e^{i\theta_1}\big]\big) \tag{1.11}$$

with $\theta_0 \in [0, 2\pi]$, $\theta_0 < \theta_1 \leqslant \theta_0 + 2\pi$, and hence $e^{i(\theta_0+\theta_1)/2} \in \mathrm{Arc}\big(\big(e^{i\theta_0}, e^{i\theta_1}\big)\big)$. Then $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}}$ is of the form,

$$\alpha_k = \alpha_0 g^k, \quad k \in \mathbb{Z}, \tag{1.12}$$

where

$$g = -\exp(i(\theta_0 + \theta_1)/2) \text{ and } |\alpha_0| = \cos((\theta_1 - \theta_0)/4). \tag{1.13}$$

Here the sequence $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}$ is called *reflectionless* if

$$\text{for all } k \in \mathbb{Z},\ M_+(\zeta, k) = -\overline{M_-(\zeta, k)} \text{ for } \mu_0\text{-a.e. } \zeta \in \sigma_{\mathrm{ess}}(U), \tag{1.14}$$

where $M_\pm(\cdot, k)$, $k \in \mathbb{Z}$, denote the half-lattice Weyl–Titchmarsh functions of U in (2.136) (cf. [20] for further details). The case of reflectionless Verblunsky coefficients includes the periodic case and certain quasi-periodic and almost periodic cases.

2. Weyl–Titchmarsh theory for CMV operators on half-lattices

In this section, we describe the Weyl–Titchmarsh theory for CMV operators on half-lattices.

In the following, let $\ell^2(\mathbb{Z})$ be the usual Hilbert space of all square summable complex-valued sequences with scalar product $(\cdot, \cdot)$ linear in the second argument. The *standard basis* in $\ell^2(\mathbb{Z})$ is denoted by

$$\{\delta_k\}_{k\in\mathbb{Z}}, \quad \delta_k = (\dots, 0, \dots, 0, \underbrace{1}_{k}, 0, \dots, 0, \dots)^\top, \quad k \in \mathbb{Z}. \tag{2.1}$$

$\ell_0^\infty(\mathbb{Z})$ denotes the set of sequences of compact support (i.e., $f = \{f(k)\}_{k\in\mathbb{Z}} \in \ell_0^\infty(\mathbb{Z})$ if there exist $M(f), N(f) \in \mathbb{Z}$ such that $f(k) = 0$ for $k < M(f)$ and $k > N(f)$). We use the analogous notation for compactly supported sequences on half-lattices $[k_0, \pm\infty) \cap \mathbb{Z}$, $k_0 \in \mathbb{Z}$, and then write $\ell_0^\infty([k_0, \pm\infty) \cap \mathbb{Z})$, etc. For $J \subseteq \mathbb{R}$ an interval, we will identify $\ell^2(J \cap \mathbb{Z}) \oplus \ell^2(J \cap \mathbb{Z})$ and $\ell^2(J \cap \mathbb{Z}) \otimes \mathbb{C}^2$ and then use the simplified notation $\ell^2(J \cap \mathbb{Z})^2$. For simplicity, the identity operator on $\ell^2(J \cap \mathbb{Z})$ is abbreviated by I without separately indicating its dependence on J.

Moreover, we denote by $\mathbb{D} = \{z \in \mathbb{C} \mid |z| < 1\}$ the open unit disk in the complex plane $\mathbb{C}$, by $\partial\mathbb{D} = \{\zeta \in \mathbb{C} \mid |\zeta| = 1\}$ its counterclockwise oriented boundary, and we freely use the notation employed in Appendix A. By a *Laurent polynomial* we denote a finite linear combination of terms z^k, $k \in \mathbb{Z}$, with complex-valued coefficients.

Throughout this paper we make the following basic assumption:

Hypothesis 2.1. Let α be a sequence of complex numbers such that

$$\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} \subset \mathbb{D}. \tag{2.2}$$

Given a sequence α satisfying (2.2), we define the sequence of positive real numbers $\{\rho_k\}_{k\in\mathbb{Z}}$ and two sequences of complex numbers with positive real parts $\{a_k\}_{k\in\mathbb{Z}}$ and $\{b_k\}_{k\in\mathbb{Z}}$ by

$$\rho_k = \sqrt{1-|\alpha_k|^2}, \quad k \in \mathbb{Z}, \tag{2.3}$$
$$a_k = 1+\alpha_k, \quad k \in \mathbb{Z}, \tag{2.4}$$
$$b_k = 1-\alpha_k, \quad k \in \mathbb{Z}. \tag{2.5}$$

Following Simon [33], we call α_k the Verblunsky coefficients in honor of Verblunsky's pioneering work in the theory of orthogonal polynomials on the unit circle [39,40].

Next, we also introduce a sequence of 2×2 unitary matrices θ_k by

$$\theta_k = \begin{pmatrix} -\alpha_k & \rho_k \\ \rho_k & \overline{\alpha_k} \end{pmatrix}, \quad k \in \mathbb{Z} \tag{2.6}$$

and two unitary operators V and W on $\ell^2(\mathbb{Z})$ by their matrix representations in the standard basis of $\ell^2(\mathbb{Z})$ as follows

$$V = \begin{pmatrix} \ddots & & & \mathbf{0} \\ & \theta_{2k-2} & & \\ & & \theta_{2k} & \\ \mathbf{0} & & & \ddots \end{pmatrix}, \quad W = \begin{pmatrix} \ddots & & & \mathbf{0} \\ & \theta_{2k-1} & & \\ & & \theta_{2k+1} & \\ \mathbf{0} & & & \ddots \end{pmatrix}, \tag{2.7}$$

where

$$\begin{pmatrix} V_{2k-1,2k-1} & V_{2k-1,2k} \\ V_{2k,2k-1} & V_{2k,2k} \end{pmatrix} = \theta_{2k}, \quad \begin{pmatrix} W_{2k,2k} & W_{2k,2k+1} \\ W_{2k+1,2k} & W_{2k+1,2k+1} \end{pmatrix} = \theta_{2k+1}, \quad k \in \mathbb{Z}. \tag{2.8}$$

Moreover, we introduce the unitary operator U on $\ell^2(\mathbb{Z})$ by

$$U = VW \tag{2.9}$$

or in matrix form, in the standard basis of $\ell^2(\mathbb{Z})$, by

$$U = \begin{pmatrix} \ddots & \ddots & \ddots & \ddots & \ddots & & & & \mathbf{0} \\ & 0 & -\alpha_0\rho_{-1} & -\overline{\alpha_{-1}}\alpha_0 & -\alpha_1\rho_0 & \rho_0\rho_1 & & & \\ & & \rho_{-1}\rho_0 & \overline{\alpha_{-1}}\rho_0 & -\overline{\alpha_0}\alpha_1 & \overline{\alpha_0}\rho_1 & 0 & & \\ & & & 0 & -\alpha_2\rho_1 & -\overline{\alpha_1}\alpha_2 & -\alpha_3\rho_2 & \rho_2\rho_3 & \\ & \mathbf{0} & & & \rho_1\rho_2 & \overline{\alpha_1}\rho_2 & -\overline{\alpha_2}\alpha_3 & \overline{\alpha_2}\rho_3 & 0 \\ & & & & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}. \tag{2.10}$$

Here terms of the form $-\overline{\alpha_k}\alpha_{k+1}$, $k \in \mathbb{Z}$, represent the diagonal entries in the infinite matrix (2.10). We will call the operator U on $\ell^2(\mathbb{Z})$ the CMV operator since (2.6)–(2.10) in the context of the semi-infinite (i.e., half-lattice) case were first obtained by Cantero et al. [8].

Finally, let $\mathbb{U}$ denote the unitary operator on $\ell^2(\mathbb{Z})^2$ defined by

$$\mathbb{U} = \begin{pmatrix} U & 0 \\ 0 & U^\top \end{pmatrix} = \begin{pmatrix} VW & 0 \\ 0 & WV \end{pmatrix} = \begin{pmatrix} 0 & V \\ W & 0 \end{pmatrix}^2. \tag{2.11}$$

One observes remnants of a certain "supersymmetric" structure in $\left(\begin{smallmatrix} 0 & V \\ W & 0 \end{smallmatrix}\right)$ which is also reflected in the following result.

Lemma 2.2. *Let $z \in \mathbb{C}\backslash\{0\}$ and $\{u(z,k)\}_{k\in\mathbb{Z}}$, $\{v(z,k)\}_{k\in\mathbb{Z}}$ be sequences of complex functions. Then the following items* (i)–(vi) *are equivalent*:

$$\text{(i)} \quad Uu(z,\cdot) = zu(z,\cdot), \quad (Wu)(z,\cdot) = zv(z,\cdot), \tag{2.12}$$

$$\text{(ii)} \quad U^\top v(z,\cdot) = zv(z,\cdot), \quad (Vv)(z,\cdot) = u(z,\cdot), \tag{2.13}$$

$$\text{(iii)} \quad (Wu)(z,\cdot) = zv(z,\cdot), \quad (Vv)(z,\cdot) = u(z,\cdot), \tag{2.14}$$

$$\text{(iv)} \quad \mathbb{U}\begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix} = z\begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix}, \quad (Wu)(z,\cdot) = zv(z,\cdot), \tag{2.15}$$

$$\text{(v)} \quad \mathbb{U}\begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix} = z\begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix}. \quad (Vv)(z,\cdot) = u(z,\cdot), \tag{2.16}$$

$$\text{(vi)} \quad \begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = T(z,k)\begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}, \quad k \in \mathbb{Z}, \tag{2.17}$$

where the transfer matrices $T(z,k)$, $z \in \mathbb{C}\backslash\{0\}$, $k \in \mathbb{Z}$, are given by

$$T(z,k) = \begin{cases} \frac{1}{\rho_k}\begin{pmatrix} \alpha_k & z \\ 1/z & \overline{\alpha_k} \end{pmatrix}, & k \text{ odd}, \\[2mm] \frac{1}{\rho_k}\begin{pmatrix} \overline{\alpha_k} & 1 \\ 1 & \alpha_k \end{pmatrix}, & k \text{ even}. \end{cases} \tag{2.18}$$

Proof. The equivalence of (2.12) and (2.14) follows from (2.9) after one defines $v(z,\cdot) = \frac{1}{z}(Wu)(z,\cdot)$. Since $\theta_k^\top = \theta_k$, one has $V^\top = V$, $W^\top = W$ and hence, $U^\top = (VW)^\top = WV$. Thus, defining $u(z,\cdot) = (Vv)(z,\cdot)$, one gets the equivalence of (2.13) and (2.14). The equivalence of (2.14), (2.15), and (2.16) follows immediately from (2.11).

Next, we will prove that (2.14) is equivalent to (2.17). Assuming k to be odd one obtains the equivalence of the following items (i)–(v):

$$\text{(i)} \quad \begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = T(z,k)\begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}, \tag{2.19}$$

$$\text{(ii)} \quad \rho_k\begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = \begin{pmatrix} \alpha_k & z \\ 1/z & \overline{\alpha_k} \end{pmatrix}\begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}, \tag{2.20}$$

$$\text{(iii)} \quad \begin{cases} zv(z,k-1) = -\alpha_k u(z,k-1) + \rho_k u(z,k), \\ z\rho_k v(z,k) = u(z,k-1) + \overline{\alpha_k} zv(z,k-1), \end{cases} \tag{2.21}$$

$$\text{(iv)} \quad \begin{cases} zv(z,k-1) = -\alpha_k u(z,k-1) + \rho_k u(z,k), \\ zv(z,k) = \rho_k u(z,k-1) + \overline{\alpha_k} u(z,k), \end{cases} \tag{2.22}$$

$$\text{(v)} \quad z\begin{pmatrix} v(z,k-1) \\ v(z,k) \end{pmatrix} = \theta_k\begin{pmatrix} u(z,k-1) \\ u(z,k) \end{pmatrix}. \tag{2.23}$$

If k is even, one similarly proves that the following items (vi)–(viii) are equivalent:

$$\text{(vi)} \quad \begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = T(z,k)\begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}, \tag{2.24}$$

$$\text{(vii)} \quad \rho_k\begin{pmatrix} v(z,k) \\ u(z,k) \end{pmatrix} = \begin{pmatrix} \alpha_k & 1 \\ 1 & \overline{\alpha_k} \end{pmatrix}\begin{pmatrix} v(z,k-1) \\ u(z,k-1) \end{pmatrix}, \tag{2.25}$$

$$\text{(viii)} \quad \begin{pmatrix} u(z,k-1) \\ u(z,k) \end{pmatrix} = \theta_k\begin{pmatrix} v(z,k-1) \\ v(z,k) \end{pmatrix}. \tag{2.26}$$

Thus, taking into account (2.7), one concludes that

$$\begin{cases} Wu(z,\cdot) = zv(z,\cdot), \\ Vv(z,\cdot) = u(z,\cdot) \end{cases} \tag{2.27}$$

is equivalent to

$$\begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = T(z,k) \begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}, \quad k \in \mathbb{Z}. \qquad \square \tag{2.28}$$

We note that in studying solutions of $Uu(z,\cdot) = zu(z,\cdot)$ as in Lemma 2.2(i), the purpose of the additional relation $(Wu)(z,\cdot) = zv(z,\cdot)$ in (2.12) is to introduce a new variable v that improves our understanding of the structure of such solutions u. An analogous comment applies to solutions of $U^\top v(z,\cdot) = zv(z,\cdot)$ and the relation $(Vv)(z,\cdot) = u(z,\cdot)$ in Lemma 2.2(ii).

If one sets $\alpha_{k_0} = e^{is}$, $s \in [0, 2\pi)$, for some reference point $k_0 \in \mathbb{Z}$, then the operator U splits into a direct sum of two half-lattice operators $U^{(s)}_{-,k_0-1}$ and $U^{(s)}_{+,k_0}$ acting on $\ell^2((-\infty, k_0-1] \cap \mathbb{Z})$ and on $\ell^2([k_0, \infty) \cap \mathbb{Z})$, respectively. Explicitly, one obtains

$$\begin{aligned} &U = U^{(s)}_{-,k_0-1} \oplus U^{(s)}_{+,k_0} \ \text{ in } \ \ell^2((-\infty, k_0-1] \cap \mathbb{Z}) \oplus \ell^2([k_0, \infty) \cap \mathbb{Z}) \\ &\text{if } \ \alpha_{k_0} = e^{is}, \ s \in [0, 2\pi). \end{aligned} \tag{2.29}$$

(Strictly, speaking, setting $\alpha_{k_0} = e^{is}$, $s \in [0, 2\pi)$, for some reference point $k_0 \in \mathbb{Z}$ contradicts our basic Hypothesis 2.1. However, as long as the exception to Hypothesis 2.1 refers to only one or two sites (cf. also (2.181)), we will safely ignore this inconsistency in favor of the notational simplicity it provides by avoiding the introduction of a properly modified hypothesis on $\{\alpha_k\}_{k\in\mathbb{Z}}$.) Similarly, one obtains $W^{(s)}_{-,k_0-1}$, $V^{(s)}_{-,k_0-1}$ and $W^{(s)}_{+,k_0}$, $V^{(s)}_{+,k_0}$ such that

$$U^{(s)}_{\pm,k_0} = V^{(s)}_{\pm,k_0} W^{(s)}_{\pm,k_0}. \tag{2.30}$$

For simplicity we will abbreviate

$$U_{\pm,k_0} = U^{(s=0)}_{\pm,k_0} = V^{(s=0)}_{\pm,k_0} W^{(s=0)}_{\pm,k_0} = V_{\pm,k_0} W_{\pm,k_0}. \tag{2.31}$$

In addition, we introduce on $\ell^2([k_0, \pm\infty) \cap \mathbb{Z})^2$ the half-lattice operators $\mathbb{U}^{(s)}_{\pm,k_0}$ by

$$\mathbb{U}^{(s)}_{\pm,k_0} = \begin{pmatrix} U^{(s)}_{\pm,k_0} & 0 \\ 0 & (U^{(s)}_{\pm,k_0})^\top \end{pmatrix} = \begin{pmatrix} V^{(s)}_{\pm,k_0} W^{(s)}_{\pm,k_0} & 0 \\ 0 & W^{(s)}_{\pm,k_0} V^{(s)}_{\pm,k_0} \end{pmatrix}. \tag{2.32}$$

By $\mathbb{U}_{\pm,k_0}$ we denote the half-lattice operators defined for $s = 0$,

$$\mathbb{U}_{\pm,k_0} = \mathbb{U}^{(s=0)}_{\pm,k_0} = \begin{pmatrix} U_{\pm,k_0} & 0 \\ 0 & (U_{\pm,k_0})^\top \end{pmatrix} = \begin{pmatrix} V_{\pm,k_0} W_{\pm,k_0} & 0 \\ 0 & W_{\pm,k_0} V_{\pm,k_0} \end{pmatrix}. \tag{2.33}$$

Lemma 2.3. *Let $z \in \mathbb{C}\backslash\{0\}$, $k_0 \in \mathbb{Z}$, and $\{\widehat{p}_+(z,k,k_0)\}_{k\geqslant k_0}$, $\{\widehat{r}_+(z,k,k_0)\}_{k\geqslant k_0}$ be sequences of complex functions. Then, the following items* (i)–(vi) *are equivalent*:

$$\text{(i)}\quad U_{+,k_0}\widehat{p}_+(z,\cdot,k_0) = z\widehat{p}_+(z,\cdot,k_0), \quad W_{+,k_0}\widehat{p}_+(z,\cdot,k_0) = z\widehat{r}_+(z,\cdot,k_0), \tag{2.34}$$

$$\text{(ii)}\quad (U_{+,k_0})^\top\widehat{r}_+(z,\cdot,k_0) = z\widehat{r}_+(z,\cdot,k_0), \quad V_{+,k_0}\widehat{r}_+(z,\cdot,k_0) = \widehat{p}_+(z,\cdot,k_0), \tag{2.35}$$

$$\text{(iii)}\quad W_{+,k_0}\widehat{p}_+(z,\cdot,k_0) = z\widehat{r}_+(z,\cdot,k_0), \quad V_{+,k_0}\widehat{r}_+(z,\cdot,k_0) = \widehat{p}_+(z,\cdot,k_0), \tag{2.36}$$

$$\text{(iv)}\quad \mathbb{U}_{+,k_0}\begin{pmatrix}\widehat{p}_+(z,\cdot,k_0)\\ \widehat{r}_+(z,\cdot,k_0)\end{pmatrix}=z\begin{pmatrix}\widehat{p}_+(z,\cdot,k_0)\\ \widehat{r}_+(z,\cdot,k_0)\end{pmatrix}, \quad W_{+,k_0}\widehat{p}_+(z,\cdot,k_0)=z\widehat{r}_+(z,\cdot,k_0), \tag{2.37}$$

$$\text{(v)}\quad \mathbb{U}_{+,k_0}\begin{pmatrix}\widehat{p}_+(z,\cdot,k_0)\\ \widehat{r}_+(z,\cdot,k_0)\end{pmatrix} = z\begin{pmatrix}\widehat{p}_+(z,\cdot,k_0)\\ \widehat{r}_+(z,\cdot,k_0)\end{pmatrix}, \quad V_{+,k_0}\widehat{r}_+(z,\cdot,k_0) = \widehat{p}_+(z,\cdot,k_0), \tag{2.38}$$

$$\text{(vi)}\quad \begin{pmatrix}\widehat{p}_+(z,k,k_0)\\ \widehat{r}_+(z,k,k_0)\end{pmatrix} = T(z,k)\begin{pmatrix}\widehat{p}_+(z,k-1,k_0)\\ \widehat{r}_+(z,k-1,k_0)\end{pmatrix}, \quad k > k_0, \tag{2.39}$$

$$\textit{assuming } \widehat{p}_+(z,k_0,k_0) = \begin{cases} z\widehat{r}_+(z,k_0,k_0), & k_0 \textit{ odd},\\ \widehat{r}_+(z,k_0,k_0), & k_0 \textit{ even}.\end{cases} \tag{2.40}$$

Next, consider sequences $\{\widehat{p}_-(z,k,k_0)\}_{k\leqslant k_0}$, $\{\widehat{r}_-(z,k,k_0)\}_{k\leqslant k_0}$. Then, the following items (vii)–(xii) *are equivalent*:

$$\text{(vii)}\quad U_{-,k_0}\widehat{p}_-(z,\cdot,k_0) = z\widehat{p}_-(z,\cdot,k_0), \quad W_{-,k_0}\widehat{p}_-(z,\cdot,k_0) = z\widehat{r}_-(z,\cdot,k_0), \tag{2.41}$$

$$\text{(viii)}\quad (U_{-,k_0})^\top\widehat{r}_-(z,\cdot,k_0) = z\widehat{r}_-(z,\cdot,k_0), \quad V_{-,k_0}\widehat{r}_-(z,\cdot,k_0) = \widehat{p}_-(z,\cdot,k_0), \tag{2.42}$$

$$\text{(ix)}\quad W_{-,k_0}\widehat{p}_-(z,\cdot,k_0) = z\widehat{r}_-(z,\cdot,k_0), \quad V_{-,k_0}\widehat{r}_-(z,\cdot,k_0) = \widehat{p}_-(z,\cdot,k_0), \tag{2.43}$$

$$\text{(x)}\quad \mathbb{U}_{-,k_0}\begin{pmatrix}\widehat{p}_-(z,\cdot,k_0)\\ \widehat{r}_-(z,\cdot,k_0)\end{pmatrix} = z\begin{pmatrix}\widehat{p}_-(z,\cdot,k_0)\\ \widehat{r}_-(z,\cdot,k_0)\end{pmatrix}, \quad W_{-,k_0}\widehat{p}_-(z,\cdot,k_0) = z\widehat{r}_-(z,\cdot,k_0), \tag{2.44}$$

$$\text{(xi)}\quad \mathbb{U}_{-,k_0}\begin{pmatrix}\widehat{p}_-(z,\cdot,k_0)\\ \widehat{r}_-(z,\cdot,k_0)\end{pmatrix} = z\begin{pmatrix}\widehat{p}_-(z,\cdot,k_0)\\ \widehat{r}_-(z,\cdot,k_0)\end{pmatrix}, \quad V_{-,k_0}\widehat{r}_-(z,\cdot,k_0) = \widehat{p}_-(z,\cdot,k_0), \tag{2.45}$$

$$\text{(xii)}\quad \begin{pmatrix}\widehat{p}_-(z,k-1),k_0\\ \widehat{r}_-(z,k-1,k_0)\end{pmatrix} = T(z,k)^{-1}\begin{pmatrix}\widehat{p}_-(z,k,k_0)\\ \widehat{r}_-(z,k,k_0)\end{pmatrix}, \quad k\leqslant k_0, \tag{2.46}$$

$$\textit{assuming } \widehat{p}_-(z,k_0,k_0) = \begin{cases} -\widehat{r}_-(z,k_0,k_0), & k_0 \textit{ odd},\\ -z\widehat{r}_-(z,k_0,k_0), & k_0 \textit{ even}.\end{cases} \tag{2.47}$$

Proof. Repeating the first part of the proof of Lemma 2.2 one obtains the equivalence of (2.34), (2.35), (2.36), (2.37), and (2.38). Moreover, repeating the second part of the proof of Lemma 2.2 one obtains that

$$(W_{+,k_0}\widehat{p}_+(z,\cdot,k_0))(k) = z\widehat{r}_+(z,k,k_0), \tag{2.48}$$

$$(V_{+,k_0}\widehat{r}_+(z,\cdot,k_0))(k) = \widehat{p}_+(z,k,k_0), \quad k > k_0 \tag{2.49}$$

is equivalent to

$$\begin{pmatrix}\widehat{p}_+(z,k,k_0)\\ \widehat{r}_+(z,k,k_0)\end{pmatrix} = T(z,k)\begin{pmatrix}\widehat{p}_+(z,k-1,k_0)\\ \widehat{r}_+(z,k-1,k_0)\end{pmatrix}, \quad k > k_0. \tag{2.50}$$

If k_0 is odd, then the operators V_{+,k_0} and W_{+,k_0} have the following structure:

$$V_{+,k_0} = \begin{pmatrix} \theta_{k_0+1} & & 0 \\ & \theta_{k_0+3} & \\ 0 & & \ddots \end{pmatrix}, \quad W_{+,k_0} = \begin{pmatrix} 1 & & 0 \\ & \theta_{k_0+2} & \\ 0 & & \ddots \end{pmatrix} \tag{2.51}$$

and hence,

$$W_{+,k_0}\widehat{p}_+(z,\cdot,k_0))(k_0) = z\widehat{r}_+(z,k_0,k_0) \tag{2.52}$$

is equivalent to

$$\widehat{p}_+(z,k_0,k_0) = z\widehat{r}_+(z,k_0,k_0). \tag{2.53}$$

Thus, one infers that (2.36) is equivalent to (2.39), (2.40) for k_0 odd. If k_0 is even, then the operators V_{+,k_0} and W_{+,k_0} have the following structure:

$$V_{+,k_0} = \begin{pmatrix} 1 & & 0 \\ & \theta_{k_0+2} & \\ 0 & & \ddots \end{pmatrix}, \quad W_{+,k_0} = \begin{pmatrix} \theta_{k_0+1} & & 0 \\ & \theta_{k_0+3} & \\ 0 & & \ddots \end{pmatrix} \tag{2.54}$$

and hence,

$$(V_{+,k_0}\widehat{r}_+(z,\cdot,k_0))(k_0) = \widehat{p}_+(z,k_0,k_0) \tag{2.55}$$

is equivalent to

$$\widehat{p}_+(z,k_0,k_0) = \widehat{r}_+(z,k_0,k_0). \tag{2.56}$$

Thus, one infers that (2.36) is equivalent to (2.39), (2.40) for k_0 even.

