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# Spectral decomposition and matrix-valued orthogonal polynomials

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**Abstract**

The relation between the spectral decomposition of a self-adjoint operator which is realizable as a higher order recurrence operator and matrix-valued orthogonal polynomials is investigated. A general construction of such operators from scalar-valued orthogonal polynomials is presented. Two examples of matrix-valued orthogonal polynomials with explicit orthogonality relations and three-term recurrence relation are presented, which both can be considered as $2 \times 2$-matrix-valued analogues of subfamilies of Askey–Wilson polynomials.


*Keywords:* Matrix-valued orthogonal polynomials; Spectral theory

## 1. Introduction

Matrix-valued orthogonal polynomials date back to the 1950s in the work of M.G. Krein; see e.g. references in [2,3]. More recently, matrix-valued orthogonal polynomials are studied from an analytic point of view. In particular, analogues of many classical results in the theory of ordinary

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(scalar-valued) orthogonal polynomials have been generalized to the situation of the matrix-valued orthogonal polynomials, such as e.g. the three-term recurrence relation, the spectral theorem (Favard), theorems of Markov, Blumenthal, etc.; see the overviews [2,3] and references given there. Many examples of the general theory of matrix-valued orthogonal polynomials are motivated by matrix-valued differential equations; see also [8]. Some of these examples are motivated from the well-known families of orthogonal polynomials in the Askey scheme [14], so the matrix-valued weight function is given by the scalar weight function times a suitable matrix-valued function. So in this case matrix-valued analogues of classical orthogonal polynomials, such as Jacobi, Laguerre and Hermite polynomials, are obtained. This theory so far gives matrix-valued analogues of hypergeometric orthogonal polynomials. Very little is known about matrix-valued analogues of $q$-orthogonal polynomials.

Another way of obtaining matrix-valued orthogonal polynomials is from group theory using matrix-valued spherical functions. An important case study has been given by Grünbaum, Pacharoni and Tirao [7], in which they obtain matrix-valued orthogonal polynomials from the symmetric pair $(SU(3), U(2))$ by studying eigenfunctions to invariant matrix-valued differential operators. Again these matrix-valued orthogonal polynomials are analogues of a subfamily of Jacobi polynomials. In [15,16] a different approach to such a group-theoretic approach has led to matrix-valued Chebyshev polynomials including relevant group theoretic interpretations of the construction, the three-term recurrence relation, weight function, differential equations, etc., using the symmetric pair $(SU(2) \times SU(2), SU(2))$. Again, in these cases the weight function resembles the corresponding scalar weight function times a suitable matrix-valued function. Again, no $q$-matrix-valued orthogonal polynomials have yet emerged from this approach.

In this paper, we discuss a new way to obtain matrix-valued orthogonal polynomials with an explicit three-term recurrence relation as well as explicit orthogonality relations. In the examples it is clear that the weight function is not of the form of a classical weight function times a matrix-valued function. The idea is to look for the spectral decomposition of a self-adjoint operator which can also be realized as a higher order recurrence operator. In order to motivate the construction, we first note that if we consider an operator which can be realized as a $2N + 1$-recurrence operator, the case $N = 0$ corresponds to eigenfunctions. The case $N = 1$ is the case of the $J$-matrix (or tridiagonalization) method, which is used in physics to determine the spectrum of certain physically relevant operators; see [10,12] and references given there. In [11] a more general method to obtain suitable tridiagonalizable operators is discussed. In this paper, we restrict ourselves to self-adjoint operators that can be realized as 5-term recurrence operators and for which we have an explicit spectral decomposition. We show in Theorem 2.1 how this gives rise to $2 \times 2$-matrix-valued orthogonal polynomials with an explicit (matrix-valued) three-term recurrence relation and explicit matrix-valued orthogonality relations. Because of computability reasons we stick to the $2\times 2$-case, but we expect that it is possible to extend to larger size matrices. In Section 4, we discuss an explicit example with an easy matrix-valued three-term recurrence relation, but an involved, but explicit, expression for the matrix-valued weight function. In Section 3, we discuss a general set-up, which is motivated by [11], and we work out a specific example in Section 3.2 which is related to the example in [11, Section 4]. This motivates us to view the family of matrix-valued orthogonal polynomials discussed in the example of Section 3.2 as analogues of a subfamily of Askey–Wilson polynomials.