The results for $\widehat{p}_-(z,\cdot,k_0)$ and $\widehat{r}_-(z,\cdot,k_0)$ are proved analogously. □

Analogous comments to those made right after the proof of Lemma 2.2 apply in the present context of Lemma 2.3.

Definition 2.4. We denote by $\begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix}_{k \geqslant k_0}$ and $\begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}_{k \geqslant k_0}$, $z \in \mathbb{C}\backslash\{0\}$, two linearly independent solutions of (2.39) with the following initial conditions:

$$\begin{pmatrix} p_+(z,k_0,k_0) \\ r_+(z,k_0,k_0) \end{pmatrix} = \begin{cases} \binom{z}{1}, & k_0 \text{ odd}, \\ \binom{1}{1}, & k_0 \text{ even}, \end{cases} \quad \begin{pmatrix} q_+(z,k_0,k_0) \\ s_+(z,k_0,k_0) \end{pmatrix} = \begin{cases} \binom{z}{-1}, & k_0 \text{ odd}, \\ \binom{-1}{1}, & k_0 \text{ even}. \end{cases} \tag{2.57}$$

Similarly, we denote by $\begin{pmatrix} p_-(z,k,k_0) \\ r_-(z,k,k_0) \end{pmatrix}_{k \leqslant k_0}$ and $\begin{pmatrix} q_-(z,k,k_0) \\ s_-(z,k,k_0) \end{pmatrix}_{k \leqslant k_0}$, $z \in \mathbb{C}\backslash\{0\}$, two linearly independent solutions of (2.46) with the following initial conditions:

$$\begin{pmatrix} p_-(z,k_0,k_0) \\ r_-(z,k_0,k_0) \end{pmatrix} = \begin{cases} \binom{1}{-1}, & k_0 \text{ odd}, \\ \binom{-z}{1}, & k_0 \text{ even}, \end{cases} \quad \begin{pmatrix} q_-(z,k_0,k_0) \\ s_-(z,k_0,k_0) \end{pmatrix} = \begin{cases} \binom{1}{1}, & k_0 \text{ odd}, \\ \binom{z}{1}, & k_0 \text{ even}. \end{cases} \tag{2.58}$$

Using (2.17) one extends $\begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix}_{k \geqslant k_0}$, $\begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}_{k \geqslant k_0}$, $z \in \mathbb{C}\backslash\{0\}$, to $k < k_0$. In the same manner, one extends $\begin{pmatrix} p_-(z,k,k_0) \\ r_-(z,k,k_0) \end{pmatrix}_{k \leqslant k_0}$ and $\begin{pmatrix} q_-(z,k,k_0) \\ s_-(z,k,k_0) \end{pmatrix}_{k \leqslant k_0}$, $z \in \mathbb{C}\backslash\{0\}$, to $k > k_0$. These extensions will be denoted by $\begin{pmatrix} p_\pm(z,k,k_0) \\ r_\pm(z,k,k_0) \end{pmatrix}_{k \in \mathbb{Z}}$ and $\begin{pmatrix} q_\pm(z,k,k_0) \\ s_\pm(z,k,k_0) \end{pmatrix}_{k \in \mathbb{Z}}$. Moreover, it follows from (2.17) that $p_\pm(z,k,k_0)$, $q_\pm(z,k,k_0)$, $r_\pm(z,k,k_0)$, and $s_\pm(z,k,k_0)$, $k, k_0 \in \mathbb{Z}$, are Laurent polynomials in z.

In particular, one computes

k	$k_0 - 1$	k_0 odd	$k_0 + 1$
$\begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix}$	$\frac{1}{\rho_{k_0}}\begin{pmatrix} z(1-\overline{\alpha_{k_0}}) \\ 1-\alpha_{k_0} \end{pmatrix}$	$\begin{pmatrix} z \\ 1 \end{pmatrix}$	$\frac{1}{\rho_{k_0+1}}\begin{pmatrix} 1+\overline{\alpha_{k_0+1}}z \\ z+\alpha_{k_0+1} \end{pmatrix}$
$\begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}$	$\frac{1}{\rho_{k_0}}\begin{pmatrix} z(-1-\overline{\alpha_{k_0}}) \\ 1+\alpha_{k_0} \end{pmatrix}$	$\begin{pmatrix} z \\ -1 \end{pmatrix}$	$\frac{1}{\rho_{k_0+1}}\begin{pmatrix} -1+\overline{\alpha_{k_0+1}}z \\ z-\alpha_{k_0+1} \end{pmatrix}$
$\begin{pmatrix} p_-(z,k,k_0) \\ r_-(z,k,k_0) \end{pmatrix}$	$\frac{1}{\rho_{k_0}}\begin{pmatrix} -z-\overline{\alpha_{k_0}} \\ 1/z+\alpha_{k_0} \end{pmatrix}$	$\begin{pmatrix} 1 \\ -1 \end{pmatrix}$	$\frac{1}{\rho_{k_0+1}}\begin{pmatrix} -1+\overline{\alpha_{k_0+1}} \\ 1-\alpha_{k_0+1} \end{pmatrix}$
$\begin{pmatrix} q_-(z,k,k_0) \\ s_-(z,k,k_0) \end{pmatrix}$	$\frac{1}{\rho_{k_0}}\begin{pmatrix} z-\overline{\alpha_{k_0}} \\ 1/z-\alpha_{k_0} \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\frac{1}{\rho_{k_0+1}}\begin{pmatrix} 1+\overline{\alpha_{k_0+1}} \\ 1+\alpha_{k_0+1} \end{pmatrix}$
k	$k_0 - 1$	k_0 even	$k_0 + 1$
$\begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix}$	$\frac{1}{\rho_{k_0}}\begin{pmatrix} 1-\alpha_{k_0} \\ 1-\overline{\alpha_{k_0}} \end{pmatrix}$	$\begin{pmatrix} 1 \\ 1 \end{pmatrix}$	$\frac{1}{\rho_{k_0+1}}\begin{pmatrix} z+\alpha_{k_0+1} \\ 1/z+\overline{\alpha_{k_0+1}} \end{pmatrix}$
$\begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}$	$\frac{1}{\rho_{k_0}}\begin{pmatrix} 1+\alpha_{k_0} \\ -1-\overline{\alpha_{k_0}} \end{pmatrix}$	$\begin{pmatrix} -1 \\ 1 \end{pmatrix}$	$\frac{1}{\rho_{k_0+1}}\begin{pmatrix} z-\alpha_{k_0+1} \\ -1/z+\overline{\alpha_{k_0+1}} \end{pmatrix}$
$\begin{pmatrix} p_-(z,k,k_0) \\ r_-(z,k,k_0) \end{pmatrix}$	$\frac{1}{\rho_{k_0}}\begin{pmatrix} 1+\alpha_{k_0}z \\ -z-\overline{\alpha_{k_0}} \end{pmatrix}$	$\begin{pmatrix} -z \\ 1 \end{pmatrix}$	$\frac{1}{\rho_{k_0+1}}\begin{pmatrix} z(1-\alpha_{k_0+1}) \\ -1+\overline{\alpha_{k_0+1}} \end{pmatrix}$
$\begin{pmatrix} q_-(z,k,k_0) \\ s_-(z,k,k_0) \end{pmatrix}$	$\frac{1}{\rho_{k_0}}\begin{pmatrix} 1-\alpha_{k_0}z \\ z-\overline{\alpha_{k_0}} \end{pmatrix}$	$\begin{pmatrix} z \\ 1 \end{pmatrix}$	$\frac{1}{\rho_{k_0+1}}\begin{pmatrix} z(1+\alpha_{k_0+1}) \\ 1+\overline{\alpha_{k_0+1}} \end{pmatrix}$

Remark 2.5. We note that Lemmas 2.2 and 2.3 are crucial for many of the proofs to follow. For instance, we note that the equivalence of items (i) and (vi) in Lemma 2.2 proves that for each $z \in \mathbb{C}\backslash\{0\}$, the solutions $\{u(z,k)\}_{k\in\mathbb{Z}}$ of $Uu(z,\cdot) = zu(z,\cdot)$ form a two-dimensional space, which implies that such solutions are linear combinations of $\{p_\pm(z,k,k_0)\}_{k\in\mathbb{Z}}$ and $\{q_\pm(z,k,k_0)\}_{k\in\mathbb{Z}}$ (with z-dependent coefficients). This equivalence also proves that any solution of $Uu(z,\cdot) = zu(z,\cdot)$ is determined by its values at a site k_0 of u and the auxiliary variable v. Moreover, taking into account item (vi) of Lemma 2.2, this also implies that such a solution is determined by its values at two consecutive sites k_0-1 and k_0. Similar comments apply to the solutions of $U^\top v(z,\cdot) = zv(z,\cdot)$. In the context of Lemma 2.3, we remark that its importance lies in the fact that it shows that in the case of half-lattice CMV operators, the analogous equations have a one-dimensional space of solutions for each $z \in \mathbb{C}\backslash\{0\}$, due to the restriction on k_0 that appears in items (vi) and (xii) of Lemma 2.3. As a consequence, the corresponding solutions are determined by their value at a single site k_0.

Next, we introduce the following modified Laurent polynomials $\widetilde{p}_\pm(z,k,k_0)$ and $\widetilde{q}_\pm(z,k,k_0)$, $z\in\mathbb{C}\backslash\{0\}$, $k,k_0\in\mathbb{Z}$, as follows:

$$\widetilde{p}_+(z,k,k_0) = \begin{cases} p_+(z,k,k_0)/z, & k_0 \text{ odd},\\ p_+(z,k,k_0), & k_0 \text{ even},\end{cases} \tag{2.59}$$

$$\widetilde{q}_+(z,k,k_0) = \begin{cases} q_+(z,k,k_0)/z, & k_0 \text{ odd},\\ q_+(z,k,k_0), & k_0 \text{ even},\end{cases} \tag{2.60}$$

$$\widetilde{p}_-(z,k,k_0) = \begin{cases} p_-(z,k,k_0), & k_0 \text{ odd},\\ p_-(z,k,k_0)/z, & k_0 \text{ even},\end{cases} \tag{2.61}$$

$$\widetilde{q}_-(z,k,k_0) = \begin{cases} q_-(z,k,k_0), & k_0 \text{ odd},\\ q_-(z,k,k_0)/z, & k_0 \text{ even}.\end{cases} \tag{2.62}$$

Remark 2.6. By Lemma 2.3, $\begin{pmatrix} p_\pm(z,k,k_0)\\ r_\pm(z,k,k_0)\end{pmatrix}_{k \gtrless k_0}$, $z\in\mathbb{C}\backslash\{0\}$, $k_0\in\mathbb{Z}$, are generalized eigenvectors of the operators $\mathbb{U}_{\pm,k_0}$. Moreover, by Lemma 2.2, $\begin{pmatrix} p_\pm(z,k,k_0)\\ r_\pm(z,k,k_0)\end{pmatrix}_{k\in\mathbb{Z}}$ and $\begin{pmatrix} q_\pm(z,k,k_0)\\ s_\pm(z,k,k_0)\end{pmatrix}_{k\in\mathbb{Z}}$, $z\in\mathbb{C}\backslash\{0\}$, $k_0\in\mathbb{Z}$, are generalized eigenvectors of $\mathbb{U}$.

Lemma 2.7. *The Laurent polynomials* $\widetilde{p}_\pm(z,k,k_0)$, $r_\pm(z,k,k_0)$, $\widetilde{q}_\pm(z,k,k_0)$, *and* $s_\pm(z,k,k_0)$ *satisfy the following relations for all* $z\in\mathbb{C}\backslash\{0\}$ *and* $k,k_0\in\mathbb{Z}$:

$$r_+(z,k,k_0) = \overline{\widetilde{p}_+(1/\overline{z},k,k_0)}, \tag{2.63}$$

$$s_+(z,k,k_0) = -\overline{\widetilde{q}_+(1/\overline{z},k,k_0)}, \tag{2.64}$$

$$r_-(z,k,k_0) = -\overline{\widetilde{p}_-(1/\overline{z},k,k_0)}, \tag{2.65}$$

$$s_-(z,k,k_0) = \overline{\widetilde{q}_-(1/\overline{z},k,k_0)}. \tag{2.66}$$

Proof. Let $\{u(z,k)\}_{k\in\mathbb{Z}}$, $\{v(z,k)\}_{k\in\mathbb{Z}}$ be two sequences of complex functions, then the following items (i)–(iii) are seen to be equivalent:

$$\text{(i)}\quad Wu(z,\cdot) = zv(z,\cdot), \quad Vv(z,\cdot) = u(z,\cdot), \tag{2.67}$$

$$\text{(ii)}\quad \frac{1}{z}u(z,\cdot) = W^*v(z,\cdot), \quad v(z,\cdot) = V^*u(z,\cdot), \tag{2.68}$$

$$\text{(iii)}\quad \frac{1}{\overline{z}}\overline{u(z,\cdot)} = W\overline{v(z,\cdot)}, \quad \overline{v(z,\cdot)} = V\overline{u(z,\cdot)}, \tag{2.69}$$

where Eqs. (2.67)–(2.69) are meant in the algebraic sense and hence V, V^*, W, and W^* are considered as difference expressions rather than difference operators. Thus, the assertion of the lemma follows from Lemma 2.3, Definition 2.4, and equalities (2.59)–(2.62). □

Lemma 2.8. *Let* $k_0\in\mathbb{Z}$. *Then the sets of Laurent polynomials* $\{p_+(\cdot,k,k_0)\}_{k\geqslant k_0}$ (*resp.*, $\{p_-(\cdot,k,k_0)\}_{k\leqslant k_0}$) *and* $\{r_+(\cdot,k,k_0)\}_{k\geqslant k_0}$ (*resp.*, $\{r_-(\cdot,k,k_0)\}_{k\leqslant k_0}$) *form orthonormal bases in* $L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))$ (*resp.*, $L^2(\partial\mathbb{D};d\mu_-(\cdot,k_0))$), *where*

$$d\mu_\pm(\zeta,k_0) = d(\delta_{k_0}, E_{U_{\pm,k_0}}(\zeta)\delta_{k_0})_{\ell^2([k_0,\pm\infty)\cap\mathbb{Z})}, \quad \zeta\in\partial\mathbb{D} \tag{2.70}$$

and $dE_{U_{\pm,k_0}}(\cdot)$ *denote the operator-valued spectral measures of the operators* $U_{\pm,k_0}$,

$$U_{\pm,k_0} = \oint_{\partial\mathbb{D}} dE_{U_{\pm,k_0}}(\zeta)\,\zeta. \tag{2.71}$$

Proof. It follows from the definition of the transfer matrix $T(z,k)$ in (2.18) and the recursion relations (2.39) and (2.46) that

$$\begin{aligned}&\overline{\operatorname{span}\{p_\pm(\cdot,k,k_0)\}_{k\gtrless k_0}} = \overline{\operatorname{span}\{r_\pm(\cdot,k,k_0)\}_{k\gtrless k_0}}\\ &\quad = \overline{\operatorname{span}\{\zeta^k\}_{k\in\mathbb{Z}}} = L^2(\partial\mathbb{D};d\mu),\end{aligned} \tag{2.72}$$

where $d\mu$ is any finite (nonnegative) Borel measure on $\partial\mathbb{D}$. Thus, one concludes that the systems of Laurent polynomials $\{p_\pm(\cdot,k,k_0)\}_{k\gtrless k_0}$ and $\{r_\pm(\cdot,k,k_0)\}_{k\gtrless k_0}$ are complete in $L^2(\partial\mathbb{D};d\mu_\pm(\cdot,k_0))$.

Next, consider the following equations:

$$(U_{+,k_0})^\top\delta_k = \sum_{j=k-2}^{k+2}(U_{+,k_0})^\top(j,k)\delta_j = \sum_{j=k-2}^{k+2}(U_{+,k_0})(k,\ j)\delta_j, \tag{2.73}$$

$$(U_{+,k_0})\delta_k = \sum_{j=k-2}^{k+2}(U_{+,k_0})(j,k)\delta_j = \sum_{j=k-2}^{k+2}(U_{+,k_0})^\top(k,\ j)\delta_j. \tag{2.74}$$

Comparing these equations to

$$z\widehat{p}_+(z,k,k_0) = (U_{+,k_0}\widehat{p}_+(z,\cdot,k_0))(k) = \sum_{j=k-2}^{k+2}(U_{+,k_0})(k,j)\widehat{p}_+(z,\ j,\ k_0), \tag{2.75}$$

$$z\widehat{r}_+(z,k,k_0) = ((U_{+,k_0})^\top\widehat{r}_+(z,\cdot,k_0))(k) = \sum_{j=k-2}^{k+2}(U_{+,k_0})^\top(k,j)\widehat{r}_+(z,j,k_0), \tag{2.76}$$

which by Lemma 2.3 have unique solutions $\widetilde{p}_+(z,k,k_0)$ and $r_+(z,k,k_0)$ satisfying $\widetilde{p}_+(z,k_0,k_0) = r_+(z,k_0,k_0) = 1$. Due to the algebraic nature of the proof of Lemma 2.3, the latter remains valid if $z\in\mathbb{C}\backslash\{0\}$ is replaced by a unitary operator on a Hilbert space. Thus, $\{\tilde{p}_+((U_{+,k_0})^\top,k,k_0)\delta_{k_0}\}_{k\geqslant k_0}$ and $\{r_+(U_{+,k_0},k,k_0)\delta_{k_0}\}_{k\geqslant k_0}$ are the unique solutions of

$$(U_{+,k_0})^\top p((U_{+,k_0})^\top,\cdot,k_0) = U_{+,k_0}p((U_{+,k_0})^\top,\cdot,k_0) \tag{2.77}$$

and

$$U_{+,k_0}r(U_{+,k_0},\cdot,k_0) = (U_{+,k_0})^\top r(U_{+,k_0},\cdot,k_0) \tag{2.78}$$

with value δ_{k_0} at $k=k_0$, respectively. In particular, one concludes that for $k\geqslant k_0$,

$$\delta_k = \widetilde{p}_+((U_{+,k_0})^\top,k,k_0)\delta_{k_0}, \tag{2.79}$$
$$\delta_k = r_+(U_{+,k_0},k,k_0)\delta_{k_0}. \tag{2.80}$$

Using the spectral representation for the operators U_{+,k_0} and $(U_{+,k_0})^\top$ one obtains (all scalar products $(\cdot,\cdot)$ in the remainder of this proof are with respect to the Hilbert space $\ell^2([k_0,\pm\infty)\cap\mathbb{Z})$ and for simplicity we omit the corresponding subscript in $(\cdot,\cdot)$),

$$(\delta_k,\delta_\ell) = \oint_{\partial\mathbb{D}} d(\delta_{k_0},E_{(U_{+,k_0})^\top}(\zeta)\delta_{k_0})\,\overline{p_+(\zeta,k,k_0)}\,p_+(\zeta,\ell,k_0), \tag{2.81}$$

$$(\delta_k,\delta_\ell) = \oint_{\partial\mathbb{D}} d(\delta_{k_0},E_{U_{+,k_0}}(\zeta)\delta_{k_0})\,\overline{r_+(\zeta,k,k_0)}\,r_+(\zeta,\ell,k_0), \quad k,\ell\in\mathbb{Z}. \tag{2.82}$$

Finally, one notes that

$$d\mu_+(\zeta,k_0) = d(\delta_{k_0},E_{U_{+,k_0}}(\zeta)\delta_{k_0}) = d(\delta_{k_0},E_{(U_{+,k_0})^\top}(\zeta)\delta_{k_0}) \tag{2.83}$$

since

$$\begin{aligned} \oint_{\partial\mathbb{D}} d\mu_+(\zeta, k_0)\, \zeta^k &= \left(\delta_{k_0}, U_{+,k_0}^k \delta_{k_0}\right) = \left(\delta_{k_0}, \left(U_{+,k_0}^k\right)^\top \delta_{k_0}\right) \\ &= \left(\delta_{k_0}, \left(U_{+,k_0}^\top\right)^k \delta_{k_0}\right) = \oint_{\partial\mathbb{D}} d(\delta_{k_0}, E_{(U_{+,k_0})^\top}(\zeta)\delta_{k_0})\, \zeta^k, \quad k \in \mathbb{Z}. \end{aligned} \tag{2.84}$$

Thus, the Laurent polynomials $\{p_+(\cdot, k, k_0)\}_{k \geqslant k_0}$ and $\{r_+(\cdot, k, k_0)\}_{k \geqslant k_0}$ are orthonormal in $L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))$.