As is well-known, it is very hard in general to obtain explicit expressions for the orthogonality measures or weights for orthogonal polynomials defined by a three-term recurrence relation. The cases of associated classical orthogonal polynomials (in the Askey-scheme [14]) amply demonstrate this point; see e.g. [13] for the case of two families of the associated Askey–Wilson polynomials. It is therefore remarkable that we can obtain in this setting an explicit, even though complicated, expression for both the weight function and the three-term recurrence relations for the $2 \times 2$-matrix-valued orthogonal polynomials in the examples considered in this paper. Moreover, to our best knowledge this is the first instance of matrix-valued orthogonal polynomials that can be considered as matrix-valued orthogonal polynomials in a yet-unknown (possible) $q$-scheme of matrix-valued orthogonal polynomials; see [14] for the scalar case. Note that we do not have explicit expressions for the $2 \times 2$-matrix-valued orthogonal polynomials, and it would be of interest to obtain such expressions for these polynomials in terms of (yet to be developed) matrix-valued basic hypergeometric series of higher type; see Tirao [19] for the matrix-valued analogue of the classical hypergeometric function.

## 2. Matrix-valued orthogonal polynomials from 5-term operators

In this section, we study the relation between a self-adjoint operator realizable as 5-term operator and corresponding $2 \times 2$-matrix-valued orthogonal polynomials. The three-term matrix-valued recurrence relations for these polynomials follow from this realization of the operator, whereas the orthogonality relations for these polynomials follow from the spectral decomposition of the operator. The precise relation is given in Theorem 2.1.

We assume that we have an operator $T$ on a Hilbert space $\mathcal{H}$ of functions. For $T$ we typically consider a second-order difference or differential operator. We assume that $T$ has the following properties;

(a) $T$ is (a possibly unbounded) self-adjoint operator on $\mathcal{H}$ (with domain $D$ in case $T$ is unbounded);
(b) there exists an orthonormal basis $\{f_n\}_{n=0}^{\infty}$ of $\mathcal{H}$ so that $f_n \in D$ in case $T$ is unbounded and so that there exist sequences $(a_n)_{n=0}^{\infty}$, $(b_n)_{n=0}^{\infty}$, $(c_n)_{n=0}^{\infty}$ of numbers with $a_n > 0$, $c_n \in \mathbb{R}$, for all $n \in \mathbb{N}$ so that

$$T\, f_n = a_n f_{n+2} + b_n f_{n+1} + c_n f_n + \overline{b_{n-1}} f_{n-1} + a_{n-2} f_{n-2}. \tag{2.1}$$

In (b) we follow the convention that $a_{-1} = a_{-2} = b_{-1} = 0$. We can relax in (2.1) to $a_n \neq 0$ and replace $a_{n-2}$ by $\overline{a_{n-2}}$, and the reduction to the form (2.1) follows by changing to a new orthonormal basis by multiplying by suitable phase factors.

Next we assume that we have a suitable spectral decomposition of $T$. We assume that the spectrum $\sigma(T)$ is simple or at most of multiplicity 2, and we leave it to the reader to extend to higher order spectra. We assume that the double spectrum is contained in $\Omega_2 \subset \sigma(T) \subset \mathbb{R}$, and the simple spectrum is contained in $\Omega_1 = \sigma(T) \setminus \Omega_2 \subset \mathbb{R}$. Consider functions $f$ defined on $\sigma(T) \subset \mathbb{R}$ so that $f|_{\Omega_1} \colon \Omega_1 \to \mathbb{C}$ and $f|_{\Omega_2} \colon \Omega_2 \to \mathbb{C}^2$. We let $\sigma$ be a Borel measure on $\Omega_1$ and $V\rho$ a $2 \times 2$-matrix-valued measure on $\Omega_2$ as in [2, Section 1.2], so $V \colon \Omega_2 \to \mathrm{M}_2(\mathbb{C})$ maps into the positive semi-definite matrices and $\rho$ is a positive Borel measure on $\Omega_2$. We assume $V$ is positive definite $\rho$-a.e. Next we consider the weighted Hilbert space $L^2(\mathcal{V})$ of such functions for which

$$\int_{\Omega_1} |f(\lambda)|^2 \, d\sigma(\lambda) + \int_{\Omega_2} f^*(\lambda) V(\lambda) f(\lambda) \, d\rho(\lambda) < \infty$$

and we obtain $L^2(\mathcal{V})$ by modding out by the functions of norm zero. The inner product is given by

$$\langle f, g \rangle = \int_{\Omega_1} f(\lambda) \overline{g(\lambda)} \, d\sigma(\lambda) + \int_{\Omega_2} g^*(\lambda) V(\lambda) f(\lambda) \, d\rho(\lambda).$$

The final assumption is then

(c) there exists a unitary map $U\colon \mathcal{H} \to L^2(\mathcal{V})$ so that $UT = MU$, where $M$ is the multiplication operator by $\lambda$ on $L^2(\mathcal{V})$.

Under the assumptions (a)–(c) we link the spectral measure to an orthogonality measure for matrix-valued orthogonal polynomials. Apply $U$ to the 5-term expression (2.1) for $T$ on the basis $\{f_n\}_{n=0}^{\infty}$, so that

$$\begin{aligned}\lambda(Uf_n)(\lambda) &= a_n(Uf_{n+2})(\lambda) + b_n(Uf_{n+1})(\lambda)\\ &\quad + c_n(Uf_n)(\lambda) + \overline{b_{n-1}}(Uf_{n-1})(\lambda) + a_{n-2}(Uf_{n-2})(\lambda)\end{aligned} \tag{2.2}$$

to be interpreted as an identity in $L^2(\mathcal{V})$. Restricted to $\Omega_1$ (2.2) is a scalar identity, and restricted to $\Omega_2$ the components of $Uf(\lambda) = (U_1 f(\lambda), U_2 f(\lambda))^t$ satisfy (2.2).

In general, a $2N + 1$-term recurrence relation can be solved using $N \times N$-matrix-valued orthogonal polynomials; see Durán and Van Assche [4]. Working out the details for $N = 2$, we see that we have to generate the $2 \times 2$-matrix-valued polynomials by

$$\begin{aligned}&\lambda P_n(\lambda) = A_n P_{n+1}(\lambda) + B_n P_n(\lambda) + A_{n-1}^* P_{n-1}(\lambda),\\ &A_n = \begin{pmatrix} a_{2n} & 0 \\ b_{2n+1} & a_{2n+1}\end{pmatrix}, \qquad B_n = \begin{pmatrix} c_{2n} & b_{2n} \\ \overline{b_{2n}} & c_{2n+1}\end{pmatrix}\end{aligned} \tag{2.3}$$

with initial conditions $P_{-1}(\lambda) = 0$ and $P_0(\lambda)$ is a constant non-singular matrix, which we take to be the identity, so $P_0(\lambda) = I$. Note that $A_n$ is a non-singular matrix and $B_n$ is a Hermitian matrix for all $n \in \mathbb{N}$. Then the $\mathbb{C}^2$-valued functions

$$\mathcal{U}_n(\lambda) = \begin{pmatrix} Uf_{2n}(\lambda) \\ Uf_{2n+1}(\lambda)\end{pmatrix}, \qquad \mathcal{U}_n^1(\lambda) = \begin{pmatrix} U_1 f_{2n}(\lambda) \\ U_1 f_{2n+1}(\lambda)\end{pmatrix}, \qquad \mathcal{U}_n^2(\lambda) = \begin{pmatrix} U_2 f_{2n}(\lambda) \\ U_2 f_{2n+1}(\lambda)\end{pmatrix}$$

satisfy (2.3) for vectors for $\lambda \in \Omega_1$ in the first case and for $\lambda \in \Omega_2$ in the last cases. Hence,

$$\mathcal{U}_n(\lambda) = P_n(\lambda)\mathcal{U}_0(\lambda), \qquad \mathcal{U}_n^1(\lambda) = P_n(\lambda)\mathcal{U}_0^1(\lambda), \qquad \mathcal{U}_n^2(\lambda) = P_n(\lambda)\mathcal{U}_0^2(\lambda), \tag{2.4}$$

where the first holds $\sigma$-a.e. and the last two hold $\rho$-a.e. We can now state the orthogonality relations for the matrix-valued orthogonal polynomials.