The results for $\{p_-(\cdot, k, k_0)\}_{k \leqslant k_0}$ and $\{r_-(\cdot, k, k_0)\}_{k \leqslant k_0}$ are proved similarly. □

We note that the measures $d\mu_\pm(\cdot, k_0)$, $k_0 \in \mathbb{Z}$, are not only nonnegative but also supported on an infinite set.

Remark 2.9. In connection with our introductory remarks in (1.3)–(1.9) we note that $d\sigma_+ = d\mu_+(\cdot, 0)$ and

$$\begin{aligned} p_+(\zeta, k, 0) &= \begin{cases} \gamma_k \zeta^{-(k-1)/2} \varphi_+(\zeta, k), & k \text{ odd}, \\ \gamma_k \zeta^{-k/2} \varphi_+^*(\zeta, k), & k \text{ even}, \end{cases} \\ r_+(\zeta, k, 0) &= \begin{cases} \gamma_k \zeta^{-(k+1)/2} \varphi_+^*(\zeta, k), & k \text{ odd}, \\ \gamma_k \zeta^{-k/2} \varphi_+(\zeta, k), & k \text{ even}, \end{cases} \quad \zeta \in \partial\mathbb{D}. \end{aligned} \tag{2.85}$$

Let $\phi \in C(\partial\mathbb{D})$ and define the operator of multiplication by ϕ, $M_{\pm,k_0}(\phi)$, in $L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0))$ by

$$(M_{\pm,k_0}(\phi) f)(\zeta) = \phi(\zeta) f(\zeta), \quad f \in L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0)). \tag{2.86}$$

In the special case $\phi = id$ (where $id(\zeta) = \zeta$, $\zeta \in \partial\mathbb{D}$), the corresponding multiplication operator is denoted by $M_{\pm,k_0}(id)$. The spectrum of $M_{\pm,k_0}(\phi)$ is given by

$$\sigma(M_{\pm,k_0}(\phi)) = \text{ess.ran}_{d\mu_\pm(\cdot,k_0)}(\phi), \tag{2.87}$$

where the essential range of ϕ with respect to a measure $d\mu$ on $\partial\mathbb{D}$ is defined by

$$\text{ess.ran}_{d\mu}(\phi) = \{z \in \mathbb{C} \,|\, \text{for all } \varepsilon > 0, \mu(\{\zeta \in \partial\mathbb{D} \,|\, |\phi(\zeta) - z| < \varepsilon\}) > 0\}. \tag{2.88}$$

Corollary 2.10. *Let $k_0 \in \mathbb{Z}$ and $\phi \in C(\partial\mathbb{D})$. Then the operators $\phi(U_{\pm,k_0})$ and $\phi(U_{\pm,k_0}^\top)$ are unitarily equivalent to the operators $M_{\pm,k_0}(\phi)$ of multiplication by ϕ on $L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0))$. In particular,*

$$\sigma(\phi(U_{\pm,k_0})) = \sigma(\phi(U_{\pm,k_0}^\top)) = \text{ess.ran}_{d\mu_\pm(\cdot,k_0)}(\phi), \tag{2.89}$$

$$\sigma(U_{\pm,k_0}) = \sigma(U_{\pm,k_0}^\top) = \text{supp}\,(d\mu_\pm(\cdot, k_0)) \tag{2.90}$$

and the spectrum of $U_{\pm,k_0}$ is simple.

Proof. Consider the following linear maps $\dot{\mathcal{U}}_\pm$ from $\ell_0^\infty([k_0, \pm\infty) \cap \mathbb{Z})$ into the set of Laurent polynomials on $\partial\mathbb{D}$ defined by

$$(\dot{\mathcal{U}}_\pm f)(\zeta) = \sum_{k=k_0}^{\pm\infty} r_\pm(\zeta, k, k_0) f(k), \quad f \in \ell_0^\infty([k_0, \pm\infty) \cap \mathbb{Z}). \tag{2.91}$$

A simple calculation for $F(\zeta) = (\dot{\mathcal{U}}_\pm f)(\zeta)$, $f \in \ell_0^\infty([k_0, \pm\infty) \cap \mathbb{Z})$, shows that

$$\sum_{k=k_0}^{\pm\infty} |f(k)|^2 = \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta, k_0)\, |F(\zeta)|^2. \tag{2.92}$$

Since $\ell_0^\infty([k_0, \pm\infty) \cap \mathbb{Z})$ is dense in $\ell^2([k_0, \pm\infty) \cap \mathbb{Z})$, $\dot{\mathcal{U}}_\pm$ extend to bounded linear operators $\mathcal{U}_\pm : \ell^2([k_0, \pm\infty) \cap \mathbb{Z}) \to L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0))$. Since by (2.72), the sets of Laurent polynomials are dense in $L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0))$, the maps $\mathcal{U}_\pm$ are onto and one infers

$$(\mathcal{U}_\pm^{-1} F)(k) = \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta, k_0)\, \overline{r_\pm(\zeta, k, k_0)}\, F(\zeta), \quad F \in L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0)). \tag{2.93}$$

In particular, $\mathcal{U}_\pm$ are unitary. Moreover, we claim that $\mathcal{U}_\pm$ map the operators $\phi(U_{\pm,k_0})$ on $\ell^2([k_0, \pm\infty) \cap \mathbb{Z})$ to the operators $M_{\pm,k_0}(\phi)$ of multiplication by ϕ on $L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0))$,

$$\mathcal{U}_\pm \phi(U_{\pm,k_0}) \mathcal{U}_\pm^{-1} = M_{\pm,k_0}(\phi). \tag{2.94}$$

Indeed,

$$\begin{aligned}
&(\mathcal{U}_\pm \phi(U_{\pm,k_0}) \mathcal{U}_\pm^{-1} F(\cdot))(\zeta) = (\mathcal{U}_\pm \phi(U_{\pm,k_0}) f(\cdot))(\zeta) \\
&\quad = \sum_{k=k_0}^{\pm\infty} (\phi(U_{\pm,k_0}) f(\cdot))(k) r_\pm(\zeta, k, k_0) = \sum_{k=k_0}^{\pm\infty} (\phi(U_{\pm,k_0}^\top) r_\pm(\zeta, \cdot, k_0))(k) f(k) \\
&\quad = \sum_{k=k_0}^{\pm\infty} \phi(\zeta) r_\pm(\zeta, k, k_0) f(k) = \phi(\zeta) F(\zeta) \\
&\quad = (M_{\pm,k_0}(\phi) F)(\zeta), \quad F \in L^2(\partial\mathbb{D}; d\mu_\pm(\cdot, k_0)).
\end{aligned} \tag{2.95}$$

The result for $\phi(U_{\pm,k_0}^\top)$ is proved analogously. $\square$

Corollary 2.11. *Let $k_0 \in \mathbb{Z}$.*
The Laurent polynomials $\{p_+(\cdot, k, k_0)\}_{k \geqslant k_0}$ can be constructed by Gram–Schmidt orthogonalizing

$$\begin{cases} \zeta,\ 1,\ \zeta^2,\ \zeta^{-1},\ \zeta^3,\ \zeta^{-2}, \dots, & k_0 \text{ odd}, \\ 1,\ \zeta,\ \zeta^{-1},\ \zeta^2,\ \zeta^{-2}, \zeta^3, \dots, & k_0 \text{ even} \end{cases} \tag{2.96}$$

in $L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))$.
The Laurent polynomials $\{r_+(\cdot, k, k_0)\}_{k \geqslant k_0}$ can be constructed by Gram–Schmidt orthogonalizing

$$\begin{cases} 1,\ \zeta,\ \zeta^{-1},\ \zeta^2,\ \zeta^{-2}, \zeta^3, \dots, & k_0 \text{ odd}, \\ 1,\ \zeta^{-1},\ \zeta,\ \zeta^{-2},\ \zeta^2, \zeta^{-3}, \dots, & k_0 \text{ even} \end{cases} \tag{2.97}$$

in $L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))$.
The Laurent polynomials $\{p_-(\cdot, k, k_0)\}_{k \leqslant k_0}$ can be constructed by Gram–Schmidt orthogonalizing

$$\begin{cases} 1,\ -\zeta,\ \zeta^{-1},\ -\zeta^2,\ \zeta^{-2}, -\zeta^3, \dots, & k_0 \text{ odd}, \\ -\zeta,\ 1,\ -\zeta^2,\ \zeta^{-1},\ -\zeta^3,\ \zeta^{-2}, \dots, & k_0 \text{ even} \end{cases} \tag{2.98}$$

in $L^2(\partial\mathbb{D}; d\mu_-(\cdot, k_0))$.

The Laurent polynomials $\{r_-(\cdot,k,k_0)\}_{k\leqslant k_0}$ *can be constructed by Gram–Schmidt orthogonalizing*

$$\begin{cases} -1,\ \zeta^{-1},\ -\zeta,\ \zeta^{-2},\ -\zeta^2, \zeta^{-3},\ \dots, & k_0 \text{ odd},\\ 1,\ -\zeta,\ \zeta^{-1},\ -\zeta^2,\ \zeta^{-2},\ -\zeta^3,\ \dots, & k_0 \text{ even} \end{cases} \tag{2.99}$$

in $L^2(\partial\mathbb{D}; d\mu_-(\cdot,k_0))$.

Proof. The statements follow from Definition 2.4 and Lemma 2.8. □

The following result clarifies which measures arise as spectral measures of half-lattice CMV operators and it yields the reconstruction of Verblunsky coefficients from the spectral measures and the corresponding orthogonal polynomials.

Theorem 2.12. *Let* $k_0 \in \mathbb{Z}$ *and* $d\mu_\pm(\cdot,k_0)$ *be nonnegative finite measures on* $\partial\mathbb{D}$ *which are supported on infinite sets and normalized by*

$$\oint_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0) = 1. \tag{2.100}$$

Then $d\mu_\pm(\cdot,k_0)$ *are necessarily the spectral measures for some half-lattice CMV operators* $U_{\pm,k_0}$ *with coefficients* $\{\alpha_k\}_{k\geqslant k_0+1}$, *respectively* $\{\alpha_k\}_{k\leqslant k_0}$, *defined as follows*:

$$\alpha_k = -\begin{cases} \big(p_+(\cdot,k-1,k_0), M_{\pm,k_0}(id) r_+(\cdot,k-1,k_0)\big)_{L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))}, & k \text{ odd},\\ \big(r_+(\cdot,k-1,k_0), p_+(\cdot,k-1,k_0)\big)_{L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))}, & k \text{ even} \end{cases} \tag{2.101}$$

for all $k \geqslant k_0+1$ *and*

$$\alpha_k = -\begin{cases} \big(p_-(\cdot,k-1,k_0), M_{\pm,k_0}(id) r_-(\cdot,k-1,k_0)\big)_{L^2(\partial\mathbb{D};d\mu_-(\cdot,k_0))}, & k \text{ odd},\\ \big(r_-(\cdot,k-1,k_0), p_-(\cdot,k-1,k_0)\big)_{L^2(\partial\mathbb{D};d\mu_-(\cdot,k_0))}, & k \text{ even} \end{cases} \tag{2.102}$$

for all $k\leqslant k_0$. *Here the Laurent polynomials* $\{p_+(\cdot,k,k_0), r_+(\cdot,k,k_0)\}_{k\geqslant k_0}$ *and* $\{p_-(\cdot,k,k_0), r_-(\cdot,k,k_0)\}_{k\leqslant k_0}$ *denote the orthonormal polynomials constructed in Corollary* 2.11.

Proof. Using Corollary 2.11 one constructs the orthonormal Laurent polynomials $\{p_+(\zeta,k,k_0), r_+(\zeta,k,k_0)\}_{k\geqslant k_0}$, $\zeta \in \partial\mathbb{D}$. Because of their orthogonality properties one concludes

$$r_+(\zeta,k,k_0) = \begin{cases} \zeta\overline{p_+(\zeta,k,k_0)}, & k_0 \text{ odd},\\ \overline{p_+(\zeta,k,k_0)}, & k_0 \text{ even}, \end{cases} \quad \zeta\in\partial\mathbb{D},\ k\geqslant k_0. \tag{2.103}$$

Next we will establish the recursion relation (2.39). Consider the following Laurent polynomial $p(\zeta)$, $\zeta\in\partial\mathbb{D}$, for some fixed $k > k_0$:

$$p(\zeta) = \begin{cases} \rho_k p_+(\zeta,k,k_0) - \zeta r_+(\zeta,k-1,k_0), & k \text{ odd},\\ \rho_k p_+(\zeta,k,k_0) - r_+(\zeta,k-1,k_0), & k \text{ even}, \end{cases} \quad \zeta\in\partial\mathbb{D}, \tag{2.104}$$

where $\rho_k \in (0,\infty)$ is chosen such that the leading term of $p_+(\cdot,k,k_0)$ cancels the leading term of $r_+(\cdot,k-1,k_0)$. Using Corollary 2.11 one checks that the Laurent polynomial $p(\cdot)$ is proportional to $p_+(\cdot,k-1,k_0)$. Hence, one arrives at the following recursion relation:

$$\rho_k p_+(\zeta,k,k_0) = \begin{cases} \alpha_k p_+(\zeta,k-1,k_0) + \zeta r_+(\zeta,k-1,k_0), & k \text{ odd},\\ \overline{\alpha_k} p_+(\zeta,k-1,k_0) + r_+(\zeta,k-1,k_0), & k \text{ even}, \end{cases} \quad \zeta\in\partial\mathbb{D}, \tag{2.105}$$

where $\alpha_k \in \mathbb{C}$ is the proportionality constant. Taking the scalar product of both sides with $p_+(\zeta, k-1, k_0)$ yields the expressions for α_k, $k \geqslant k_0+1$, in (2.101). Moreover, applying (2.103) one obtains

$$\rho_k r_+(\zeta, k, k_0) = \begin{cases} \overline{\alpha_k} r_+(\zeta, k-1, k_0) + \frac{1}{\zeta} p_+(\zeta, k-1, k_0), & k \text{ odd}, \\ \alpha_k r_+(\zeta, k-1, k_0) + p_+(\zeta, k-1, k_0), & k \text{ even} \end{cases} \quad \zeta \in \partial\mathbb{D}, \tag{2.106}$$

and hence (2.39). Since $\rho_k > 0$, $k \in \mathbb{Z}$, it remains to show that $\rho_k^2 = 1 - |\alpha_k|^2$ and hence that $|\alpha_k| < 1$. This follows from the orthonormality of Laurent polynomials $\{p_+(\cdot, k, k_0)\}_{k \geqslant k_0}$ in $L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))$,

$$\begin{aligned} |\alpha_k|^2 &= \|\alpha_k p_+(\cdot, k-1, k_0)\|^2_{L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))} \\ &= \left\|\rho_k p_+(\cdot, k, k_0) - id(\cdot) r_+(\cdot, k-1, k_0)\right\|^2_{L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))} \\ &= \rho_k^2 + 1 - 2\mathrm{Re}\Big(\big(\rho_k p_+(\cdot, k, k_0), id(\cdot) r_+(\cdot, k-1, k_0)\big)_{L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))}\Big) \\ &= \rho_k^2 + 1 \\ &\quad - 2\mathrm{Re}\Big(\big(\rho_k p_+(\cdot, k, k_0), [\rho_k p_+(\cdot, k, k_0) - \alpha_k p_+(\cdot, k-1, k_0)]\big)_{L^2(\partial\mathbb{D}; d\mu_+(\cdot, k_0))}\Big) \\ &= 1 - \rho_k^2, \ k \text{ odd}. \end{aligned} \tag{2.107}$$

Similarly one treats the case k even. Finally, using Lemma 2.3 one concludes that $\begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix}_{k \geqslant k_0}$, $z \in \mathbb{C}\backslash\{0\}$, $k_0 \in \mathbb{Z}$, is a generalized eigenvector of the operator $\mathbb{U}_{+,k_0}$ defined in (2.33) associated with the coefficients α_k, ρ_k introduced above. Thus, the measure $d\mu_+(\cdot, k_0)$ is the spectral measure of the operator U_{+,k_0} in (2.31). Similarly one proves the result for $d\mu_-(\cdot, k_0)$ and (2.102) for $k \leqslant k_0$. □

Lemma 2.13. *Let $z \in \mathbb{C}\backslash(\partial\mathbb{D} \cup \{0\})$ and $k_0 \in \mathbb{Z}$. Then the sets of two-dimensional Laurent polynomials* $\begin{pmatrix} \widetilde{p}_\pm(z,k,k_0) \\ r_\pm(z,k,k_0) \end{pmatrix}_{k \gtrless k_0}$ and $\begin{pmatrix} \widetilde{q}_\pm(z,k,k_0) \\ s_\pm(z,k,k_0) \end{pmatrix}_{k \gtrless k_0}$ *are related by*

$$\begin{pmatrix} \widetilde{q}_\pm(z, k, k_0) \\ s_\pm(z, k, k_0 \end{pmatrix} = \pm \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta, k_0) \, \frac{\zeta + z}{\zeta - z} \left(\begin{pmatrix} \widetilde{p}_\pm(\zeta, k, k_0) \\ r_\pm(\zeta, k, k_0) \end{pmatrix} - \begin{pmatrix} \widetilde{p}_\pm(z, k, k_0) \\ r_\pm(z, k, k_0) \end{pmatrix} \right), \quad k \gtrless k_0. \tag{2.108}$$

Proof. First, we prove (2.108) for k_0 even, which by (2.59)–(2.62) is equivalent to

$$\begin{pmatrix} q_+(z, k, k_0) \\ s_+(z, k, k_0 \end{pmatrix} = \oint_{\partial\mathbb{D}} \frac{\zeta + z}{\zeta - z} \left(\begin{pmatrix} p_+(\zeta, k, k_0) \\ r_+(\zeta, k, k_0) \end{pmatrix} - \begin{pmatrix} p_+(z, k, k_0) \\ r_+(z, k, k_0) \end{pmatrix} \right) d\mu_+(\zeta, k_0), \quad z \in \mathbb{C}\backslash(\partial\mathbb{D} \cup \{0\}), \ k > k_0, k_0 \text{ even}. \tag{2.109}$$

Let $k_0 \in \mathbb{Z}$ be even. It suffices to show that the right-hand side of (2.109), temporarily denoted by the symbol $RHS(z, k, k_0)$, satisfies

$$T(z, k+1)^{-1} RHS(z, k+1, k_0) = RHS(z, k, k_0), \quad k > k_0, \tag{2.110}$$

$$T(z, k_0+1)^{-1} RHS(z, k_0+1, k_0) = \begin{pmatrix} q_+(z, k_0, k_0) \\ s_+(z, k_0, k_0) \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}. \tag{2.111}$$

One verifies these statements using the following equality:

$$T(z,k+1)^{-1} RHS(z,k+1,k_0) = RHS(z,k,k_0) + \oint_{\partial\mathbb{D}} \frac{\zeta+z}{\zeta-z}\Big(T(z,k+1)^{-1} - T(\zeta,k+1)^{-1}\Big)\begin{pmatrix} p_+(\zeta,k+1,k_0) \\ r_+(\zeta,k+1,k_0)\end{pmatrix} d\mu_+(\zeta,k_0), \quad k\in\mathbb{Z}. \tag{2.112}$$

For $k > k_0$, the last term on the right-hand side of (2.112) is equal to zero since for k odd, $T(z,k+1)$ does not depend on z, and for k even, by Corollary 2.11, $p_+(\zeta,k+1,k_0)$ and $r_+(\zeta,k+1,k_0)$ are orthogonal in $L^2(\partial\mathbb{D}; d\mu_+(\cdot,k_0))$ to span$\{1,\zeta\}$ and span$\{1,\zeta^{-1}\}$, respectively, hence,

$$\begin{aligned}
&\oint_{\partial\mathbb{D}} \frac{\zeta+z}{\zeta-z}\Big(T(z,k+1)^{-1} - T(\zeta,k+1)^{-1}\Big)\begin{pmatrix} p_+(\zeta,k+1,k_0) \\ r_+(\zeta,k+1,k_0)\end{pmatrix} d\mu_+(\zeta,k_0) \\
&\quad = \oint_{\partial\mathbb{D}} \frac{\zeta+z}{\zeta-z}\,\frac{1}{\rho_{k+1}}\begin{pmatrix} 0 & z-\zeta \\ (1/z)-(1/\zeta) & 0\end{pmatrix}\begin{pmatrix} p_+(\zeta,k+1,k_0) \\ r_+(\zeta,k+1,k_0)\end{pmatrix} d\mu_+(\zeta,k_0) \\
&\quad = \frac{1}{\rho_{k+1}}\oint_{\partial\mathbb{D}} \begin{pmatrix} 0 & -(\zeta+z) \\ (1/\zeta)+(1/z) & 0\end{pmatrix}\begin{pmatrix} p_+(\zeta,k+1,k_0) \\ r_+(\zeta,k+1,k_0)\end{pmatrix} d\mu_+(\zeta,k_0) \\
&\quad = \frac{1}{\rho_{k+1}}\oint_{\partial\mathbb{D}} \begin{pmatrix} -\overline{((1/\zeta)+\overline{z})}r_+(\zeta,k,k_0) \\ \overline{(\zeta+(1/\overline{z}))}p_+(\zeta,k,k_0)\end{pmatrix} d\mu_+(\zeta,k_0) = \begin{pmatrix} 0 \\ 0\end{pmatrix}.
\end{aligned} \tag{2.113}$$

This proves (2.110).

For $k = k_0$ one obtains $RHS(z,k_0,k_0) = 0$ since $p_+(\zeta,k_0,k_0) = r_+(\zeta,k_0,k_0) = 1$. By Corollary 2.11, $p_+(\zeta,k_0+1,k_0)$ and $r_+(\zeta,k_0+1,k_0)$ are orthogonal to constants in $L^2(\partial\mathbb{D}; d\mu_+(\cdot,k_0))$ and by the recursion relation (2.17),

$$p_+(\zeta,k_0+1,k_0) = (\zeta+\alpha_{k_0+1})/\rho_{k_0+1}, \quad r_+(\zeta,k_0+1,k_0) = ((1/\zeta)+\overline{\alpha_{k_0+1}})/\rho_{k_0+1}. \tag{2.114}$$

Thus,

$$\begin{aligned}
&\oint_{\partial\mathbb{D}} \frac{\zeta+z}{\zeta-z}\Big(T(z,k_0+1)^{-1} - T(\zeta,k_0+1)^{-1}\Big)\begin{pmatrix} p_+(\zeta,k_0+1,k_0) \\ r_+(\zeta,k_0+1,k_0)\end{pmatrix} d\mu_+(\zeta,k_0) \\
&\quad = \oint_{\partial\mathbb{D}} \frac{1}{\rho_{k_0+1}}\begin{pmatrix} -\overline{((1/\zeta)+\overline{z})},\, r_+(\zeta,k_0+1,k_0) \\ \overline{(\zeta+(1/\overline{z}))},\, p_+(\zeta,k_0+1,k_0)\end{pmatrix} d\mu_+(\zeta,k_0) \\
&\quad = \begin{pmatrix} -\|r_+(\zeta,k_0+1,k_0)\|^2_{L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))} \\ \|p_+(\zeta,k_0+1,k_0)\|^2_{L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))}\end{pmatrix} = \begin{pmatrix} -1 \\ 1\end{pmatrix}.
\end{aligned} \tag{2.115}$$

This proves (2.111).

Next, we prove that

$$\begin{pmatrix} s_+(z,k,k_0) \\ \widetilde{q}_+(z,k,k_0)\end{pmatrix} = \oint_{\partial\mathbb{D}} \frac{\zeta+z}{\zeta-z}\left(\begin{pmatrix} r_+(\zeta,k,k_0) \\ \widetilde{p}_+(\zeta,k,k_0)\end{pmatrix} - \begin{pmatrix} r_+(z,k,k_0) \\ \widetilde{p}_+(z,k,k_0)\end{pmatrix}\right) d\mu_+(\zeta,k_0), \quad z\in\mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}),\ k>k_0, \quad k_0 \text{ odd}. \tag{2.116}$$

Let $k_0\in\mathbb{Z}$ be odd. We note that

$$\begin{pmatrix} u(z,k) \\ v(z,k)\end{pmatrix} = T(z,k)\begin{pmatrix} u(z,k-1) \\ v(z,k-1)\end{pmatrix}$$

is equivalent to

$$\begin{pmatrix} v(z,k) \\ \widetilde{u}(z,k) \end{pmatrix} = \widetilde{T}(z,k) \begin{pmatrix} v(z,k-1) \\ \widetilde{u}(z,k-1) \end{pmatrix}, \tag{2.117}$$

where

$$\widetilde{u}(z,k) = u(z,k)/z, \quad \widetilde{T}(z,k) = \begin{pmatrix} 0 & 1 \\ 1/z & 0 \end{pmatrix} T(z,k) \begin{pmatrix} 0 & z \\ 1 & 0 \end{pmatrix}. \tag{2.118}$$

Thus, it suffices to show that the right-hand side of (2.116), temporarily denoted by $\widetilde{RHS}(z,k,k_0)$, satisfies

$$\widetilde{T}(z,k+1)^{-1}\widetilde{RHS}(z,k+1,k_0) = \widetilde{RHS}(z,k,k_0), \quad k > k_0, \tag{2.119}$$

$$\widetilde{T}(z,k_0+1)^{-1}\widetilde{RHS}(z,k_0+1,k_0) = \begin{pmatrix} s_+(z,k_0,k_0) \\ \widetilde{q}_+(z,k_0,k_0) \end{pmatrix} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}. \tag{2.120}$$

At this point one can follow the first part of the proof replacing T by $\widetilde{T}$, $\left(\begin{smallmatrix} p_+ \\ r_+ \end{smallmatrix}\right)$ by $\left(\begin{smallmatrix} r_+ \\ \widetilde{p}_+ \end{smallmatrix}\right)$, $\left(\begin{smallmatrix} q_+ \\ s_+ \end{smallmatrix}\right)$ by $\left(\begin{smallmatrix} s_+ \\ \widetilde{q}_+ \end{smallmatrix}\right)$, etc.

The result for the remaining polynomials $\widetilde{p}_-(z,k,k_0), r_-(z,k,k_0), \widetilde{q}_-(z,k,k_0)$, and $s_-(z,k,k_0)$ follows similarly. □

Corollary 2.14. *Let $k_0 \in \mathbb{Z}$. Then the sets of two-dimensional Laurent polynomials $\left(\begin{smallmatrix} p_\pm(z,k,k_0) \\ r_\pm(z,k,k_0) \end{smallmatrix}\right)_{k \gtrless k_0}$ and $\left(\begin{smallmatrix} q_\pm(z,k,k_0) \\ s_\pm(z,k,k_0) \end{smallmatrix}\right)_{k \gtrless k_0}$ satisfy the relation*

$$\begin{pmatrix} q_\pm(z,\cdot,k_0) \\ s_\pm(z,\cdot,k_0) \end{pmatrix} + m_\pm(z,k_0) \begin{pmatrix} p_\pm(z,\cdot,k_0) \\ r_\pm(z,\cdot,k_0) \end{pmatrix} \in \ell^2([k_0,\pm\infty)\cap\mathbb{Z})^2, \quad z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}), \tag{2.121}$$

for some coefficients $m_\pm(z,k_0)$ given by

$$m_\pm(z,k_0) = \pm(\delta_{k_0}, (U_{\pm,k_0}+zI)(U_{\pm,k_0}-zI)^{-1}\delta_{k_0})_{\ell^2([k_0,\pm\infty)\cap\mathbb{Z})} \tag{2.122}$$

$$= \pm \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0)\, \frac{\zeta+z}{\zeta-z}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D} \tag{2.123}$$

with

$$m_\pm(0,k_0) = \pm \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0) = \pm 1. \tag{2.124}$$

Proof. Consider the operator

$$C_{\pm,k_0}(z) = \begin{cases} \begin{pmatrix} I & 0 \\ 0 & \pm I \end{pmatrix} ((\mathbb{U}_{\pm,k_0})^\top + zI)((\mathbb{U}_{\pm,k_0})^\top - zI)^{-1}, & k_0 \text{ odd}, \\ \begin{pmatrix} \pm I & 0 \\ 0 & I \end{pmatrix} ((\mathbb{U}_{\pm,k_0})^\top + zI)((\mathbb{U}_{\pm,k_0})^\top - zI)^{-1}, & k_0 \text{ even}, \end{cases} \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \tag{2.125}$$

on $\ell^2(\mathbb{Z})^2$. Since $C_{\pm,k_0}(z)$ is bounded for $z \in \mathbb{C}\backslash\partial\mathbb{D}$ one has

$$\left\{\left(\begin{pmatrix} \delta_{k_0} \\ \delta_{k_0} \end{pmatrix}, C_{\pm,k_0}(z)\begin{pmatrix} \delta_k \\ \delta_k \end{pmatrix}\right)\right\}_{k\in\mathbb{Z}} = \left\{\left(C_{\pm,k_0}(z)^*\begin{pmatrix} \delta_{k_0} \\ \delta_{k_0} \end{pmatrix}, \begin{pmatrix} \delta_k \\ \delta_k \end{pmatrix}\right)\right\}_{k\in\mathbb{Z}} \in \ell^2(\mathbb{Z})^2. \tag{2.126}$$

Using the spectral representation for the operator $C_{\pm,k_0}(z)$, Lemma 2.13, and (2.59)–(2.62) one obtains

$$\begin{aligned}\left(\begin{pmatrix}\delta_{k_0}\\ \delta_{k_0}\end{pmatrix}, C_{\pm,k_0}(z)\begin{pmatrix}\delta_k\\ \delta_k\end{pmatrix}\right) &= \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0)\,\frac{\zeta+z}{\zeta-z}\begin{pmatrix}\widetilde{p}_\pm(\zeta,k,k_0)\\ r_\pm(\zeta,k,k_0)\end{pmatrix}\\ &= \pm\left[\begin{pmatrix}\widetilde{q}_\pm(z,k,k_0)\\ s_\pm(z,k,k_0)\end{pmatrix} + m_\pm(z,k_0)\begin{pmatrix}\widetilde{p}_\pm(z,k,k_0)\\ r_\pm(z,k,k_0)\end{pmatrix}\right], \quad k \gtrless k_0, \end{aligned} \tag{2.127}$$

where $m_\pm(z,k_0) = \pm\int_{\partial\mathbb{D}} d\mu_\pm(\zeta,k_0)\,\frac{\zeta+z}{\zeta-z}$. □

Lemma 2.15. *Let $k_0 \in \mathbb{Z}$. Then relation* (2.121) *uniquely determines the functions $m_\pm(\cdot,k_0)$ on $\mathbb{C}\backslash\partial\mathbb{D}$.*

Proof. We will prove the lemma by contradiction. Assume that there are two functions $m_+(z,k_0)$ and $\widetilde{m}_+(z,k_0)$ satisfying (2.121) such that $m_+(z_0,k_0) \neq \widetilde{m}_+(z_0,k_0)$ for some $z_0 \in \mathbb{C}\backslash\partial\mathbb{D}$. Then there are $\lambda_1, \lambda_2 \in \mathbb{C}$ such that the following vector:

$$\begin{pmatrix}w_1(z_0,\cdot,k_0)\\ w_2(z_0,\cdot,k_0)\end{pmatrix} = (\lambda_1 m_+(z_0,k_0) + \lambda_2\widetilde{m}_+(z_0,k_0))\begin{pmatrix}p_+(z_0,\cdot,k_0\\ r_+(z_0,\cdot,k_0)\end{pmatrix} \tag{2.128}$$

$$+(\lambda_1+\lambda_2)\begin{pmatrix}q_+(z_0,\cdot,k_0)\\ s_+(z_0,\cdot,k_0)\end{pmatrix} \in \ell^2([k_0,\infty)\cap\mathbb{Z})^2 \tag{2.129}$$

is nonzero and satisfies

$$w_1(z_0,k_0,k_0) = \begin{cases} z_0 w_2(z_0,k_0,k_0), & k_0 \text{ odd},\\ w_2(z_0,k_0,k_0), & k_0 \text{ even}.\end{cases} \tag{2.130}$$

By Lemma 2.3, $\begin{pmatrix}w_1(z_0,k,k_0)\\ w_2(z_0,k,k_0)\end{pmatrix}_{k\geqslant k_0}$ is an eigenvector of the operator U_{+,k_0} and $z_0 \in \mathbb{C}\backslash\partial\mathbb{D}$ is the corresponding eigenvalue which is impossible since U_{+,k_0} is unitary.

Similarly, one proves the result for $m_-(z,k_0)$. □

Corollary 2.16. *There are solutions $\begin{pmatrix}\psi_\pm(z,\cdot)\\ \chi_\pm(z,\cdot)\end{pmatrix}_{k\in\mathbb{Z}}$ of* (2.17), *unique up to constant multiples, so that for some* (*and hence for all*) $k_1 \in \mathbb{Z}$,

$$\begin{pmatrix}\psi_\pm(z,\cdot)\\ \chi_\pm(z,\cdot)\end{pmatrix} \in \ell^2([k_1,\pm\infty)\cap\mathbb{Z})^2, \quad z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}). \tag{2.131}$$

Proof. Since any solution of (2.17) can be expressed as a linear combination of the polynomials $\begin{pmatrix}p_\pm(z,k,k_0)\\ r_\pm(z,k,k_0)\end{pmatrix}_{k\in\mathbb{Z}}$ and $\begin{pmatrix}q_\pm(z,k,k_0)\\ s_\pm(z,k,k_0)\end{pmatrix}_{k\in\mathbb{Z}}$, existence and uniqueness of the solutions $\begin{pmatrix}\psi_\pm(z,\cdot)\\ \chi_\pm(z,\cdot)\end{pmatrix}_{k\in\mathbb{Z}}$ follow from Corollary 2.14 and Lemma 2.15, respectively. □

Lemma 2.17. *Let $z \in \mathbb{C}\backslash\{0\}$ and $k_0 \in \mathbb{Z}$. Then the two-dimensional Laurent polynomials* $\begin{pmatrix}p_+(z,k,k_0)\\ r_+(z,k,k_0)\end{pmatrix}_{k\in\mathbb{Z}}$, $\begin{pmatrix}q_+(z,k,k_0)\\ s_+(z,k,k_0)\end{pmatrix}_{k\in\mathbb{Z}}$, $\begin{pmatrix}p_-(z,k,k_0-1)\\ r_-(z,k,k_0-1)\end{pmatrix}_{k\in\mathbb{Z}}$, $\begin{pmatrix}q_-(z,k,k_0-1)\\ s_-(z,k,k_0-1)\end{pmatrix}_{k\in\mathbb{Z}}$ *are connected* *by the following relations*:

$$\begin{pmatrix} p_-(z,k,k_0-1) \\ r_-(z,k,k_0-1) \end{pmatrix} = \frac{i\mathrm{Im}(b_{k_0})}{\rho_{k_0}} \begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix} + \frac{\mathrm{Re}(b_{k_0})}{\rho_{k_0}} \begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}, \tag{2.132}$$

$$\begin{pmatrix} q_-(z,k,k_0-1) \\ s_-(z,k,k_0-1) \end{pmatrix} = \frac{\mathrm{Re}(a_{k_0})}{\rho_{k_0}} \begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix} + \frac{i\mathrm{Im}(a_{k_0})}{\rho_{k_0}} \begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}, \quad k \in \mathbb{Z}. \tag{2.133}$$

Proof. It follows from Definition 2.4 that the left- and right-hand sides of (2.132) and (2.133) satisfy the same recursion relation (2.17). Hence, it suffices to check (2.132) and (2.133) at one point, say, the point $k = k_0$. Using (2.4), (2.5), (2.17), and (2.58), one finds the following expressions for the left-hand sides of (2.132) and (2.133):

$$\begin{pmatrix} p_-(z,k_0,k_0-1) \\ r_-(z,k_0,k_0-1) \end{pmatrix} = \frac{1}{\rho_{k_0}} \begin{pmatrix} zb_{k_0} \\ -\overline{b_{k_0}} \end{pmatrix}, \quad \begin{pmatrix} q_-(z,k_0,k_0-1) \\ s_-(z,k_0,k_0-1) \end{pmatrix} = \frac{1}{\rho_{k_0}} \begin{pmatrix} za_{k_0} \\ \overline{a_{k_0}} \end{pmatrix}, \quad k_0 \text{ odd} \tag{2.134}$$

and

$$\begin{pmatrix} p_-(z,k_0,k_0-1) \\ r_-(z,k_0,k_0-1) \end{pmatrix} = \frac{1}{\rho_{k_0}} \begin{pmatrix} -\overline{b_{k_0}} \\ b_{k_0} \end{pmatrix}, \quad \begin{pmatrix} q_-(z,k_0,k_0-1) \\ s_-(z,k_0,k_0-1) \end{pmatrix} = \frac{1}{\rho_{k_0}} \begin{pmatrix} \overline{a_{k_0}} \\ a_{k_0} \end{pmatrix}, \quad k_0 \text{ even.} \tag{2.135}$$

The same result also follows for the right-hand side of (2.132), (2.133) using (2.4), (2.5), and the initial conditions (2.57). □

Theorem 2.18. *Let $k_0 \in \mathbb{Z}$. Then there exist unique functions $M_\pm(\cdot, k_0)$ such that*

$$\begin{pmatrix} u_\pm(z,\cdot,k_0) \\ v_\pm(z,\cdot,k_0) \end{pmatrix} = \begin{pmatrix} q_+(z,\cdot,k_0) \\ s_+(z,\cdot,k_0) \end{pmatrix} + M_\pm(z,k_0) \begin{pmatrix} p_+(z,\cdot,k_0) \\ r_+(z,\cdot,k_0) \end{pmatrix} \in \ell^2([k_0,\pm\infty) \cap \mathbb{Z})^2, \quad z \in \mathbb{C}\backslash(\partial\mathbb{D} \cup \{0\}). \tag{2.136}$$

Proof. Assertion (2.136) follows from (2.59)–(2.62), Corollaries 2.14 and 2.16, and Lemmas 2.15 and 2.17. □

We will call $u_\pm(z,\cdot,k_0)$ (resp., $v_\pm(z,\cdot,k_0)$) *Weyl–Titchmarsh solutions* of U (resp., $U^\top$). By Corollary 2.16, $u_\pm(z,\cdot,k_0)$ and $v_\pm(z,\cdot,k_0)$ are constant multiples of $\psi_\pm(z,\cdot,k_0)$ and $\chi_\pm(z,\cdot,k_0)$. Similarly, we will call $m_\pm(z,k_0)$ as well as $M_\pm(z,k_0)$ the *half-lattice Weyl–Titchmarsh m-functions* associated with $U_{\pm,k_0}$. (See also [31] for a comparison of various alternative notions of Weyl–Titchmarsh m-functions for U_{+,k_0}.)

It follows from Corollaries 2.14 and 2.16 and Lemma 2.17 that

$$M_+(z,k_0) = m_+(z,k_0), \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \tag{2.137}$$

$$M_+(0,k_0) = 1, \tag{2.138}$$

$$M_-(z,k_0) = \frac{\mathrm{Re}(a_{k_0}) + i\mathrm{Im}(b_{k_0})m_-(z,k_0-1)}{i\mathrm{Im}(a_{k_0}) + \mathrm{Re}(b_{k_0})m_-(z,k_0-1)}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \tag{2.139}$$

$$M_-(0,k_0) = \frac{\alpha_{k_0}+1}{\alpha_{k_0}-1}. \tag{2.140}$$

In particular, one infers that $M_\pm$ are analytic at $z = 0$.

Since (2.136) singles out $p_+(z,\cdot,k_0)$, $q_+(z,\cdot,k_0)$, $r_+(z,\cdot,k_0)$, and $s_+(z,\cdot,k_0)$, we now add the following observation.

Remark 2.19. One can also define functions $\widehat{M}_\pm(\cdot, k_0)$ such that the following relation holds:

$$\begin{pmatrix} \widehat{u}_\pm(z,\cdot,k_0) \\ \widehat{v}_\pm(z,\cdot,k_0) \end{pmatrix} = \begin{pmatrix} q_-(z,\cdot,k_0) \\ s_-(z,\cdot,k_0) \end{pmatrix} + \widehat{M}_\pm(z,k_0) \begin{pmatrix} p_-(z,\cdot,k_0) \\ r_-(z,\cdot,k_0) \end{pmatrix} \in \ell^2([k_0, \pm\infty) \cap \mathbb{Z})^2, \quad z \in \mathbb{C}\backslash(\partial\mathbb{D} \cup \{0\}). \tag{2.141}$$

Applying Corollary 2.16, $\widehat{u}_\pm(z,\cdot,k_0)$ and $\widehat{v}_\pm(z,\cdot,k_0)$ are also constant multiples of $\psi_\pm(z,\cdot,k_0)$ and $\chi_\pm(z,\cdot,k_0)$ (hence they are constant multiples of $u_\pm(z,\cdot,k_0)$ and $v_\pm(z,\cdot,k_0)$). It follows from Corollaries 2.14 and 2.16 and Lemmas 2.15 and 2.17, that $\widehat{M}_\pm(\cdot, k_0)$ are uniquely defined and satisfy the relations

$$\widehat{M}_+(z, k_0 - 1) = \frac{\mathrm{Re}(a_{k_0}) - i\,\mathrm{Im}(a_{k_0}) m_+(z,k_0)}{-i\,\mathrm{Im}(a_{k_0}) + \mathrm{Re}(b_{k_0}) m_+(z,k_0)}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \tag{2.142}$$

$$\widehat{M}_-(z,k_0) = m_-(z,k_0), \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{2.143}$$

Moreover, one derives from (2.139) and (2.143) that

$$M_\pm(z,k_0) = \frac{\mathrm{Re}(a_{k_0}) + i\,\mathrm{Im}(b_{k_0}) \widehat{M}_\pm(z,k_0-1)}{i\,\mathrm{Im}(a_{k_0}) + \mathrm{Re}(b_{k_0}) \widehat{M}_\pm(z,k_0-1)}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{2.144}$$

In this paper we will only use $\begin{pmatrix} u_\pm(z,\cdot,k_0) \\ v_\pm(z,\cdot,k_0) \end{pmatrix}$ and $M_\pm(z,k_0)$.

Lemma 2.20. *Let $k \in \mathbb{Z}$. Then the functions $M_+(\cdot,k)|_{\mathbb{D}}$ (resp., $M_-(\cdot,k)|_{\mathbb{D}}$) are Caratheodory (resp., anti-Caratheodory) functions. Moreover, $M_\pm$ satisfy the following Riccati-type equation*:

$$(z\overline{b_k} - b_k) M_\pm(z,k-1) M_\pm(z,k) + (z\overline{b_k} + b_k) M_\pm(z,k) - (z\overline{a_k} + a_k) M_\pm(z,k-1) = z\overline{a_k} - a_k, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{2.145}$$

Proof. It follows from (2.123) and Theorem A.2 that $m_\pm(z,k_0)$ are Caratheodory and anti-Caratheodory functions, respectively. From (2.137) one concludes that $M_+(z,k_0)$ is also a Caratheodory function. Using (2.139) one verifies that $M_-(z,k_0)$ is analytic in $\mathbb{D}$ since $\mathrm{Re}(m_-(z,k_0)) < 0$ and that

$$\begin{aligned} \mathrm{Re}(M_-(z,k_0)) &= \mathrm{Re}\left(\frac{\mathrm{Re}(a_{k_0}) + i\,\mathrm{Im}(b_{k_0}) m_-(z,k_0-1)}{i\,\mathrm{Im}(a_{k_0}) + \mathrm{Re}(b_{k_0}) m_-(z,k_0-1)}\right) \\ &= \frac{\mathrm{Re}(a_{k_0})\mathrm{Re}(b_{k_0}) + \mathrm{Im}(a_{k_0})\mathrm{Im}(b_{k_0})}{|i\,\mathrm{Im}(a_{k_0}) + \mathrm{Re}(b_{k_0}) m_-(z,k_0-1)|^2} \mathrm{Re}(m_-(z,k_0-1)) \\ &= \frac{\rho_{k_0}^2 \mathrm{Re}(m_-(z,k_0-1))}{|i\,\mathrm{Im}(a_{k_0}) + \mathrm{Re}(b_{k_0}) m_-(z,k_0-1)|^2} < 0. \end{aligned} \tag{2.146}$$

Hence, $M_-(z,k_0)$ is an anti-Caratheodory function.