**Theorem 2.1.** *With the assumptions* (a)–(c) *as given above, the* $2\times 2$*-matrix-valued polynomials* $P_n$ *generated by* (2.3) *and* $P_{-1}(\lambda) = 0$, $P_0(\lambda) = I$ *satisfy*

$$\int_{\Omega_1} P_n(\lambda)\, W_1(\lambda)\, P_m(\lambda)^*\, d\sigma(\lambda) + \int_{\Omega_2} P_n(\lambda)\, W_2(\lambda)\, P_m(\lambda)^*\, d\rho(\lambda) = \delta_{nm} I$$

*where*

$$W_1(\lambda) = \begin{pmatrix} |Uf_0(\lambda)|^2 & Uf_0(\lambda)\overline{Uf_1(\lambda)} \\ \overline{Uf_0(\lambda)}Uf_1(\lambda) & |Uf_1(\lambda)|^2\end{pmatrix}, \quad \sigma\text{-a.e.}$$

*and*

$$W_2(\lambda) = \begin{pmatrix} \langle Uf_0(\lambda), Uf_0(\lambda)\rangle_{V(\lambda)} & \langle Uf_0(\lambda), Uf_1(\lambda)\rangle_{V(\lambda)} \\ \langle Uf_1(\lambda), Uf_0(\lambda)\rangle_{V(\lambda)} & \langle Uf_1(\lambda), Uf_1(\lambda)\rangle_{V(\lambda)}\end{pmatrix}, \quad \rho\text{-a.e.}$$

*where* $\langle x, y\rangle_{V(\lambda)} = x^* V(\lambda) y$.

Theorem 2.1 can be phrased more compactly, and then the generalization to self-adjoint operators $T$ realizable as higher order recurrence relations can be phrased compactly as well.

Since we stick to the situation with the assumptions (a), (b), (c), the multiplicity of $T$ cannot be higher than 2. Note that the matrices $W_1(\lambda)$ and $W_2(\lambda)$ are Gram matrices. In particular, $\det(W_1(\lambda)) = 0$ for all $\lambda$. So the weight matrix $W_1(\lambda)$ is semi-definite positive with eigenvalues 0 and $\operatorname{tr}(W_1(\lambda)) = |Uf_0(\lambda)|^2 + |Uf_1(\lambda)|^2 > 0$. Note that

$$\ker(W_1(\lambda)) = \mathbb{C}\begin{pmatrix} \overline{Uf_1(\lambda)} \\ -\overline{Uf_0(\lambda)} \end{pmatrix} = \begin{pmatrix} Uf_0(\lambda) \\ Uf_1(\lambda) \end{pmatrix}^{\perp},$$

$$\ker(W_1(\lambda) - \operatorname{tr}(W_1(\lambda))) = \mathbb{C}\begin{pmatrix} Uf_0(\lambda) \\ Uf_1(\lambda) \end{pmatrix}.$$

Moreover, $\det(W_2(\lambda)) = 0$ if and only if $Uf_0(\lambda)$ and $Uf_1(\lambda)$ are multiples of each other.

Denoting the integral in Theorem 2.1 as $\langle P_n, P_m\rangle_W$, we see that all the assumptions on the weights for matrix-valued orthogonal polynomials, as in e.g. [8, Section 2, p.453] are trivially satisfied, except for $\langle Q, Q\rangle_W = 0$ implies $Q = 0$ for a matrix-valued polynomial $Q$. Instead of using [8, Prop. 2.2] to conclude this, we can proceed by writing $Q = \sum_{k=1}^{n} C_k P_k$ for suitable matrices $C_k$, since the leading coefficient of $P_k$ is non-singular by (2.3). Then by Theorem 2.1 we have $\langle Q, Q\rangle_W = \sum_{k=0}^{n} C_k C_k^*$, so that $\langle Q, Q\rangle_W = 0$ implies $C_k = 0$ for all $k$, hence $Q = 0$.

**Proof.** Start using the unitarity

$$\begin{aligned}\delta_{nm}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} &= \begin{pmatrix} \langle f_{2n}, f_{2m}\rangle_{\mathcal{H}} & \langle f_{2n}, f_{2m+1}\rangle_{\mathcal{H}} \\ \langle f_{2n+1}, f_{2m}\rangle_{\mathcal{H}} & \langle f_{2n+1}, f_{2m+1}\rangle_{\mathcal{H}} \end{pmatrix} \\ &= \begin{pmatrix} \langle Uf_{2n}, Uf_{2m}\rangle_{L^2(\mathcal{V})} & \langle Uf_{2n}, Uf_{2m+1}\rangle_{L^2(\mathcal{V})} \\ \langle Uf_{2n+1}, Uf_{2m}\rangle_{L^2(\mathcal{V})} & \langle Uf_{2n+1}, Uf_{2m+1}\rangle_{L^2(\mathcal{V})} \end{pmatrix}. \qquad (2.5)\end{aligned}$$