Next, consider the 2×2 matrix

$$D(z,k_0) = \big(d_{\ell,\ell'}(z,k_0)\big)_{\ell,\ell'=1,2} = \frac{1}{2\rho_{k_0}} \begin{cases} \begin{pmatrix} \overline{a_{k_0}} + a_{k_0}/z & \overline{a_{k_0}} - a_{k_0}/z \\ \overline{b_{k_0}} - b_{k_0}/z & \overline{b_{k_0}} + b_{k_0}/z \end{pmatrix}, & k_0 \text{ odd}, \\ \begin{pmatrix} z\overline{a_{k_0}} + a_{k_0} & z\overline{a_{k_0}} - a_{k_0} \\ z\overline{b_{k_0}} - b_{k_0} & z\overline{b_{k_0}} + b_{k_0} \end{pmatrix}, & k_0 \text{ even}, \end{cases} \quad z \in \mathbb{C}\backslash\{0\}, \; k_0 \in \mathbb{Z}. \tag{2.147}$$

It follows from (2.4), (2.5), and Definition 2.4 that $D(z,k_0)$ satisfies

$$\begin{pmatrix} p_+(z,\cdot,k_0-1) & q_+(z,\cdot,k_0-1) \\ r_+(z,\cdot,k_0-1) & s_+(z,\cdot,k_0-1) \end{pmatrix} = \begin{pmatrix} p_+(z,\cdot,k_0) & q_+(z,\cdot,k_0) \\ r_+(z,\cdot,k_0) & s_+(z,\cdot,k_0) \end{pmatrix} D(z,k_0). \tag{2.148}$$

Thus, using Theorem 2.18 one finds

$$M_\pm(z,k_0) = \frac{d_{1,2}(z,k_0) + d_{1,1}(z,k_0)M_\pm(z,k_0-1)}{d_{2,2}(z,k_0) + d_{2,1}(z,k_0)M_\pm(z,k_0-1)}. \qquad \square \tag{2.149}$$

In addition, we introduce the functions $\Phi_\pm(\cdot,k)$, $k \in \mathbb{Z}$, by

$$\Phi_\pm(z,k) = \frac{M_\pm(z,k)-1}{M_\pm(z,k)+1}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{2.150}$$

One then verifies,

$$M_\pm(z,k) = \frac{1+\Phi_\pm(z,k)}{1-\Phi_\pm(z,k)}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{2.151}$$

Moreover, we extend these functions to the unit circle $\partial\mathbb{D}$ by taking the radial limits which exist and are finite for μ_0-almost every $\zeta \in \partial\mathbb{D}$,

$$M_\pm(\zeta,k) = \lim_{r\uparrow 1} M_\pm(r\zeta,k), \tag{2.152}$$

$$\Phi_\pm(\zeta,k) = \lim_{r\uparrow 1} \Phi_\pm(r\zeta,k), \quad k \in \mathbb{Z}. \tag{2.153}$$

Lemma 2.21. *Let $z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\})$, $k_0, k \in \mathbb{Z}$. Then the functions $\Phi_\pm(\cdot,k)$ satisfy*

$$\Phi_\pm(z,k) = \begin{cases} z\frac{v_\pm(z,k,k_0)}{u_\pm(z,k,k_0)}, & k \text{ odd}, \\ \frac{u_\pm(z,k,k_0)}{v_\pm(z,k,k_0)}, & k \text{ even}, \end{cases} \tag{2.154}$$

where $u_\pm(\cdot,k,k_0)$ and $v_\pm(\cdot,k,k_0)$ are the polynomials defined in (2.136).

Proof. Using Corollary 2.16 it suffices to assume $k = k_0$. Then the statement follows immediately from (2.57) and (2.150). $\square$

Lemma 2.22. *Let $k \in \mathbb{Z}$. Then the functions $\Phi_+(\cdot,k)|_{\mathbb{D}}$ (resp., $\Phi_-(\cdot,k)|_{\mathbb{D}}$) are Schur (resp., anti-Schur) functions. Moreover, $\Phi_\pm$ satisfy the following Riccati-type equation*:

$$\alpha_k\Phi_\pm(z,k-1)\Phi_\pm(z,k) - \Phi_\pm(z,k-1) + z\Phi_\pm(z,k) = \overline{\alpha_k}z, \quad z \in \mathbb{C}\backslash\partial\mathbb{D},\ k \in \mathbb{Z}. \tag{2.155}$$

Proof. It follows from Lemma 2.20 and (2.150) that the functions $\Phi_+(\cdot,k)|_{\mathbb{D}}$ (resp., $\Phi_-(\cdot,k)|_{\mathbb{D}}$) are Schur (resp., anti-Schur) functions.

Let k be odd. Then applying Lemma 2.21 and the recursion relation (2.17) one obtains

$$\begin{aligned} \Phi_\pm(z,k) &= \frac{zv_\pm(z,k,k_0)}{u_\pm(z,k,k_0)} = \frac{u_\pm(z,k-1,k_0) + z\overline{\alpha_k}v_\pm(z,k-1,k_0)}{\alpha_k u_\pm(z,k-1,k_0) + zv_\pm(z,k-1,k_0)} \\ &= \frac{\Phi_\pm(z,k-1) + z\overline{\alpha_k}}{\alpha_k\Phi_\pm(z,k-1) + z}. \end{aligned} \tag{2.156}$$

For k even, one similarly obtains

$$\Phi_\pm(z,k) = \frac{u_\pm(z,k,k_0)}{v_\pm(z,k,k_0)} = \frac{\overline{\alpha_k} u_\pm(z,k-1,k_0) + v_\pm(z,k-1,k_0)}{u_\pm(z,k-1,k_0) + \alpha_k v_\pm(z,k-1,k_0)}$$
$$= \frac{z\overline{\alpha_k} + \Phi_\pm(z,k-1)}{z + \alpha_k \Phi_\pm(z,k-1)}. \qquad \square \tag{2.157}$$

Remark 2.23. (i) In the special case $\alpha = \{\alpha_k\}_{k\in\mathbb{Z}} = 0$, one obtains

$$M_\pm(z,k) = \pm 1, \quad \Phi_+(z,k) = 0, \quad 1/\Phi_-(z,k) = 0, \quad z \in \mathbb{C}, \ k \in \mathbb{Z}. \tag{2.158}$$

Thus, strictly speaking, one should always consider $1/\Phi_-$ rather than Φ_- and hence refer to the Riccati-type equation of $1/\Phi_-$,

$$\overline{\alpha_k} z \frac{1}{\Phi_-(z,k-1)} \frac{1}{\Phi_-(z,k)} + \frac{1}{\Phi_-(z,k)} - z\frac{1}{\Phi_-(z,k-1)} = \alpha_k, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \ k \in \mathbb{Z}, \tag{2.159}$$

rather than that of Φ_-, etc. For simplicity of notation, we will avoid this distinction between Φ_- and $1/\Phi_-$ and usually just invoke Φ_- whenever confusions are unlikely.

(ii) We note that $M_\pm(z,k)$ and $\Phi_\pm(z,k)$, $z \in \partial\mathbb{D}$, $k \in \mathbb{Z}$, have nontangential limits to $\partial\mathbb{D}$ μ_0-a.e. In particular, the Riccati-type equations (2.145), (2.155), and (2.159) extend to $\partial\mathbb{D}$ μ_0-a.e.

The Riccati-type equation for the Caratheodory function Φ_+ implies the following absolutely convergent expansion:

$$\Phi_+(z,k) = \sum_{j=1}^{\infty} \phi_{+,j}(k) z^j, \quad z \in \mathbb{D}, \ k \in \mathbb{Z}, \tag{2.160}$$

$$\begin{aligned} \phi_{+,1}(k) &= -\overline{\alpha_{k+1}}, \\ \phi_{+,2}(k) &= -\rho_{k+1}^2 \overline{\alpha_{k+2}}, \\ \phi_{+,j}(k) &= \alpha_{k+1} \sum_{\ell=1}^{j} \phi_{+,j-\ell}(k+1)\phi_{+,\ell}(k) + \phi_{+,j-1}(k+1), \ j \geqslant 3. \end{aligned} \tag{2.161}$$

The corresponding Riccati-type equation for the Caratheodory function $1/\Phi_-(z,k)$ implies the absolutely convergent expansion

$$1/\Phi_-(z,k) = \sum_{j=0}^{\infty} [1/\phi_{-,j}(k)] z^j, \quad z \in \mathbb{D}, \ k \in \mathbb{Z}, \tag{2.162}$$

$$\begin{aligned} 1/\phi_{-,0}(k) &= \alpha_k, \\ 1/\phi_{-,1}(k) &= \rho_k^2 \alpha_{k-1}, \\ 1/\phi_{-,j}(k) &= -\overline{\alpha_k} \sum_{\ell=0}^{j-1} [1/\phi_{-,j-1-\ell}(k-1)][1/\phi_{-,\ell}(k)] + [1/\phi_{-,j-1}(k-1)], \ j \geqslant 2. \end{aligned} \tag{2.163}$$

Next, we introduce the following notation for the half-open arc on the unit circle,

$$\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2}]\big) = \big\{e^{i\theta} \in \partial\mathbb{D} \mid \theta_1 < \theta \leqslant \theta_2\big\}, \quad \theta_1 \in [0, 2\pi), \ \theta_1 < \theta_2 \leqslant \theta_1 + 2\pi. \tag{2.164}$$

In the same manner we also introduce open and closed arcs on $\partial\mathbb{D}$, $\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big)\big)$ and $\mathrm{Arc}\big(\big[e^{i\theta_1}, e^{i\theta_2}\big]\big)$, respectively. Moreover, we identify the unit circle $\partial\mathbb{D}$ with the arcs of the form $\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_1+2\pi}\big]\big)$, $\theta_1 \in [0, 2\pi)$.

The following result is the unitary operator analog of a version of Stone's formula relating resolvents of self-adjoint operators with spectral projections in the weak sense (cf., e.g., [9, p. 1203]).

Lemma 2.24. *Let U be a unitary operator in a complex separable Hilbert space $\mathcal{H}$ (with scalar product denoted by $(\cdot,\cdot)_{\mathcal{H}}$, linear in the second factor), $f, g \in \mathcal{H}$, and denote by $\{E_U(\zeta)\}_{\zeta\in\partial\mathbb{D}}$ the family of self-adjoint right-continuous spectral projections associated with U, that is, $(f, Ug)_{\mathcal{H}} = \int_{\partial\mathbb{D}} d(f, E_U(\zeta)g)_{\mathcal{H}}\,\zeta$. Moreover, let $\theta_1 \in [0, 2\pi)$, $\theta_1 < \theta_2 \leqslant \theta_1 + 2\pi$, $F \in C(\partial\mathbb{D})$, and denote by $C(U,z)$ the operator*

$$C(U,z) = (U + zI_{\mathcal{H}})(U - zI_{\mathcal{H}})^{-1} = I_{\mathcal{H}} + 2z(U - zI_{\mathcal{H}})^{-1}, \quad z \in \mathbb{C}\backslash\sigma(U) \tag{2.165}$$

with $I_{\mathcal{H}}$ the identity operator in $\mathcal{H}$. Then,

$$\begin{aligned}&\big(f, F(U)E_U\big(\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big]\big)\big)g\big)_{\mathcal{H}}\\ &\quad= \lim_{\delta\downarrow 0}\lim_{r\uparrow 1}\int_{\theta_1+\delta}^{\theta_2+\delta}\frac{d\theta}{4\pi}\,F\big(e^{i\theta}\big)\big[\big(f, C\big(U, re^{i\theta}\big)g\big)_{\mathcal{H}} - \big(f, C\big(U, r^{-1}e^{i\theta}\big)g\big)_{\mathcal{H}}\big].\end{aligned} \tag{2.166}$$

Similar formulas hold for $\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big)\big)$ *and* $\mathrm{Arc}\big(\big[e^{i\theta_1}, e^{i\theta_2}\big]\big)$.

Proof. First one notices that

$$C\big(U, re^{i\theta}\big)^* = -C\big(U, r^{-1}e^{i\theta}\big), \quad r \in (0,\infty)\backslash\{1\},\ \theta \in [0, 2\pi]. \tag{2.167}$$

Next, introducing the characteristic function χ_A of a set $A \subseteq \partial\mathbb{D}$ and assuming $F \geqslant 0$, one obtains that

$$\begin{aligned}&\big(F(U)^{1/2}E_U\big(\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big]\big)\big)f, C(U,z)F(U)^{1/2}E_U\big(\mathrm{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big]\big)\big)f\big)_{\mathcal{H}}\\ &\quad= \int_{\partial\mathbb{D}} d\big(f, E_U\big(e^{i\theta}\big)f\big)_{\mathcal{H}}\,F\big(e^{i\theta}\big)\chi_{(e^{i\theta_1},e^{i\theta_2}]}\big(e^{i\theta}\big)\frac{e^{i\theta}+z}{e^{i\theta}-z}\\ &\quad= \int_{\partial\mathbb{D}} d\Big(F(U)^{1/2}\chi_{(e^{i\theta_1},e^{i\theta_2}]}(U)f, E_U\big(e^{i\theta}\big)F(U)^{1/2}\chi_{(e^{i\theta_1},e^{i\theta_2}]}(U)f\Big)_{\mathcal{H}}\frac{e^{i\theta}+z}{e^{i\theta}-z},\\ &\qquad z \in \partial\mathbb{D}\end{aligned} \tag{2.168}$$

is a Caratheodory function and hence (2.166) for $g = f$ follows from (A.5). If F is not nonnegative, one decomposes F as $F = (F_1 - F_2) + i(F_3 - F_4)$ with $F_j \geqslant 0$ and applies (2.168) to each F_j, $j \in \{1,2,3,4\}$. The general case $g \neq f$ then follows from the special case $g = f$ by polarization. □

Next, in addition to the definition of $\widetilde{p}_\pm$ and $\widetilde{q}_\pm$ in (2.59)–(2.62) we introduce $\widetilde{u}_+$ by

$$\begin{pmatrix}\widetilde{u}_+(z,\cdot,k_0)\\ v_+(z,\cdot,k_0)\end{pmatrix} = \begin{pmatrix}\widetilde{q}_+(z,\cdot,k_0)\\ s_+(z,\cdot,k_0)\end{pmatrix} + m_+(z,k_0)\begin{pmatrix}\widetilde{p}_+(z,\cdot,k_0)\\ r_+(z,\cdot,k_0)\end{pmatrix} \in \ell^2([k_0,\infty)\cap\mathbb{Z})^2,$$
$$z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}) \tag{2.169}$$

and the functions $\widetilde{t}_-$ and w_- by

$$\begin{pmatrix}\widetilde{t}_-(z,\cdot,k_0)\\ w_-(z,\cdot,k_0)\end{pmatrix} = \begin{pmatrix}\widetilde{q}_-(z,\cdot,k_0)\\ s_-(z,\cdot,k_0)\end{pmatrix} + m_-(z,k_0)\begin{pmatrix}\widetilde{p}_-(z,\cdot,k_0)\\ r_-(z,\cdot,k_0)\end{pmatrix} \in \ell^2((-\infty,k_0]\cap\mathbb{Z})^2,$$
$$z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}). \tag{2.170}$$

One then computes for the resolvent of $U_{\pm,k_0}$ in terms of its matrix representation in the standard basis of $\ell^2([k_0,\pm\infty)\cap\mathbb{Z})$,

$$(U_{+,k_0} - zI)^{-1}(k,k') = \frac{1}{2z}\begin{cases}\widetilde{p}_+(z,k,k_0)v_+(z,k',k_0), & k<k' \text{ and } k=k' \text{ odd},\\ r_+(z,k',k_0)\widetilde{u}_+(z,k,k_0), & k'<k \text{ and } k=k' \text{ even},\end{cases}$$
$$z\in\mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}),\ k_0\in\mathbb{Z},\ k,k'\in[k_0,\infty)\cap\mathbb{Z}, \tag{2.171}$$

$$(U_{-,k_0} - zI)^{-1}(k,k') = \frac{1}{2z}\begin{cases}\widetilde{t}_-(z,k,k_0)r_-(z,k',k_0), & k<k' \text{ and } k=k' \text{ odd},\\ w_-(z,k',k_0)\widetilde{p}_-(z,k,k_0), & k'<k \text{ and } k=k' \text{ even},\end{cases}$$
$$z\in\mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}),\ k_0\in\mathbb{Z},\ k,k'\in(-\infty,k_0]\cap\mathbb{Z}. \tag{2.172}$$

The proof of these formulas repeats the proof of the analogous result, Lemma 3.1, for the full-lattice CMV operator U and hence we omit it here.

We finish this section with an explicit connection between the family of spectral projections of $U_{\pm,k_0}$ and the spectral function $\mu_\pm(\cdot,k_0)$, supplementing relation (2.70).

Lemma 2.25. *Let $f,g\in\ell_0^\infty([k_0,\pm\infty)\cap\mathbb{Z})$, $F\in C(\partial\mathbb{D})$, and $\theta_1\in[0,2\pi)$, $\theta_1<\theta_2\leqslant\theta_1+2\pi$. Then,*

$$\begin{aligned}&\big(f, F(U_{\pm,k_0})E_{U_{\pm,k_0}}\big(\mathrm{Arc}\big(\big(e^{i\theta_1},e^{i\theta_2}\big]\big)\big)g\big)_{\ell^2([k_0,\pm\infty)\cap\mathbb{Z})}\\ &\quad = \big(\widehat{f}_\pm(\cdot,k_0), M_F M_{\chi_{\mathrm{Arc}((e^{i\theta_1},e^{i\theta_2}])}}\widehat{g}_\pm(\cdot,k_0)\big)_{L^2(\partial\mathbb{D};d\mu_\pm(\cdot,k_0))},\end{aligned} \tag{2.173}$$

where we introduced the notation

$$\widehat{h}_\pm(\zeta,k_0) = \sum_{k=k_0}^{\pm\infty} r_\pm(\zeta,k,k_0)h(k), \quad \zeta\in\partial\mathbb{D},\ h\in\ell_0^\infty([k_0,\pm\infty)\cap\mathbb{Z}) \tag{2.174}$$

and M_G denotes the maximally defined operator of multiplication by the $d\mu_\pm(\cdot,k_0)$-measurable function G in the Hilbert space $L^2(\partial\mathbb{D};d\mu_\pm(\cdot,k_0))$,

$$\begin{aligned}&(M_G\widehat{h})(\zeta) = G(\zeta)\widehat{h}(\zeta) \text{ for a.e. } \zeta\in\partial\mathbb{D},\\ &\widehat{h}\in\mathrm{dom}(M_G) = \{\widehat{k}\in L^2(\partial\mathbb{D};d\mu_\pm(\cdot,k_0))\,|\,G\widehat{k}\in L^2(\partial\mathbb{D};d\mu_\pm(\cdot,k_0))\}.\end{aligned} \tag{2.175}$$

Proof. It suffices to consider U_{+,k_0} only. Inserting (2.171) into (2.166) and observing (2.169) leads to

$$\begin{aligned}
&\big(f, F(U_{+,k_0})E_{U_{+,k_0}}\big(\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2}]\big)\big)g\big)_{\ell^2([k_0,\infty)\cap\mathbb{Z})}\\
&= \lim_{\delta\downarrow 0}\lim_{r\uparrow 1}\int_{\theta_1+\delta}^{\theta_2+\delta}\frac{d\theta}{4\pi}\,F\big(e^{i\theta}\big)\Bigg[\sum_{k=k_0}^{\infty}\sum_{k'=k_0}^{\infty}\overline{f(k)}g(k')[C\big(U_{+,k_0}, re^{i\theta}\big)(k,k')\\
&\quad -C\big(U_{+,k_0}, r^{-1}e^{i\theta}\big)(k,k')\Bigg]\\
&= \sum_{k=k_0}^{\infty}\overline{f(k)}\Bigg\{\sum_{\substack{k_0\leqslant k'<k\\ k'=k\text{ even}}} g(k')\lim_{\delta\downarrow 0}\lim_{r\uparrow 1}\frac{1}{4\pi}\int_{\theta_1+\delta}^{\theta_2+\delta}d\theta\,F\big(e^{i\theta}\big)\widetilde{p}_+\big(e^{i\theta},k,k_0\big)\\
&\quad\times r_+\big(e^{i\theta},k',k_0\big)\big[m_+\big(re^{i\theta},k_0\big)-m_+\big(r^{-1}e^{i\theta},k_0\big)\big]\\
&\quad\times\sum_{\substack{k_0\leqslant k<k'\\ k'=k\text{ odd}}} g(k')\lim_{\delta\downarrow 0}\lim_{r\uparrow 1}\frac{1}{4\pi}\int_{\theta_1+\delta}^{\theta_2+\delta}d\theta\,F\big(e^{i\theta}\big)\widetilde{p}_+\big(e^{i\theta},k,k_0\big)\\
&\quad\times r_+\big(e^{i\theta},k',k_0\big)\big[m_+\big(re^{i\theta},k_0\big)-m_+\big(r^{-1}e^{i\theta},k_0\big)\big]\Bigg\}.
\end{aligned}\tag{2.176}$$

Here we freely interchanged the θ-integral with the sums over k and k' (the latter are finite) and also replaced $\widetilde{p}_+\big(r^{\pm 1}e^{i\theta},k,k_0\big)$ and $r_+\big(r^{\pm 1}e^{i\theta},k,k_0\big)$ by $\widetilde{p}_+\big(e^{i\theta},k,k_0\big)$ and $r_+\big(e^{i\theta},k,k_0\big)$. The latter is permissible since by (A.16),

$$\big|(1-r^{\pm 1})\mathrm{Re}\big(m_+\big(r^{\pm 1}e^{i\theta}\big)\big)\big| \underset{r\to 1}{=} O(1),\quad \big|(1-r^{\pm 1})\mathrm{Im}\big(m_+\big(r^{\pm 1}e^{i\theta}\big)\big)\big| \underset{r\to 1}{=} o(1).\tag{2.177}$$

Finally, since $\widetilde{p}_+(\zeta,k,k_0) = \overline{r_+(\zeta,k,k_0)}$, $\zeta\in\partial\mathbb{D}$ by (2.63) and $m_+(re^{i\theta},k_0) = -m_+(\frac{1}{r}e^{i\theta},k_0)$ by (A.19), one infers

$$\begin{aligned}
&\big(f, F(U_{+,k_0})E_{U_{+,k_0}}\big(\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2}]\big)\big)g\big)_{\ell^2([k_0,\infty)\cap\mathbb{Z})}\\
&\quad= \sum_{k=k_0}^{\infty}\sum_{k'=k_0}^{\infty}\overline{f(k)}g(k')\lim_{\delta\downarrow 0}\lim_{r\uparrow 1}\int_{\theta_1+\delta}^{\theta_2+\delta}\frac{d\theta}{2\pi}\,F\big(e^{i\theta}\big)\widetilde{p}_+\big(e^{i\theta},k,k_0\big)r_+\big(e^{i\theta},k',k_0\big)\\
[-1pt]&\qquad\times\mathrm{Re}\big(m_+\big(re^{i\theta},k_0\big)\big)\\
&\quad= \sum_{k=k_0}^{\infty}\sum_{k'=k_0}^{\infty}\overline{f(k)}g(k')\int_{(\theta_1,\theta_2]}d\mu_+\big(e^{i\theta},k_0\big)\,F\big(e^{i\theta}\big)\overline{r_+\big(e^{i\theta},k,k_0\big)}r_+\big(e^{i\theta},k',k_0\big)\\
&\quad= \int_{(\theta_1,\theta_2]}d\mu_+\big(e^{i\theta},k_0\big)\,F\big(e^{i\theta}\big)\overline{\widehat{f}_+\big(e^{i\theta},k_0\big)}\widehat{g}_+\big(e^{i\theta},k_0\big)\\
&\quad= \big(\widehat{f}_+(\cdot,k_0), M_F M_{\chi_{\mathrm{Arc}((e^{i\theta_1},e^{i\theta_2}])}}\widehat{g}_+(\cdot,k_0)\big)_{L^2(\partial\mathbb{D};d\mu_+(\cdot,k_0))},
\end{aligned}\tag{2.178}$$

interchanging the (finite) sums over k and k' and the $d\mu(\cdot,k_0)$-integral once more. □