Split each of the inner products on the right hand side of (2.5) as a sum over two integrals, one over $\Omega_1$ and the other over $\Omega_2$. First the integral over $\Omega_1$ equals

$$\begin{aligned}&\begin{pmatrix} \int_{\Omega_1} Uf_{2n}(\lambda)\overline{Uf_{2m}(\lambda)}\,d\sigma(\lambda) & \int_{\Omega_1} Uf_{2n}(\lambda)\overline{Uf_{2m+1}(\lambda)}\,d\sigma(\lambda) \\ \int_{\Omega_1} Uf_{2n+1}(\lambda)\overline{Uf_{2m}(\lambda)}\,d\sigma(\lambda) & \int_{\Omega_1} Uf_{2n+1}(\lambda)\overline{Uf_{2m+1}(\lambda)}\,d\sigma(\lambda) \end{pmatrix} \\ &= \int_{\Omega_1} \begin{pmatrix} Uf_{2n}(\lambda)\overline{Uf_{2m}(\lambda)} & Uf_{2n}(\lambda)\overline{Uf_{2m+1}(\lambda)} \\ Uf_{2n+1}(\lambda)\overline{Uf_{2m}(\lambda)} & Uf_{2n+1}(\lambda)\overline{Uf_{2m+1}(\lambda)} \end{pmatrix} d\sigma(\lambda) \\ &= \int_{\Omega_1} \begin{pmatrix} Uf_{2n}(\lambda) \\ Uf_{2n+1}(\lambda) \end{pmatrix} \begin{pmatrix} Uf_{2m}(\lambda) \\ Uf_{2m+1}(\lambda) \end{pmatrix}^* d\sigma(\lambda) \\ &= \int_{\Omega_1} P_n(\lambda) \begin{pmatrix} Uf_0(\lambda) \\ Uf_1(\lambda) \end{pmatrix} \begin{pmatrix} Uf_0(\lambda) \\ Uf_1(\lambda) \end{pmatrix}^* P_m(\lambda)^*\,d\sigma(\lambda) \\ &= \int_{\Omega_1} P_n(\lambda) W_1(\lambda) P_m(\lambda)^*\,d\sigma(\lambda), \qquad (2.6)\end{aligned}$$

where we have used (2.4). For the integral over $\Omega_2$ we write $Uf(\lambda) = (U_1 f(\lambda), U_2 f(\lambda))^t$ and $V(\lambda) = (v_{ij}(\lambda))_{i,j=1}^2$, so that the integral over $\Omega_2$ can be written as

$$\sum_{i,j=1}^{2} \int_{\Omega_2} \begin{pmatrix} U_j f_{2n}(\lambda) v_{ij}(\lambda)\overline{U_i f_{2m}(\lambda)} & U_j f_{2n}(\lambda) v_{ij}(\lambda)\overline{U_i f_{2m+1}(\lambda)} \\ U_j f_{2n+1}(\lambda) v_{ij}(\lambda)\overline{U_i f_{2m}(\lambda)} & U_j f_{2n+1}(\lambda) v_{ij}(\lambda)\overline{U_i f_{2m+1}(\lambda)} \end{pmatrix} d\rho(\lambda)$$

$$= \sum_{i,j=1}^{2} \int_{\Omega_2} \begin{pmatrix} U_j f_{2n}(\lambda) \\ U_j f_{2n+1}(\lambda) \end{pmatrix} \begin{pmatrix} U_i f_{2m}(\lambda) \\ U_i f_{2m+1}(\lambda) \end{pmatrix}^* v_{ij}(\lambda)\, d\rho(\lambda)$$

$$= \sum_{i,j=1}^{2} \int_{\Omega_2} P_n(\lambda) \begin{pmatrix} U_j f_0(\lambda) \\ U_j f_1(\lambda) \end{pmatrix} \begin{pmatrix} U_i f_0(\lambda) \\ U_i f_1(\lambda) \end{pmatrix}^* P_m(\lambda)^* v_{ij}(\lambda)\, d\rho(\lambda)$$

$$= \int_{\Omega_2} P_n(\lambda) W_2(\lambda) P_m(\lambda)^*\, d\rho(\lambda), \tag{2.7}$$

where we have used (2.4) again and with

$$W_2(\lambda) = \sum_{i,j=1}^{2} \begin{pmatrix} U_j f_0(\lambda) \\ U_j f_1(\lambda) \end{pmatrix} \begin{pmatrix} U_i f_0(\lambda) \\ U_i f_1(\lambda) \end{pmatrix}^* v_{ij}(\lambda)$$