Finally, this section would not be complete if we would not briefly mention the analogs of Weyl disks for finite interval problems and their behavior in the limit where the finite interval tends to a half-lattice. Before starting the analysis, we note the following geometric fact: Let $p, q, r, s \in \mathbb{C}$, $|p| \neq |r|$. Then, the set of points $m(\theta) \in \mathbb{C}$ given by

$$m(\theta) = -\frac{q + se^{i\theta}}{p + re^{i\theta}}, \quad \theta \in [0, 2\pi), \tag{2.179}$$

describes a circle in $\mathbb{C}$ with radius $R > 0$ and center $C \in \mathbb{C}$ given by

$$R = \frac{|qr - ps|}{\big||p|^2 - |r|^2\big|}, \quad C = -\frac{s}{r} - \frac{\overline{p}}{r}\frac{qr - ps}{|p|^2 - |r|^2}. \tag{2.180}$$

To introduce the analog of $\mathbb{U}_{+,k_0}^{(s)}$ and $\big(\mathbb{U}_{+,k_0}^{(s)}\big)^\top$ on a finite interval $[k_0, k_1] \cap \mathbb{Z}$, we choose $\alpha_{k_0} = e^{is_0}$, $\alpha_{k_1+1} = e^{is_1}$, $s_0, s_1 \in [0, 2\pi)$. Then the operator $\mathbb{U}_{+,k_0}^{(s_0)}$ splits into a direct sum of two operators $\mathbb{U}_{[k_0,k_1]}^{(s_0,s_1)}$ and $\mathbb{U}_{+,k_1+1}^{(s_1)}$

$$\mathbb{U}_{+,k_0}^{(s_0)} = \mathbb{U}_{[k_0,k_1]}^{(s_0,s_1)} \oplus \mathbb{U}_{+,k_1+1}^{(s_1)} \tag{2.181}$$

acting on $\ell^2([k_0, k_1] \cap \mathbb{Z})$ and $\ell^2([k_1 + 1, \infty) \cap \mathbb{Z})$, respectively. Then, repeating the proof of Lemma 2.3 one obtains the following result for the CMV operator $\mathbb{U}_{[k_0,k_1]}^{(s_0,s_1)}$:

$$\mathbb{U}_{[k_0,k_1]}^{(s_0,s_1)} \begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix} = z \begin{pmatrix} u(z,\cdot) \\ v(z,\cdot) \end{pmatrix}, \quad z \in \mathbb{C}\backslash\{0\} \tag{2.182}$$

is satisfied by $\begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix}_{k\in[k_0,k_1]\cap\mathbb{Z}}$ such that

$$\begin{pmatrix} u(z,k) \\ v(z,k) \end{pmatrix} = T(z,k) \begin{pmatrix} u(z,k-1) \\ v(z,k-1) \end{pmatrix}, \quad k \in [k_0 + 1, k_1] \cap \mathbb{Z}, \tag{2.183}$$

$$u(z,k_0) = \begin{cases} ze^{is_0} v(z,k_0), & k_0 \text{ odd}, \\ e^{-is_0} v(z,k_0), & k_0 \text{ even}, \end{cases} \tag{2.184}$$

$$u(z,k_1) = \begin{cases} -e^{is_1} v(z,k_1), & k_1 \text{ odd}, \\ -ze^{-is_1} v(z,k_1), & k_1 \text{ even}. \end{cases} \tag{2.185}$$

To simplify matters we now put $s_0 = 0$ in the following. Moreover, we first treat the case k_0 even and k_1 odd. Then $\begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix}$ satisfies (2.183) and (2.184) and hence there exists a coefficient $m_{+,s_1}(z, k_1, k_0)$ such that

$$\begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix} + m_{+,s_1}(z,k_0,k_1) \begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix} \tag{2.186}$$

satisfies (2.185). One computes

$$m_{+,s_1}(z,k_1,k_0) = -\frac{q_+(z,k_1,k_0) + s_+(z,k_1,k_0)e^{is_1}}{p_+(z,k_1,k_0) + r_+(z,k_1,k_0)e^{is_1}}. \tag{2.187}$$

By (2.179), this describes a (Weyl–Titchmarsh) circle as s_1 varies in $[0, 2\pi)$ of radius

$$\begin{aligned} R(z,k_1) &= \frac{|q_+(z,k_1,k_0)r_+(z,k_1,k_0) - p_+(z,k_1,k_0)s_+(z,k_1,k_0))|}{\big||p_+(z,k_1,k_0)|^2 - |r_+(z,k_1,k_0)|^2\big|} \\ &= \frac{2}{\big||p_+(z,k_1,k_0)|^2 - |r_+(z,k_1,k_0)|^2\big|} \end{aligned} \tag{2.188}$$

since

$$W\left(\begin{pmatrix} p_+(z,k_1,k_0) \\ r_+(z,k_1,k_0) \end{pmatrix} \begin{pmatrix} q_+(z,k_1,k_0) \\ s_+(z,k_1,k_0) \end{pmatrix} \right) = 2 \tag{2.189}$$

if k_0 is even and k_1 is odd (cf. also (3.3)).

Thus far our computations are subject to $|p_+(z,k_1,k_0)| \neq |r_+(z,k_1.k_0)|$. To clarify this point we now state the following result.

Lemma 2.26. *Let $z \in \mathbb{C}\backslash(\partial\mathbb{D} \cup \{0\})$ and $k_0, k_1 \in \mathbb{Z}$, $k_1 > k_0$. Then,*

$$\left(1-|z|^{-2}\right)\sum_{k=k_0}^{k_1}|p_+(z,k,k_0)|^2 = \begin{cases} |p_+(z,k_1,k_0)|^2 - |r_+(z,k_1.k_0)|^2, & k_1 \text{ odd}, \\ |r_+(z,k_1.k_0)|^2 - |z|^{-2}|p_+(z,k_1,k_0)|^2, & k_1 \text{ even}. \end{cases} \tag{2.190}$$

Proof. It suffices to prove the case k_1 odd. The computation

$$\begin{aligned}
\overline{z}\sum_{k=k_0}^{k_1}|p_+(z,k,k_0)|^2 &= \sum_{k=k_0}^{k_1}\overline{(U_{+,k_0}p_+(z,\cdot,k_0))(k)}\,p_+(z,k,k_0) \\
&= \sum_{k=k_0}^{k_1-1}\overline{(V_{+,k_0}W_{+,k_0}p_+(z,\cdot,k_0))(k)}\,p_+(z,k,k_0) + \overline{z}|p_+(z,k_1,k_0)|^2 \\
&= \sum_{k=k_0}^{k_1-1}\overline{(W_{+,k_0}p_+(z,\cdot,k_0))(k)}(V_{+,k_0}^*p_+(z,\cdot,k_0))(k) + \overline{z}|p_+(z,k_1,k_0)|^2 \\
&= \sum_{k=k_0}^{k_1}\overline{p_+(z,k,k_0)}(W_{+,k_0}^*V_{+,k_0}^*p_+(z,\cdot,k_0))(k) \\
&\quad -\overline{(W_{+,k_0}p_+(z,\cdot,k_0))(k_1)}(V_{+,k_0}^*p_+(z,\cdot,k_0))(k_1) + \overline{z}|p_+(z,k_1,k_0)|^2 \\
&= \sum_{k=k_0}^{k_1}\overline{p_+(z,k,k_0)}(U_{+,k_0}^*p_+(z,\cdot,k_0))(k) - \overline{z}|r_+(z,k_1,k_0))|^2 + \overline{z}|p_+(z,k_1,k_0)|^2 \\
&= z^{-1}\sum_{k=k_0}^{k_1}|p_+(z,k,k_0)|^2 - \overline{z}|r_+(z,k_1,k_0))|^2 + \overline{z}|p_+(z,k_1,k_0)|^2
\end{aligned} \tag{2.191}$$

proves (2.190) for k_1 odd. □

A systematic investigation of all even/odd possibilities for k_0 and k_1 then yields the following result.

Theorem 2.27. *Let $z \in \mathbb{C}\backslash(\partial\mathbb{D} \cup \{0\})$ and $k_0, k_1 \in \mathbb{Z}$, $k_1 > k_0$. Then,*

$$m_{+,s_1}(z,k_1,k_0) = \begin{cases} -\frac{q_+(z,k_1,k_0)+s_+(z,k_1,k_0)e^{is_1}}{p_+(z,k_1,k_0)+r_+(z,k_1,k_0)e^{is_1}}, & k_1 \text{ odd}, \\ -\frac{z^{-1}q_+(z,k_1,k_0)+s_+(z,k_1,k_0)e^{-is_1}}{z^{-1}p_+(z,k_1,k_0)+r_+(z,k_1,k_0)e^{-is_1}}, & k_1 \text{ even} \end{cases} \tag{2.192}$$

lies on a circle of radius

$$R(z,k_1,k_0) = \left[\left|1-|z|^{-2}\right| \sum_{k=k_0}^{k_1} |p_+(z,k_1,k_0)|^2\right]^{-1} \begin{cases} 2|z|, & k_0 \text{ odd},\ k_1 \text{ odd}, \\ 2, & k_0 \text{ even},\ k_1 \text{ odd}, \\ 2, & k_0 \text{ odd},\ k_1 \text{ even}, \\ 2|z|^{-1}, & k_0 \text{ even},\ k_1 \text{ even} \end{cases} \tag{2.193}$$

with center

$$C(z,k_1,k_0) = \begin{cases} -\frac{s_+(z,k_1,k_0)}{r_+(z,k_1,k_0)} - \overline{\frac{p_+(z,k_1,k_0)}{r_+(z,k_1,k_0)}} \\ \quad \times \frac{2z}{|p_+(z,k_1,k_0)|^2-|r_+(z,k_1,k_0)|^2}, & k_0 \text{ odd},\ k_1 \text{ odd}, \\ -\frac{s_+(z,k_1,k_0)}{r_+(z,k_1,k_0)} - \overline{\frac{p_+(z,k_1,k_0)}{r_+(z,k_1,k_0)}} \\ \quad \times \frac{2}{|p_+(z,k_1,k_0)|^2-|r_+(z,k_1,k_0)|^2}, & k_0 \text{ even},\ k_1 \text{ odd}, \\ -\frac{s_+(z,k_1,k_0)}{r_+(z,k_1,k_0)} - \overline{\frac{z^{-1}p_+(z,k_1,k_0)}{r_+(z,k_1,k_0)}} \\ \quad \times \frac{-2}{|z|^{-2}|p_+(z,k_1,k_0)|^2-|r_+(z,k_1,k_0)|^2}, & k_0 \text{ odd},\ k_1 \text{ even}, \\ -\frac{s_+(z,k_1,k_0)}{r_+(z,k_1,k_0)} - \overline{\frac{z^{-1}p_+(z,k_1,k_0)}{r_+(z,k_1,k_0)}} \\ \quad \times \frac{-2z^{-1}}{|z|^{-2}|p_+(z,k_1,k_0)|^2-|r_+(z,k_1,k_0)|^2}, & k_0 \text{ even},\ k_1 \text{ even}. \end{cases} \tag{2.194}$$

In particular, the limit point case holds at $+\infty$ *since*

$$\lim_{k_1\uparrow\infty} R(z,k_1,k_0) = 0. \tag{2.195}$$

Proof. The case k_0 even, k_1 odd has been discussed explicitly in (2.186)–(2.190). The remaining cases follow similarly using Lemma 2.26 for k_1 even and the Wronski relations (3.3). Relation (2.195) follows since $p_+(z,\cdot,k_0) \notin \ell^2([k_0,\infty)\cap\mathbb{Z})$, $z\in\mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\})$. The latter follows from $(U_{+,k_0}p(z,\cdot,k_0))(k) = zp_+(z,k,k_0)$, $z\in\mathbb{C}\backslash\{0\}$, in the weak sense (cf. Remark 2.6) and the fact that U_{+,k_0} is unitary. □

3. Weyl–Titchmarsh theory for CMV operators on $\mathbb{Z}$

In this section, we describe the Weyl–Titchmarsh theory for the CMV operator U on $\mathbb{Z}$. We note that in a context different from orthogonal polynomials on the unit circle, Bourget et al. [7] introduced a set of doubly infinite family of matrices with three sets of parameters which for special choices of the parameters reduces to two-sided CMV matrices on $\mathbb{Z}$.

We denote by

$$W\left(\begin{pmatrix} u_1(z,k,k_0) \\ v_1(z,k,k_0)\end{pmatrix}, \begin{pmatrix} u_2(z,k,k_0) \\ v_2(z,k,k_0)\end{pmatrix}\right) = \det\left(\begin{pmatrix} u_1(z,k,k_0) & u_2(z,k,k_0) \\ v_1(z,k,k_0) & v_2(z,k,k_0)\end{pmatrix}\right), \quad k\in\mathbb{Z}, \tag{3.1}$$

the Wronskian of two solutions $\begin{pmatrix} u_1(z,\cdot,k_0) \\ v_1(z,\cdot,k_0)\end{pmatrix}$ and $\begin{pmatrix} u_2(z,\cdot,k_0) \\ v_2(z,\cdot,k_0)\end{pmatrix}$ of (2.17) for $z\in\mathbb{C}\backslash\{0\}$. Then, since

$$\det(T(z,k)) = -1, \quad k\in\mathbb{Z}, \tag{3.2}$$

it follows from Definition 2.4 that

$$W\left(\begin{pmatrix} p_+(z,k,k_0) \\ r_+(z,k,k_0) \end{pmatrix}, \begin{pmatrix} q_+(z,k,k_0) \\ s_+(z,k,k_0) \end{pmatrix}\right) = (-1)^k \begin{cases} 2z, & k_0 \text{ odd}, \\ 2, & k_0 \text{ even}, \end{cases} \tag{3.3}$$

$$W\left(\begin{pmatrix} p_-(z,k,k_0) \\ r_-(z,k,k_0) \end{pmatrix}, \begin{pmatrix} q_-(z,k,k_0) \\ s_-(z,k,k_0) \end{pmatrix}\right) = (-1)^{k+1} \begin{cases} 2, & k_0 \text{ odd}, \\ 2z, & k_0 \text{ even}, \end{cases} \quad z \in \mathbb{C}\backslash\{0\},\ k \in \mathbb{Z}. \tag{3.4}$$

Next, in order to compute the resolvent of U, we introduce in addition to $\widetilde{p}_\pm$ and $\widetilde{q}_\pm$ in (2.59)–(2.62) the functions $\widetilde{u}_\pm$ by

$$\begin{pmatrix} \widetilde{u}_\pm(z,\cdot,k_0) \\ v_\pm(z,\cdot,k_0) \end{pmatrix} = \begin{pmatrix} \widetilde{q}_+(z,\cdot,k_0) \\ s_+(z,\cdot,k_0) \end{pmatrix} + M_\pm(z,k_0) \begin{pmatrix} \widetilde{p}_+(z,\cdot,k_0) \\ r_+(z,\cdot,k_0) \end{pmatrix} \in \ell^2([k_0,\pm\infty)\cap\mathbb{Z})^2, \quad z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\}). \tag{3.5}$$

Lemma 3.1. *Let $z \in \mathbb{C}\backslash(\partial\mathbb{D}\cup\{0\})$ and fix $k_0, k_1 \in \mathbb{Z}$. Then the resolvent $(U - zI)^{-1}$ of the unitary CMV operator U on $\ell^2(\mathbb{Z})$ is given in terms of its matrix representation in the standard basis of $\ell^2(\mathbb{Z})$ by*

$$\begin{aligned} &(U - zI)^{-1}(k,k') \\ &= \frac{(-1)^{k_1+1}}{zW\left(\begin{pmatrix} u_+(z,k_1,k_0) \\ v_+(z,k_1,k_0) \end{pmatrix}, \begin{pmatrix} u_-(z,k_1,k_0) \\ v_-(z,k_1,k_0) \end{pmatrix}\right)} \\ &\quad \times \begin{cases} u_-(z,k,k_0)v_+(z,k',k_0), & k < k' \text{ and } k = k' \text{ odd}, \\ v_-(z,k',k_0)u_+(z,k,k_0), & k' < k \text{ and } k = k' \text{ even}, \end{cases} \quad k,k' \in \mathbb{Z}, \end{aligned} \tag{3.6}$$

$$\begin{aligned} &= \frac{-1}{2z[M_+(z,k_0) - M_-(z,k_0)]} \\ &\quad \times \begin{cases} \widetilde{u}_-(z,k,k_0)v_+(z,k',k_0), & k < k' \text{ and } k = k' \text{ odd}, \\ v_-(z,k',k_0)\widetilde{u}_+(z,k,k_0), & k' < k \text{ and } k = k' \text{ even}, \end{cases} \quad k,k' \in \mathbb{Z}, \end{aligned} \tag{3.7}$$

where

$$\begin{aligned} &W\left(\begin{pmatrix} u_+(z,k_1,k_0) \\ v_+(z,k_1,k_0) \end{pmatrix}, \begin{pmatrix} u_-(z,k_1,k_0) \\ v_-(z,k_1,k_0) \end{pmatrix}\right) = \det\left(\begin{pmatrix} u_+(z,k_1,k_0) & u_-(z,k_1,k_0) \\ v_+(z,k_1,k_0) & v_-(z,k_1,k_0) \end{pmatrix}\right) \\ &= (-1)^{k_1}[M_+(z,k_0) - M_-(z,k_0)] \begin{cases} 2z, & k_0 \text{ odd}, \\ 2, & k_0 \text{ even} \end{cases} \end{aligned} \tag{3.8}$$

and

$$W\left(\begin{pmatrix} \widetilde{u}_+(z,k_1,k_0) \\ v_+(z,k_1,k_0) \end{pmatrix}, \begin{pmatrix} \widetilde{u}_-(z,k_1,k_0) \\ v_-(z,k_1,k_0) \end{pmatrix}\right) = 2(-1)^{k_1}[M_+(z,k_0) - M_-(z,k_0)]. \tag{3.9}$$

Moreover, since $0 \in \mathbb{C}\backslash\sigma(U)$, (3.6) *and* (3.7) *analytically extend to* $z = 0$.

Proof. Denote

$$w(z,k,k',k_0) = \begin{cases} u_-(z,k,k_0)v_+(z,k',k_0), & k < k',\ k = k' \text{ odd}, \\ u_+(z,k,k_0)v_-(z,k',k_0), & k' < k,\ k = k' \text{ even}, \end{cases} \quad k,k',k_0 \in \mathbb{Z}. \tag{3.10}$$

We will prove that

$$(U - zI)w(z,\cdot,k',k_0) = (-1)^{k'+1} z \det\left(\begin{pmatrix} u_+(z,k',k_0) & u_-(z,k',k_0) \\ v_+(z,k',k_0) & v_-(z,k',k_0)\end{pmatrix}\right)\delta_{k'}, \quad k',k_0\in\mathbb{Z} \tag{3.11}$$

and hence, using (3.2), one obtains

$$(U - zI)w(z,\cdot,k',k_0) = (-1)^{k_1+1} z \det\left(\begin{pmatrix} u_+(z,k_1,k_0) & u_-(z,k_1,k_0) \\ v_+(z,k_1,k_0) & v_-(z,k_1,k_0)\end{pmatrix}\right)\delta_{k'}, \quad k',k_0,k_1\in\mathbb{Z}. \tag{3.12}$$

First, let $k_0 \in \mathbb{Z}$ and assume k' to be odd. Then,

$$\big((U-zI)w(z,\cdot,k',k_0)\big)(\ell)=\big((VW-zI)w(z,\cdot,k',k_0)\big)(\ell)=0, \quad \ell\in\mathbb{Z}\backslash\{k',k'+1\} \tag{3.13}$$

and

$$\begin{aligned}
\begin{pmatrix} ((U-zI)w(z,\cdot,k',k_0))(k') \\ ((U-zI)w(z,\cdot,k',k_0))(k'+1)\end{pmatrix} &= \begin{pmatrix} ((VW-zI)w(z,\cdot,k',k_0))(k') \\ ((VW-zI)w(z,\cdot,k',k_0))(k'+1)\end{pmatrix} \\
&= \theta_{k'+1} z \begin{pmatrix} (v_+(z,k',k_0)v_-(z,\cdot,k_0))(k') \\ (v_-(z,k',k_0)v_+(z,\cdot,k_0))(k'+1)\end{pmatrix} - z\begin{pmatrix} w(z,k',k',k_0) \\ w(z,k'+1,k',k_0)\end{pmatrix} \\
&= z v_-(z,k',k_0)\begin{pmatrix} u_+(z,k',k_0) \\ u_+(z,k'+1,k_0)\end{pmatrix} - z\begin{pmatrix} v_+(z,k',k_0)u_-(z,k',k_0) \\ v_-(z,k',k_0)u_+(z,k'+1,k_0)\end{pmatrix} \\
&= z\begin{pmatrix} \det\left(\begin{pmatrix} u_+(z,k',k_0) & u_-(z,k',k_0) \\ v_+(z,k',k_0) & v_-(z,k',k_0)\end{pmatrix}\right) \\ 0\end{pmatrix}.
\end{aligned} \tag{3.14}$$

Next, assume k' to be even. Then,

$$\big((U - zI)w(z,\cdot,k',k_0)\big)(\ell) = \big((VW - zI)w(z,\cdot,k',k_0)\big)(\ell) = 0, \quad \ell\in\mathbb{Z}\backslash\{k'-1,k'\} \tag{3.15}$$

and

$$\begin{aligned}
\begin{pmatrix} ((U-zI)w(z,\cdot,k',k_0))(k'-1) \\ ((U-zI)w(z,\cdot,k',k_0))(k')\end{pmatrix} &= \begin{pmatrix} ((VW-zI)w(z,\cdot,k',k_0))(k'-1) \\ ((VW-zI)w(z,\cdot,k',k_0))(k')\end{pmatrix} \\
&= \theta_{k'} z \begin{pmatrix} (v_+(z,k',k_0)v_-(z,\cdot,k_0))(k'-1) \\ (v_-(z,k',k_0)v_+(z,\cdot,k_0))(k')\end{pmatrix} - z\begin{pmatrix} w(z,k'-1,k',k_0) \\ w(z,k',k',k_0)\end{pmatrix} \\
&= z v_+(z,k',k_0)\begin{pmatrix} u_-(z,k'-1,k_0) \\ u_-(z,k',k_0)\end{pmatrix} - z\begin{pmatrix} v_+(z,k',k_0)u_-(z,k'-1,k_0) \\ v_-(z,k',k_0)u_+(z,k',k_0)\end{pmatrix} \\
&= z\begin{pmatrix} 0 \\ -\det\left(\begin{pmatrix} u_+(z,k',k_0) & u_-(z,k',k_0) \\ v_+(z,k',k_0) & v_-(z,k',k_0)\end{pmatrix}\right)\end{pmatrix}.
\end{aligned} \tag{3.16}$$

Thus, one obtains (3.11). □

Next, we denote by $d\Omega(\cdot,k)$, $k\in\mathbb{Z}$, the 2×2 matrix-valued measure,

$$\begin{aligned}
d\Omega(\zeta,k) &= d\begin{pmatrix} \Omega_{0,0}(\zeta,k) & \Omega_{0,1}(\zeta,k) \\ \Omega_{1,0}(\zeta,k) & \Omega_{1,1}(\zeta,k)\end{pmatrix} \\
&= d\begin{pmatrix} (\delta_{k-1},E_U(\zeta)\delta_{k-1})_{\ell^2(\mathbb{Z})} & (\delta_{k-1},E_U(\zeta)\delta_k)_{\ell^2(\mathbb{Z})} \\ (\delta_k,E_U(\zeta)\delta_{k-1})_{\ell^2(\mathbb{Z})} & (\delta_k,E_U(\zeta)\delta_k)_{\ell^2(\mathbb{Z})}\end{pmatrix}, \quad \zeta\in\partial\mathbb{D},
\end{aligned} \tag{3.17}$$

where $dE_U(\cdot)$ denotes the operator-valued spectral measure of the unitary CMV operator U on $\ell^2(\mathbb{Z})$,

$$U = \oint_{\partial\mathbb{D}} dE_U(\zeta)\,\zeta. \tag{3.18}$$

We note that by (3.17) $d\Omega_{0,0}(\cdot,k)$ and $d\Omega_{1,1}(\cdot,k)$ are nonnegative measures on $\partial\mathbb{D}$ and $d\Omega_{0,1}(\cdot,k)$ and $d\Omega_{1,0}(\cdot,k)$ are complex-valued measures on $\partial\mathbb{D}$.