$$= \sum_{i,j=1}^{2} v_{ij}(\lambda) \begin{pmatrix} U_j f_0(\lambda)\overline{U_i f_0(\lambda)} & U_j f_0(\lambda)\overline{U_i f_1(\lambda)} \\ U_j f_1(\lambda)\overline{U_i f_0(\lambda)} & U_j f_1(\lambda)\overline{U_i f_1(\lambda)} \end{pmatrix}$$

$$= \begin{pmatrix} (Uf_0(\lambda))^* V(\lambda) U f_0(\lambda) & (Uf_1(\lambda))^* V(\lambda) U f_0(\lambda) \\ (Uf_0(\lambda))^* V(\lambda) U f_1(\lambda) & (Uf_1(\lambda))^* V(\lambda) U f_1(\lambda) \end{pmatrix} \tag{2.8}$$

and putting (2.6) and (2.7), (2.8) into (2.5) proves the result. □

In case we additionally assume $T$ is bounded, so that the measures $\sigma$ and $\rho$ have compact support, the coefficients in (2.1) and (2.3) are bounded. In this case the corresponding moment problem is determinate, see [2, Theorem 2.11], and Theorem 2.1 gives the explicit expression for the weight function.

**Remark 2.2.** Assume that $\Omega_1 = \sigma(T)$ or $\Omega_2 = \emptyset$, so that $T$ has simple spectrum. Then

$$\mathcal{L}^2(W_1 d\sigma) = \left\{ f : \mathbb{R} \to \mathbb{C}^2 \;\middle|\; \int_{\mathbb{R}} f(\lambda)^* W_1(\lambda) f(\lambda)\, d\sigma(\lambda) < \infty \right\} \tag{2.9}$$

has the subspace of null-vectors

$$\mathcal{N} = \left\{ f \in \mathcal{L}^2(W_1 d\sigma) \;\middle|\; \int_{\mathbb{R}} f(\lambda)^* W_1(\lambda) f(\lambda)\, d\sigma(\lambda) = 0 \right\}$$

$$= \left\{ f \in \mathcal{L}^2(W_1 d\sigma) \;\middle|\; f(\lambda) = c(\lambda) \begin{pmatrix} \overline{Uf_1(\lambda)} \\ -\overline{Uf_0(\lambda)} \end{pmatrix} \sigma\text{-a.e.} \right\},$$

where $c$ is a scalar-valued function. In this case $L^2(\mathcal{V}) = \mathcal{L}^2(W_1 d\sigma)/\mathcal{N}$. Note that $\mathcal{U}_n : \mathbb{R} \to L^2(W_1 d\sigma)$ is completely determined by $Uf_0(\lambda)$, which is a restatement of $T$ having simple spectrum. From Theorem 2.1 we see that

$$\langle P_n(\cdot) v_1, P_m(\cdot) v_2 \rangle_{L^2(W_1 d\sigma)} = \delta_{nm} \langle v_1, v_2 \rangle$$

so that $\{P_n(\cdot) e_i\}_{i \in \{1,2\}, n \in \mathbb{N}}$ is linearly independent in $L^2(W_1 d\sigma)$ for any basis $\{e_1, e_2\}$ of $\mathbb{C}^2$.

## 3. A general class of examples

In [11] we have studied a general procedure to obtain self-adjoint tridiagonalizable operators, and in this section we show how to extend this to obtain self-adjoint operators which can be realized as 5-term recurrence. This brings us back to the situation of Section 2, hence leading to $2 \times 2$-matrix-valued orthogonal polynomials. Of course, we still need to obtain the spectral decomposition of such operators as well. We extend [11, Section 2] in Section 3.1 and we present an example of the construction using little $q$-Jacobi polynomials in Section 3.2. The analogue of the Jacobi polynomials is rather involved, in particular the spectral decomposition, and this is worked out in [6].