We also introduce the 2×2 matrix-valued function $\mathcal{M}(\cdot,k)$, $k\in\mathbb{Z}$, by

$$\begin{aligned}\mathcal{M}(z,k) &= \begin{pmatrix} M_{0,0}(z,k) & M_{0,1}(z,k) \\ M_{1,0}(z,k) & M_{1,1}(z,k)\end{pmatrix} \\ &= \begin{pmatrix} (\delta_{k-1},(U+zI)(U-zI)^{-1}\delta_{k-1})_{\ell^2(\mathbb{Z})} & (\delta_{k-1},(U+zI)(U-zI)^{-1}\delta_{k})_{\ell^2(\mathbb{Z})} \\ (\delta_{k},(U+zI)(U-zI)^{-1}\delta_{k-1})_{\ell^2(\mathbb{Z})} & (\delta_{k},(U+zI)(U-zI)^{-1}\delta_{k})_{\ell^2(\mathbb{Z})}\end{pmatrix} \\ &= \oint_{\partial\mathbb{D}} d\Omega(\zeta,k)\,\frac{\zeta+z}{\zeta-z}, \quad z\in\mathbb{C}\backslash\partial\mathbb{D}. \end{aligned} \tag{3.19}$$

We note that,

$$M_{0,0}(\cdot,k+1) = M_{1,1}(\cdot,k), \quad k\in\mathbb{Z} \tag{3.20}$$

and

$$M_{1,1}(z,k) = (\delta_k,(U+zI)(U-zI)^{-1}\delta_k)_{\ell^2(\mathbb{Z})} \tag{3.21}$$

$$= \oint_{\partial\mathbb{D}} d\Omega_{1,1}(\zeta,k)\,\frac{\zeta+z}{\zeta-z}, \quad z\in\mathbb{C}\backslash\partial\mathbb{D},\ k\in\mathbb{Z}, \tag{3.22}$$

where

$$d\Omega_{1,1}(\zeta,k) = d(\delta_k, E_U(\zeta)\delta_k)_{\ell^2(\mathbb{Z})}, \quad \zeta\in\partial\mathbb{D}. \tag{3.23}$$

Thus, $M_{0,0}|_{\mathbb{D}}$ and $M_{1,1}|_{\mathbb{D}}$ are Caratheodory functions. Moreover, by (3.21) one infers that

$$M_{1,1}(0,k) = 1, \quad k\in\mathbb{Z}. \tag{3.24}$$

Lemma 3.2. *Let $z\in\mathbb{C}\backslash\partial\mathbb{D}$. Then the functions $M_{1,1}(\cdot,k)$ and $M_\pm(\cdot,k)$, $k\in\mathbb{Z}$, satisfy the following relations*:

$$M_{0,0}(z,k) = 1 + \frac{[\overline{a_k} - \overline{b_k}M_+(z,k)][a_k + b_kM_-(z,k)]}{\rho_k^2[M_+(z,k) - M_-(z,k)]}, \tag{3.25}$$

$$M_{1,1}(z,k) = \frac{1 - M_+(z,k)M_-(z,k)}{M_+(z,k) - M_-(z,k)}, \tag{3.26}$$

$$M_{0,1}(z,k) = \frac{-1}{\rho_k[M_+(z,k) - M_-(z,k)]}\begin{cases}[1 - M_+(z,k)][\overline{a_k} - \overline{b_k}M_-(z,k)], & k \text{ odd},\\ [1 + M_+(z,k)][a_k + b_kM_-(z,k)], & k \text{ even},\end{cases} \tag{3.27}$$

$$M_{1,0}(z,k) = \frac{-1}{\rho_k[M_+(z,k) - M_-(z,k)]}\begin{cases}[1 + M_+(z,k)][a_k + b_kM_-(z,k)], & k \text{ odd},\\ [1 - M_+(z,k)][\overline{a_k} - \overline{b_k}M_-(z,k)], & k \text{ even}.\end{cases} \tag{3.28}$$

Proof. Using (2.4), (2.5), (2.17), and (2.57) one finds

$$\begin{pmatrix} p_+(z,k_0-1,k_0) \\ r_+(z,k_0-1,k_0) \end{pmatrix} = \begin{cases} \frac{1}{\rho_{k_0}} \begin{pmatrix} z\overline{b_{k_0}} \\ b_{k_0} \end{pmatrix}, & k_0 \text{ odd}, \\ \frac{1}{\rho_{k_0}} \begin{pmatrix} b_{k_0} \\ \overline{b_{k_0}} \end{pmatrix}, & k_0 \text{ even}, \end{cases} \tag{3.29}$$

$$\begin{pmatrix} q_+(z,k_0-1,k_0) \\ s_+(z,k_0-1,k_0) \end{pmatrix} = \begin{cases} \frac{1}{\rho_{k_0}} \begin{pmatrix} -z\overline{a_{k_0}} \\ a_{k_0} \end{pmatrix}, & k_0 \text{ odd}, \\ \frac{1}{\rho_{k_0}} \begin{pmatrix} a_{k_0} \\ -\overline{a_{k_0}} \end{pmatrix}, & k_0 \text{ even}. \end{cases} \tag{3.30}$$

It follows from (3.19) that

$$\begin{aligned} M_{\ell,\ell'}(z,k_0) &= \delta_{\ell,\ell'} + 2z\big(\delta_{k_0+\ell-1}, (U-zI)^{-1}\delta_{k_0+\ell'-1}\big)_{\ell^2(\mathbb{Z})} \\ &= \delta_{\ell,\ell'} + 2z(U-zI)^{-1}(k_0+\ell-1, k_0+\ell'-1), \quad \ell,\ell'=0,1. \end{aligned} \tag{3.31}$$

Thus, by Lemma 3.1 and equalities (2.57), (2.136), (3.29), and (3.30), one finds

$$(U-zI)^{-1}(k_0,k_0) = \frac{[1-M_+(z,k_0)][1+M_-(z,k_0)]}{2z[M_+(z,k_0)-M_-(z,k_0)]}, \tag{3.32}$$

$$(U-zI)^{-1}(k_0-1,k_0-1) = \frac{[\overline{a_{k_0}} - \overline{b_{k_0}}M_+(z,k_0)][a_{k_0}+b_{k_0}M_-(z,k_0)]}{2z\rho_{k_0}^2[M_+(z,k_0)-M_-(z,k_0)]}, \tag{3.33}$$

$$(U-zI)^{-1}(k_0-1,k_0) = \frac{\begin{cases} [1-M_+(z,k_0)][\overline{a_{k_0}}-\overline{b_{k_0}}M_-(z,k_0)], & k_0 \text{ odd}, \\ [1+M_+(z,k_0)][a_{k_0}+b_{k_0}M_-(z,k_0)], & k_0 \text{ even} \end{cases}}{2z\rho_{k_0}[M_+(z,k_0)-M_-(z,k_0)]}, \tag{3.34}$$

$$(U-zI)^{-1}(k_0,k_0-1) = \frac{\begin{cases} [1+M_+(z,k_0)][a_{k_0}+b_{k_0}M_-(z,k_0)], & k_0 \text{ odd}, \\ [1-M_+(z,k_0)][\overline{a_{k_0}}-\overline{b_{k_0}}M_-(z,k_0)], & k_0 \text{ even} \end{cases}}{2z\rho_{k_0}[M_+(z,k_0)-M_-(z,k_0)]}, \tag{3.35}$$

and hence (3.25)–(3.28). □

Finally, introducing the functions $\Phi_{1,1}(\cdot,k)$, $k \in \mathbb{Z}$, by

$$\Phi_{1,1}(z,k) = \frac{M_{1,1}(z,k)-1}{M_{1,1}(z,k)+1}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \tag{3.36}$$

then,

$$M_{1,1}(z,k) = \frac{1+\Phi_{1,1}(z,k)}{1-\Phi_{1,1}(z,k)}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{3.37}$$

Both, $M_{1,1}(z,k)$ and $\Phi_{1,1}(z,k)$, $z \in \mathbb{C}\backslash\partial\mathbb{D}$, $k \in \mathbb{Z}$, have nontangential limits to $\partial\mathbb{D}$ μ_0-a.e.

Lemma 3.3. *The function $\Phi_{1,1}|_{\mathbb{D}}$ is a Schur function and $\Phi_{1,1}$ is related to $\Phi_\pm$ by*

$$\Phi_{1,1}(z,k) = \frac{\Phi_+(z,k)}{\Phi_-(z,k)}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}, \; k \in \mathbb{Z}. \tag{3.38}$$

Proof. The assertion follows from (2.150), (3.36) and Lemma 3.2. □

Lemma 3.4. *Let $\zeta \in \partial\mathbb{D}$ and $k_0 \in \mathbb{Z}$. Then the following sets of two-dimensional Laurent polynomials $\{P(\zeta,k,k_0)\}_{k\in\mathbb{Z}}$ and $\{R(\zeta,k,k_0)\}_{k\in\mathbb{Z}}$:*

$$P(\zeta,k,k_0) = \begin{pmatrix} P_0(\zeta,k,k_0) \\ P_1(\zeta,k,k_0) \end{pmatrix} = \begin{cases} \frac{1}{2\zeta}\begin{pmatrix} -\rho_{k_0} & \rho_{k_0} \\ \overline{b_{k_0}} & \overline{a_{k_0}} \end{pmatrix}\begin{pmatrix} q_+(\zeta,k,k_0) \\ p_+(\zeta,k,k_0) \end{pmatrix}, & k_0 \text{ odd}, \\ \frac{1}{2}\begin{pmatrix} \rho_{k_0} & \rho_{k_0} \\ -b_{k_0} & a_{k_0} \end{pmatrix}\begin{pmatrix} q_+(\zeta,k,k_0) \\ p_+(\zeta,k,k_0) \end{pmatrix}, & k_0 \text{ even}, \end{cases} \tag{3.39}$$

$$R(\zeta,k,k_0) = \begin{pmatrix} R_0(\zeta,k,k_0) \\ R_1(\zeta,k,k_0) \end{pmatrix} = \begin{cases} \frac{1}{2}\begin{pmatrix} \rho_{k_0} & \rho_{k_0} \\ -b_{k_0} & a_{k_0} \end{pmatrix}\begin{pmatrix} s_+(\zeta,k,k_0) \\ r_+(\zeta,k,k_0) \end{pmatrix}, & k_0 \text{ odd}, \\ \frac{1}{2}\begin{pmatrix} -\rho_{k_0} & \rho_{k_0} \\ \overline{b_{k_0}} & \overline{a_{k_0}} \end{pmatrix}\begin{pmatrix} s_+(\zeta,k,k_0) \\ r_+(\zeta,k,k_0) \end{pmatrix}, & k_0 \text{ even} \end{cases} \tag{3.40}$$

form complete orthonormal systems in $L^2(\partial\mathbb{D}; d\Omega(\cdot,k_0)^\top)$ and $L^2(\partial\mathbb{D}; d\Omega(\cdot,k_0))$, respectively.

Proof. Consider the following relation:

$$U^\top\delta_k = \sum_{j\in\mathbb{Z}} U^\top(j,k)\delta_j = \sum_{j\in\mathbb{Z}} U(k,j)\delta_j, \quad k \in \mathbb{Z}. \tag{3.41}$$

By Lemma 2.2 any solution u of

$$zu(z,k,k_0) = \sum_{j\in\mathbb{Z}} U(k,j)u(z,j,k_0), \quad k \in \mathbb{Z}, \tag{3.42}$$

is a linear combination of $p_+(z,\cdot,k_0)$ and $q_+(z,\cdot,k_0)$, and hence, (3.42) has a unique solution $\{u(z,k,k_0)\}_{k\in\mathbb{Z}}$ with prescribed values at k_0-1 and k_0,

$$u\ (z,\cdot,k_0) = P_0(z,\cdot,k_0)u(z,k_0-1,k_0) + P_1(z,\cdot,k_0)u(z,k_0,k_0). \tag{3.43}$$

Due to the algebraic nature of the proof of Lemma 2.2 and the algebraic similarity of equations (3.41) and (3.42), one concludes from (3.43) that

$$\delta_k = P_0(U^\top,k,k_0)\delta_{k_0-1} + P_1(U^\top,k,k_0)\delta_{k_0}, \quad k \in \mathbb{Z}. \tag{3.44}$$

Using the spectral representation for the operator $U^\top$ one then obtains

$$P_\ell(U^\top,k,k_0) = \oint_{\partial\mathbb{D}} dE_{U^\top}(\zeta)\, P_\ell(\zeta,k,k_0), \quad \ell = 0,1 \tag{3.45}$$

and by (3.44),

$$\begin{aligned}(\delta_k,\delta_{k'})_{\ell^2(\mathbb{Z})} &= \sum_{\ell,\ell'=0}^{1} \Big(P_\ell(U^\top,k,k_0)\delta_{k_0+\ell-1}, P_{\ell'}(U^\top,k',k_0)\delta_{k_0+\ell'-1}\Big)_{\ell^2(\mathbb{Z})} \\ &= \oint_{\partial\mathbb{D}} P(\zeta,k,k_0)^*\, d\Omega(\zeta,k_0)^\top P(\zeta,k',k_0). \end{aligned} \tag{3.46}$$

Similarly, one obtains the orthonormality relation for the two-dimensional Laurent polynomials $\{R(\zeta,k,k_0)\}_{k\in\mathbb{Z}}$ in $L^2(\partial\mathbb{D}; d\Omega(\cdot,k_0))$.

To prove completeness of $\{P(\zeta,k,k_0)\}_{k\in\mathbb{Z}}$ we first note the following fact:

$$\begin{aligned}\operatorname{span}\{P(z,k,k_0)\}_{k\in\mathbb{Z}} &= \operatorname{span}\left\{\begin{pmatrix} z^k \\ z^{k-1}\end{pmatrix}, \begin{pmatrix} z^{k-1} \\ z^k\end{pmatrix}, \begin{pmatrix} 1 \\ 0\end{pmatrix}, \begin{pmatrix} 0 \\ 1\end{pmatrix}\right\}_{k\in\mathbb{Z}} \\ &= \operatorname{span}\left\{\begin{pmatrix} z^k \\ 0\end{pmatrix}, \begin{pmatrix} 0 \\ z^k\end{pmatrix}\right\}_{k\in\mathbb{Z}}, \quad k_0 \in \mathbb{Z}. \end{aligned} \tag{3.47}$$

This follows by investigating the leading coefficients of $p_+(z,k,k_0)$ and $q_+(z,k,k_0)$. Thus, it suffices to prove that $\left\{\begin{pmatrix}\zeta^k\\0\end{pmatrix},\begin{pmatrix}0\\\zeta^k\end{pmatrix}\right\}_{k\in\mathbb{Z}}$ form a basis in $L^2(\partial\mathbb{D};d\Omega(\cdot,k_0)^\top)$ for all $k_0\in\mathbb{Z}$.

Let $k_0\in\mathbb{Z}$ and suppose that $F=\begin{pmatrix}f_0\\f_1\end{pmatrix}\in L^2(\partial\mathbb{D};d\Omega(\cdot,k_0)^\top)$ is orthogonal to $\left\{\begin{pmatrix}\zeta^k\\0\end{pmatrix},\begin{pmatrix}0\\\zeta^k\end{pmatrix}\right\}_{k\in\mathbb{Z}}$ in $L^2(\partial\mathbb{D};d\Omega(\cdot,k_0)^\top)$, that is,

$$\begin{aligned}0&=\oint_{\partial\mathbb{D}}\overline{(\zeta^k\quad 0)}\,d\Omega(\zeta,k_0)^\top F(\zeta)\\&=\oint_{\partial\mathbb{D}}\overline{\zeta^k}\,[f_0(\zeta)d\Omega_{0,0}(\zeta,k_0)+f_1(\zeta)d\Omega_{1,0}(\zeta,k_0)],\end{aligned}\tag{3.48}$$

and

$$\begin{aligned}0&=\oint_{\partial\mathbb{D}}\overline{(0\quad \zeta^k)}\,d\Omega(\zeta,k_0)^\top F(\zeta)\\&=\oint_{\partial\mathbb{D}}\overline{\zeta^k}\,[f_0(\zeta)d\Omega_{0,1}(\zeta,k_0)+f_1(\zeta)d\Omega_{1,1}(\zeta,k_0)]\end{aligned}\tag{3.49}$$

for all $k\in\mathbb{Z}$. Hence (cf., e.g., [10, p. 24]),

$$f_0d\Omega_{0,0}+f_1d\Omega_{1,0}=0,\tag{3.50}$$

$$f_0d\Omega_{0,1}+f_1d\Omega_{1,1}=0.\tag{3.51}$$

Multiplying (3.50) by $\overline{f_0}$ and (3.51) by $\overline{f_1}$ then yields

$$|f_0|^2d\Omega_{0,0}+\overline{f_0}f_1d\Omega_{1,0}+\overline{f_1}f_0d\Omega_{0,1}+|f_1|^2d\Omega_{1,1}=0\tag{3.52}$$

and hence

$$\|F\|^2_{L^2(\partial\mathbb{D};d\Omega(\cdot,k_0)^\top)}=\oint_{\partial\mathbb{D}}F(\zeta)^*\,d\Omega(\zeta,k_0)^\top F(\zeta)=0.\tag{3.53}$$

Similarly, one proves completeness of $\{R(\zeta,k,k_0)\}_{k\in\mathbb{Z}}$ in $L^2(\partial\mathbb{D};d\Omega(\cdot,k_0))$. $\square$

Denoting by I_2 the identity operator in $\mathbb{C}^2$, we state the following result.

Corollary 3.5. *Let $k_0\in\mathbb{Z}$. Then the operators U and $U^\top$ are unitarily equivalent to the operator of multiplication by $I_2 id$ (where $id(\zeta)=\zeta$, $\zeta\in\partial\mathbb{D}$) on $L^2(\partial\mathbb{D};d\Omega(\cdot,k_0))$ and $L^2(\partial\mathbb{D};d\Omega(\cdot,k_0)^\top)$, respectively. Thus,*

$$\sigma(U)=\operatorname{supp}(d\Omega(\cdot,k_0))=\operatorname{supp}(d\Omega^{\mathrm{tr}}(\cdot,k_0))=\operatorname{supp}(d\Omega(\cdot,k_0)^\top)=\sigma(U^\top),\tag{3.54}$$

where

$$d\Omega^{\mathrm{tr}}(\cdot,k_0)=d\Omega_{0,0}(\cdot,k_0)+d\Omega_{1,1}(\cdot,k_0)\tag{3.55}$$

denotes the trace measure of $d\Omega(\cdot,k_0)$.

Proof. Consider the linear map $\dot{\mathcal{U}}$ from $\ell_0^\infty(\mathbb{Z})$ into the set of two-dimensional Laurent polynomials on $\partial\mathbb{D}$ defined by

$$(\dot{\mathcal{U}}f)(\zeta)=\sum_{k\in\mathbb{Z}}R(\zeta,k,k_0)f(k),\qquad f\in\ell_0^\infty(\mathbb{Z}).\tag{3.56}$$

A simple calculation for $F(\zeta) = (\dot{\mathcal{U}} f)(\zeta)$, $f \in \ell_0^\infty(\mathbb{Z})$, shows that

$$\sum_{k\in\mathbb{Z}} |f(k)|^2 = \oint_{\partial\mathbb{D}} F(\zeta)^* d\Omega(\zeta, k_0) F(\zeta). \tag{3.57}$$

Since $\ell_0^\infty(\mathbb{Z})$ is dense in $\ell^2(\mathbb{Z})$, $\mathcal{U}$ extends to a bounded linear operator $\mathcal{U}\colon \ell^2(\mathbb{Z}) \to L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0))$. By Lemma 3.4, $\mathcal{U}$ is onto and one verifies that

$$(\mathcal{U}^{-1} F)(k) = \oint_{\partial\mathbb{D}} R(\zeta, k, k_0)^* d\Omega(\zeta, k_0) F(\zeta). \tag{3.58}$$

In particular, $\mathcal{U}$ is unitary. Moreover, we claim that $\mathcal{U}$ maps the operator U on $\ell^2(\mathbb{Z})$ to the operator of multiplication by $id(\zeta) = \zeta$, $\zeta \in \partial\mathbb{D}$, denoted by $M(id)$, on $L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0))$,

$$\mathcal{U} U \mathcal{U}^{-1} = M(id), \tag{3.59}$$

where

$$(M(id)F)(\zeta) = \zeta F(\zeta), \quad F \in L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0)). \tag{3.60}$$

Indeed,

$$\begin{aligned}
&(\mathcal{U} U \mathcal{U}^{-1} F(\cdot))(\zeta) = (\mathcal{U} U f(\cdot))(\zeta) \\
&\quad = \sum_{k\in\mathbb{Z}} (U f(\cdot))(k) R(\zeta, k, k_0) = \sum_{k\in\mathbb{Z}} (U^\top R(\zeta, \cdot, k_0))(k) f(k) \\
&\quad = \sum_{k\in\mathbb{Z}} \zeta R(\zeta, k, k_0) f(k) = \zeta F(\zeta) \\
&\quad = (M(id)F(\cdot))(\zeta), \quad F \in L^2(\partial\mathbb{D}; d\Omega(\cdot, k_0)).
\end{aligned} \tag{3.61}$$

The result for the operator $U^\top$ is proved analogously. □

Finally, we note an alternative approach to (a variant of) the 2×2 matrix-valued spectral function $\Omega(\cdot, k_0)$ associated with U.

First we introduce $\widetilde{\mathcal{M}}(z, k)$, $z \in \mathbb{C}\backslash\partial\mathbb{D}$, $k \in \mathbb{Z}$, defined by

$$\begin{aligned}
\widetilde{\mathcal{M}}(z, k) &= \begin{pmatrix} \widetilde{M}_{0,0}(z, k) & \widetilde{M}_{0,1}(z, k) \\ \widetilde{M}_{1,0}(z, k) & \widetilde{M}_{1,1}(z, k) \end{pmatrix} \\
&= \begin{cases} \frac{1}{4} \begin{pmatrix} \rho_k & \rho_k \\ -b_k & a_k \end{pmatrix}^* \mathcal{M}(z, k) \begin{pmatrix} \rho_k & \rho_k \\ -b_k & a_k \end{pmatrix}, & k \text{ odd}, \\ \frac{1}{4} \begin{pmatrix} -\rho_k & \rho_k \\ \overline{b_k} & \overline{a_k} \end{pmatrix}^* \mathcal{M}(z, k) \begin{pmatrix} -\rho_k & \rho_k \\ \overline{b_k} & \overline{a_k} \end{pmatrix}, & k \text{ even} \end{cases} \\
&= \begin{pmatrix} \frac{1}{M_+(z,k) - M_-(z,k)} + \frac{i}{2}\operatorname{Im}(\alpha_k) & \frac{1}{2}\frac{M_+(z,k) + M_-(z,k)}{M_+(z,k) - M_-(z,k)} + \frac{1}{2}\operatorname{Re}(\alpha_k) \\ -\frac{1}{2}\frac{M_+(z,k) + M_-(z,k)}{M_+(z,k) - M_-(z,k)} - \frac{1}{2}\operatorname{Re}(\alpha_k) & -\frac{M_+(z,k) M_-(z,k)}{M_+(z,k) - M_-(z,k)} - \frac{i}{2}\operatorname{Im}(\alpha_k) \end{pmatrix} \\
&\qquad z \in \mathbb{C}\backslash\partial\mathbb{D}, \; k \in \mathbb{Z}.
\end{aligned} \tag{3.62}$$

Clearly, $\mathcal{M}(\cdot, k)$, and hence, $\widetilde{\mathcal{M}}(\cdot, k)$, $k \in \mathbb{Z}$, are 2×2 matrix-valued Caratheodory functions. Since by (3.19) $\mathcal{M}(0, k) = I$, $k \in \mathbb{Z}$, one computes

$$\widetilde{\mathcal{M}}(0, k) = \frac{1}{4} \begin{pmatrix} \rho_k^2 + |b_k|^2 & -2i\operatorname{Im}(\alpha_k) \\ 2i\operatorname{Im}(\alpha_k) & \rho_k^2 + |a_k|^2 \end{pmatrix} = [\widetilde{\mathcal{M}}(0, k)]^*, \quad k \in \mathbb{Z}. \tag{3.63}$$

Hence, the Herglotz representation of $\widetilde{\mathcal{M}}(\cdot,k)$ is given by

$$\widetilde{\mathcal{M}}(z,k) = \int_{\partial\mathbb{D}} d\widetilde{\Omega}(\zeta,k)\,\frac{\zeta+z}{\zeta-z}, \quad z\in\mathbb{C}\backslash\partial\mathbb{D},\ k\in\mathbb{Z}, \tag{3.64}$$

where the measure $d\widetilde{\Omega}(\cdot,k)$ can be reconstructed from the boundary values of $\mathrm{Re}(\widetilde{\mathcal{M}}(\cdot,k))$ via

$$\begin{aligned}\widetilde{\Omega}\big(\big(e^{i\theta_1},e^{i\theta_2}\big],k\big) &= \lim_{\delta\downarrow 0}\lim_{r\uparrow 1}\frac{1}{2\pi}\int_{\theta_1+\delta}^{\theta_2+\delta} d\theta \\ &\times\begin{pmatrix} \mathrm{Re}\left(\frac{1}{M_+(re^{i\theta},k)-M_-(re^{i\theta},k)}\right) & \frac{i}{2}\mathrm{Im}\left(\frac{M_+(re^{i\theta},k)+M_-(re^{i\theta},k)}{M_+(re^{i\theta},k)-M_-(re^{i\theta},k)}\right) \\ -\frac{i}{2}\mathrm{Im}\left(\frac{M_+(re^{i\theta},k)+M_-(re^{i\theta},k)}{M_+(re^{i\theta},k)-M_-(re^{i\theta},k)}\right) & -\mathrm{Re}\left(\frac{M_+(re^{i\theta},k)M_-(re^{i\theta},k)}{M_+(re^{i\theta},k)-M_-(re^{i\theta},k)}\right)\end{pmatrix}, \\ &\qquad \theta_1\in[0,2\pi),\ \theta_1<\theta_2<\theta_1+2\pi,\ k\in\mathbb{Z}.\end{aligned} \tag{3.65}$$

Finally, the analog of Lemma 2.25 in the full-lattice context reads as follows.

Lemma 3.6. *Let $f,g\in\ell_0^\infty(\mathbb{Z})$, $F\in C(\partial\mathbb{D})$, and $\theta_1\in[0,2\pi)$, $\theta_1<\theta_2\leqslant\theta_1+2\pi$. Then,*

$$\begin{aligned}&\big(f,F(U)E_U\big(\mathrm{Arc}\big(\big(e^{i\theta_1},e^{i\theta_2}\big]\big)\big)g\big)_{\ell^2(\mathbb{Z})} \\ &\quad = \big(\widehat{f}(\cdot,k_0),M_F M_{\chi_{\mathrm{Arc}((e^{i\theta_1},e^{i\theta_2}])}}\widehat{g}(\cdot,k_0)\big)_{L^2(\partial\mathbb{D};d\widetilde{\Omega}_\pm(\cdot,k_0))},\end{aligned} \tag{3.66}$$

where we introduced the notation

$$\widehat{h}(\zeta,k_0) = \sum_{k\in\mathbb{Z}}\begin{pmatrix} s_+(\zeta,k,k_0) \\ r_+(\zeta,k,k_0)\end{pmatrix} h(k), \quad \zeta\in\partial\mathbb{D},\ h\in\ell_0^\infty(\mathbb{Z}) \tag{3.67}$$

and M_G denotes the maximally defined operator of multiplication by the $d\widetilde{\Omega}(\cdot,k_0)$-measurable function G in the Hilbert space $L^2(\partial\mathbb{D};d\widetilde{\Omega}(\cdot,k_0))$,

$$\begin{aligned}&(M_G\widehat{h})(\zeta) = G(\zeta)\widehat{h}(\zeta) \text{ for a.e. } \zeta\in\partial\mathbb{D}, \\ &\widehat{h}\in\mathrm{dom}(M_G) = \{\widehat{k}\in L^2(\partial\mathbb{D};d\widetilde{\Omega}(\cdot,k_0))\,|\,G\widehat{k}\in L^2(\partial\mathbb{D};d\widetilde{\Omega}(\cdot,k_0))\}.\end{aligned} \tag{3.68}$$

Using Lemma 2.24, (2.63), (2.64), (2.169), and (3.7) one can follow the proof of Lemma 2.25 step by step and so we omit the details (cf. also [21]).

Finally, Weyl–Titchmarsh circles associated with finite intervals $[k_-,k_+]\cap\mathbb{Z}$ and the ensuing limits $k_\pm\to\pm\infty$ can be discussed in analogy to the half-lattice case at the end of Section 2. Without entering into details, we mention that U is of course in the limit point case at $\pm\infty$.

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Appendix A. Basic facts on Caratheodory and Schur functions

In this appendix, we summarize a few basic properties of Caratheodory and Schur functions used throughout this manuscript.

We denote by $\mathbb{D}$ and $\partial\mathbb{D}$ the open unit disk and the counterclockwise oriented unit circle in the complex plane $\mathbb{C}$,

$$\mathbb{D} = \{z \in \mathbb{C} \mid |z| < 1\}, \quad \partial\mathbb{D} = \{\zeta \in \mathbb{C} \mid |\zeta| = 1\} \tag{A.1}$$

and by

$$\mathbb{C}_\ell = \{z \in \mathbb{C} \mid \mathrm{Re}(z) < 0\}, \quad \mathbb{C}_r = \{z \in \mathbb{C} \mid \mathrm{Re}(z) > 0\} \tag{A.2}$$

the open left and right complex half-planes, respectively.

Definition A.1. Let $f_\pm$, φ_+, and $1/\varphi_-$ be analytic in $\mathbb{D}$.

(i) f_+ is called a *Caratheodory function* if $f_+ : \mathbb{D} \to \mathbb{C}_r$ and f_- is called an *anti-Caratheodory function* if $-f_-$ is a Caratheodory function.

(ii) φ_+ is called a *Schur function* if $\varphi_+ : \mathbb{D} \to \mathbb{D}$. φ_- is called an *anti-Schur function* if $1/\varphi_-$ is a Schur function.

Theorem A.2. (*Akhiezer [3, Sect. 3.1], Akhiezer and Glazman [4, Sect. 69], Simon [33, Sect. 1.3] Let f be a Caratheodory function. Then f admits the Herglotz representation*

$$f(z) = ic + \oint_{\partial\mathbb{D}} d\mu(\zeta)\, \frac{\zeta + z}{\zeta - z}, \quad z \in \mathbb{D}, \tag{A.3}$$

$$c = \mathrm{Im}(f(0)), \quad \oint_{\partial\mathbb{D}} d\mu(\zeta) = \mathrm{Re}(f(0)) < \infty, \tag{A.4}$$

where $d\mu$ denotes a nonnegative measure on $\partial\mathbb{D}$. The measure $d\mu$ can be reconstructed from f by the formula

$$\mu\big(\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2}]\big)\big) = \lim_{\delta\downarrow 0} \lim_{r\uparrow 1} \frac{1}{2\pi} \oint_{\theta_1+\delta}^{\theta_2+\delta} d\theta\, \mathrm{Re}\big(f\big(re^{i\theta}\big)\big), \tag{A.5}$$

where

$$\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2}]\big) = \big\{e^{i\theta} \in \partial\mathbb{D} \mid \theta_1 < \theta \leqslant \theta_2\big\}, \quad \theta_1 \in [0, 2\pi),\ \theta_1 < \theta_2 \leqslant \theta_1 + 2\pi. \tag{A.6}$$

Conversely, the right-hand side of (A.3) *with $c \in \mathbb{R}$ and $d\mu$ a finite* (*nonnegative*) *measure on $\partial\mathbb{D}$ defines a Caratheodory function.*

We note that additive nonnegative constants on the right-hand side of (A.3) can be absorbed into the measure $d\mu$ since

$$\oint_{\partial\mathbb{D}} d\mu_0(\zeta)\, \frac{\zeta + z}{\zeta - z} = 1, \quad z \in \mathbb{D}, \tag{A.7}$$

where

$$d\mu_0(\zeta) = \frac{d\theta}{2\pi}, \quad \zeta = e^{i\theta},\ \theta \in [0, 2\pi] \tag{A.8}$$

denotes the normalized Lebesgue measure on the unit circle $\partial\mathbb{D}$.

A useful fact on Caratheodory functions f is a certain monotonicity property they exhibit on open connected arcs of the unit circle away from the support of the measure $d\mu$ in the Herglotz representation (A.3). More precisely, suppose $\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2})\big) \subset (\partial\mathbb{D} \backslash \mathrm{supp}(d\mu))$, $\theta_1 < \theta_2$, then f has an analytic continuation through $\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2})\big)$ and it is purely imaginary on $\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2})\big)$. Moreover,

$$\frac{d}{d\theta} f\big(e^{i\theta}\big) = -\frac{i}{2}\int_{[0,2\pi]\backslash(\theta_1,\theta_2)} d\mu\big(e^{it}\big)\frac{1}{\sin^2((t-\theta)/2)}, \quad \theta \in (\theta_1, \theta_2). \tag{A.9}$$

In particular,

$$-i\frac{d}{d\theta} f\big(e^{i\theta}\big) < 0, \quad \theta \in (\theta_1, \theta_2). \tag{A.10}$$

We recall that any Caratheodory function f has finite radial limits to the unit circle μ_0-almost everywhere, that is,

$$f(\zeta) = \lim_{r\uparrow 1} f(r\zeta) \text{ exists and is finite for } \mu_0\text{-a.e. } \zeta \in \partial\mathbb{D}. \tag{A.11}$$

The absolutely continuous part $d\mu_{\mathrm{ac}}$ of the measure $d\mu$ in the Herglotz representation (A.3) of the Caratheodory function f is given by

$$d\mu_{\mathrm{ac}}(\zeta) = \lim_{r\uparrow 1} \mathrm{Re}(f(r\zeta))\, d\mu_0(\zeta), \quad \zeta \in \partial\mathbb{D}. \tag{A.12}$$

The set

$$S_{\mu_{\mathrm{ac}}} = \{\zeta \in \partial\mathbb{D} \mid \lim_{r\uparrow 1} \mathrm{Re}(f(r\zeta)) = \mathrm{Re}(f(\zeta)) > 0 \text{ exists finitely}\} \tag{A.13}$$

is an essential support of $d\mu_{\mathrm{ac}}$ and its essential closure, $\overline{S_{\mu_{\mathrm{ac}}}}^{e}$, coincides with the topological support, $\mathrm{supp}(d\mu_{\mathrm{ac}})$ (the smallest closed support), of $d\mu_{\mathrm{ac}}$,

$$\overline{S_{\mu_{\mathrm{ac}}}}^{e} = \mathrm{supp}\,(d\mu_{\mathrm{ac}}). \tag{A.14}$$

Moreover, the set

$$S_{\mu_{\mathrm{s}}} = \{\zeta \in \partial\mathbb{D} \mid \lim_{r\uparrow 1} \mathrm{Re}(f(r\zeta)) = \infty\} \tag{A.15}$$

is an essential support of the singular part $d\mu_{\mathrm{s}}$ of the measure $d\mu$, and

$$\lim_{r\uparrow 1}(1-r)f(r\zeta) = \lim_{r\uparrow 1}(1-r)\mathrm{Re}(f(r\zeta)) \geqslant 0 \text{ exists for all } \zeta \in \partial\mathbb{D}. \tag{A.16}$$

In particular, $\zeta_0 \in \partial\mathbb{D}$ is a pure point of $d\mu$ if and only if

$$\mu(\{\zeta_0\}) = \lim_{r\uparrow 1}\left(\frac{1-r}{2}\right) f(r\zeta_0) > 0. \tag{A.17}$$

Given a Caratheodory (resp., anti-Caratheodory) function f_+ (resp. f_-) defined in $\mathbb{D}$ as in (A.3), one extends $f_\pm$ to all of $\mathbb{C}\backslash\partial\mathbb{D}$ by

$$f_\pm(z) = ic_\pm \pm \oint_{\partial\mathbb{D}} d\mu_\pm(\zeta)\,\frac{\zeta+z}{\zeta-z}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D},\ c_\pm \in \mathbb{R}. \tag{A.18}$$

In particular,

$$f_\pm(z) = -\overline{f_\pm(1/\overline{z})}, \quad z \in \mathbb{C}\backslash\overline{\mathbb{D}}. \tag{A.19}$$

Of course, this continuation of $f_\pm|_{\mathbb{D}}$ to $\mathbb{C}\backslash\overline{\mathbb{D}}$, in general, is not an analytic continuation of $f_\pm|_{\mathbb{D}}$. With $f_\pm$ defined on $\mathbb{C}\backslash\partial\mathbb{D}$ by (A.18) one infers the mapping properties

$$f_+ : \mathbb{D} \to \mathbb{C}_r, \quad f_+ : \mathbb{C}\backslash\overline{\mathbb{D}} \to \mathbb{C}_\ell, \quad f_- : \mathbb{D} \to \mathbb{C}_\ell, \quad f_- : \mathbb{C}\backslash\overline{\mathbb{D}} \to \mathbb{C}_r. \tag{A.20}$$

Next, given the functions $f_\pm$ defined in $\mathbb{C}\backslash\partial\mathbb{D}$ as in (A.18), we introduce the functions $\varphi_\pm$ by

$$\varphi_\pm(z) = \frac{f_\pm(z) - 1}{f_\pm(z) + 1}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{A.21}$$

Then $\varphi_\pm$ have the mapping properties

$$\begin{aligned} &\varphi_+ : \mathbb{D} \to \mathbb{D}, \quad 1/\varphi_+ : \mathbb{C}\backslash\overline{\mathbb{D}} \to \mathbb{D} \quad (\varphi_+ : \mathbb{C}\backslash\overline{\mathbb{D}} \to (\mathbb{C}\backslash\overline{\mathbb{D}}) \cup \{\infty\}), \\ &\varphi_- : \mathbb{C}\backslash\overline{\mathbb{D}} \to \mathbb{D}, \quad 1/\varphi_- : \mathbb{D} \to \mathbb{D} \quad (\varphi_- : \mathbb{D} \to (\mathbb{C}\backslash\overline{\mathbb{D}}) \cup \{\infty\}), \end{aligned} \tag{A.22}$$

in particular, $\varphi_+|_{\mathbb{D}}$ (resp., $\varphi_-|_{\mathbb{D}}$) is a Schur (resp., anti-Schur) function. Moreover,

$$f_\pm(z) = \frac{1 + \varphi_\pm(z)}{1 - \varphi_\pm(z)}, \quad z \in \mathbb{C}\backslash\partial\mathbb{D}. \tag{A.23}$$

We also recall the following useful result (see [33, Lemma 10.11.17, 20] for a proof). To fix some notation we denote by f_+ and f_- a Caratheodory and anti-Caratheodory function, respectively, and by φ_+ and φ_- the corresponding Schur and anti-Schur functions as defined in (A.21). We also introduce the following notation for open arcs on the unit circle $\partial\mathbb{D}$:

$$\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2})\big) = \big\{e^{i\theta} \in \partial\mathbb{D} \,|\, \theta_1 < \theta < \theta_2\big\}, \quad \theta_1 \in [0, 2\pi], \ \theta_1 < \theta_2 \leqslant \theta_1 + 2\pi. \tag{A.24}$$

An open arc $A \subseteq \partial\mathbb{D}$ then either coincides with $\mathrm{Arc}\big((e^{i\theta_1}, e^{i\theta_2})\big)$ for some $\theta_1 \in [0, 2\pi]$, $\theta_1 < \theta_2 \leqslant \theta_1 + 2\pi$, or else, $A = \partial\mathbb{D}$.

Lemma A.3. *Let $A \subseteq \partial\mathbb{D}$ be an open arc and assume that f_+ (resp., f_-) is a Caratheodory (resp., anti-Caratheodory) function satisfying the reflectionless condition*

$$\lim_{r\uparrow 1} \big[f_+(r\zeta) + \overline{f_-(r\zeta)}\big] = 0 \quad \mu_0\text{-a.e. on } A. \tag{A.25}$$

Then,

(i) $f_+(\zeta) = -\overline{f_-(\zeta)}$ *for all* $\zeta \in A$.
(ii) *For* $z \in \mathbb{D}$, $-\overline{f_-(1/\overline{z})}$ *is the analytic continuation of* $f_+(z)$ *through the arc* A.
(iii) $d\mu_\pm$ *are purely absolutely continuous on* A *and*

$$\frac{d\mu_\pm}{d\mu_0}(\zeta) = \mathrm{Re}(f_+(\zeta)) = -\mathrm{Re}(f_-(\zeta)), \quad \zeta \in A. \tag{A.26}$$

In analogy to the exponential representation of Nevanlinna–Herglotz functions (i.e., functions analytic in the open complex upper half-plane $\mathbb{C}_+$ with a strictly positive imaginary part on $\mathbb{C}_+$, cf. [5,6,19,24]) one obtains the following result.

Theorem A.4. *Let f be a Caratheodory function. Then $-i\ln(if)$ is a Caratheodory function and f has the exponential Herglotz representation,*

$$-i\ln(if(z)) = id + \oint_{\partial\mathbb{D}} d\mu_0(\zeta)\, \Upsilon(\zeta)\, \frac{\zeta + z}{\zeta - z}, \quad z \in \mathbb{D}, \tag{A.27}$$

$$d = -\mathrm{Re}(\ln(f(0))), \quad 0 \leqslant \Upsilon(\zeta) \leqslant \pi \text{ for } \mu_0\text{-a.e. } \zeta \in \partial\mathbb{D}. \tag{A.28}$$

Υ can be reconstructed from f by

$$\Upsilon(\zeta) = \lim_{r\uparrow 1} \operatorname{Re}[-i\ln(if(r\zeta))]$$
$$= (\pi/2) + \lim_{r\uparrow 1} \operatorname{Im}[\ln(f(r\zeta))] \text{ for } \mu_0\text{-a.e. } \zeta \in \partial\mathbb{D}. \tag{A.29}$$

Next we briefly turn to matrix-valued Caratheodory functions. We denote as usual $\operatorname{Re}(A) = (A + A^*)/2$, $\operatorname{Im}(A) = (A - A^*)/(2i)$, etc., for square matrices A.

Definition A.5. Let $m \in \mathbb{N}$ and $\mathcal{F}$ be an $m \times m$ matrix-valued function analytic in $\mathbb{D}$. $\mathcal{F}$ is called a *Caratheodory matrix* if $\operatorname{Re}(\mathcal{F}(z)) \geqslant 0$ for all $z \in \mathbb{D}$.

Theorem A.6. *Let $\mathcal{F}$ be an $m \times m$ Caratheodory matrix, $m \in \mathbb{N}$. Then $\mathcal{F}$ admits the Herglotz representation*

$$\mathcal{F}(z) = iC + \oint_{\partial\mathbb{D}} d\Omega(\zeta)\, \frac{\zeta + z}{\zeta - z}, \quad z \in \mathbb{D}, \tag{A.30}$$

$$C = \operatorname{Im}(\mathcal{F}(0)), \quad \oint_{\partial\mathbb{D}} d\Omega(\zeta) = \operatorname{Re}(\mathcal{F}(0)), \tag{A.31}$$

where $d\Omega$ denotes a nonnegative $m \times m$ matrix-valued measure on $\partial\mathbb{D}$. The measure $d\Omega$ can be reconstructed from $\mathcal{F}$ by the formula

$$\Omega\big(\operatorname{Arc}\big(\big(e^{i\theta_1}, e^{i\theta_2}\big]\big)\big) = \lim_{\delta\downarrow 0} \lim_{r\uparrow 1} \frac{1}{2\pi} \oint_{\theta_1+\delta}^{\theta_2+\delta} d\theta \operatorname{Re}\big(\mathcal{F}\big(re^{i\theta}\big)\big), \tag{A.32}$$
$$\theta_1 \in [0, 2\pi],\ \theta_1 < \theta_2 \leqslant \theta_1 + 2\pi.$$

Conversely, the right-hand side of Eq. (A.30) *with $C = C^*$ and $d\Omega$ a finite nonnegative $m \times m$ matrix-valued measure on $\partial\mathbb{D}$ defines a Caratheodory matrix.*

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