### *3.1. Self-adjoint penta-diagonalizable operators*

Let $\mu$ and $\nu$ be positive Borel measures with finite moments on the real line $\mathbb{R}$ so that $\mu$ is absolutely continuous with respect to $\nu$. Let $r = \frac{d\mu}{d\nu}$ be the Radon–Nikodym derivative, so $r \geq 0$. We assume that we have a (possibly unbounded) self-adjoint operator $L$ on $L^2(\mu)$ preserving the space of polynomials in $L^2(\mu)$ and the existence of an orthonormal basis $\{\Phi_n\}_{n\in\mathbb{N}}$ of $L^2(\mu)$ of polynomial eigenfunctions of $L$, so $L\Phi_n = \lambda_n \Phi_n$, $\lambda_n \in \mathbb{R}$. Moreover, we assume the existence of an orthonormal basis $\{\phi_n\}_{n=0}^{\infty}$ of polynomials of $L^2(\nu)$ such that for all $n \in \mathbb{N}$

$$\phi_n = \alpha_n \Phi_n + \beta_n \Phi_{n-1} + \gamma_n \Phi_{n-2}, \quad \alpha_n, \beta_n, \gamma_n \in \mathbb{R} \tag{3.1}$$

(with the convention $\beta_0 = \gamma_0 = \gamma_1 = 0$). We assume that the polynomials are dense in $L^2(\mu)$ and $L^2(\nu)$. Finally we assume that the Radon–Nikodym derivative $r$ is a polynomial, necessarily at most of degree 2 by (3.1). We denote by $M(r)$ and $M(x)$ the multiplication operator by $r$ and by $x$. From (3.1) we find $M(r)\Phi_n = \alpha_n\phi_n + \beta_{n+1}\phi_{n+1} + \gamma_{n+2}\phi_{n+2}$, so that the coefficients can also be calculated from Christoffel's formula; see [9, Theorem 2.7.1].

**Lemma 3.1.** *$T^\rho = M(r)(L + \rho)$, $\rho \in \mathbb{R}$, is a symmetric five-diagonal operator on $L^2(\nu)$ with respect to the orthonormal basis $\{\phi_n\}_{n=0}^{\infty}$;*

$$T^\rho \phi_n = a_n\phi_{n+2} + \tilde{b}_n\phi_{n+1} + \tilde{c}_n\phi_n + \tilde{b}_{n-1}\phi_{n-1} + a_{n-2}\phi_{n-2}$$

*where*

$$a_n = \alpha_n\gamma_{n+2}(\lambda_n + \rho), \qquad \tilde{b}_n = \alpha_n\beta_{n+1}(\lambda_n + \rho) + \beta_n(\lambda_{n-1} + \rho)\gamma_{n+1},$$
$$\tilde{c}_n = \alpha_n^2(\lambda_n + \rho) + \beta_n^2(\lambda_{n-1} + \rho) + \gamma_n^2(\lambda_{n-2} + \rho).$$

**Proof.** This is completely analogous to [11, Section 2.1]. Indeed,

$$\langle T^\rho\phi_n, \phi_m\rangle_{L^2(\nu)} = \langle M(r)(L + \rho)\phi_n, \phi_m\rangle_{L^2(\nu)} = \langle (L + \rho)\phi_n, \phi_m\rangle_{L^2(\mu)}$$

and next apply (3.1) and $\Phi_n$ being eigenfunctions of $L$. □

Since the orthonormal basis $\{\phi_n\}_{n=0}^{\infty}$ of $L^2(\nu)$ consists of polynomials, we have

$$x\phi_n(x) = \theta_n\phi_{n+1}(x) + \xi_n\phi_n(x) + \theta_{n-1}\phi_{n-1}(x), \tag{3.2}$$

for $\theta_n, \xi_n \in \mathbb{R}$, $\theta_n \neq 0$ for all $n \in \mathbb{N}$ and the convention $\theta_{-1} = 0$.

**Corollary 3.2.** *$T^{\rho,\tau} = M(r)(L + \rho) + \tau M(x)$, $\rho, \tau \in \mathbb{R}$, is a symmetric five-diagonal operator on $L^2(\nu)$ with respect to the orthonormal basis $\{\phi_n\}_{n=0}^{\infty}$;*

$$T^{\rho,\tau} \phi_n = a_n\phi_{n+2} + b_n\phi_{n+1} + c_n\phi_n + b_{n-1}\phi_{n-1} + a_{n-2}\phi_{n-2}$$

*where $b_n = \tilde{b}_n + \tau\theta_n$, $c_n = \tilde{c}_n + \tau\xi_n$, and the notation as in Lemma 3.1.*

Note that in case $L$ is a second-order differential or difference operator, then so is $T$. However, the coefficients of $T$ get more complicated and in order to carry through the programme of

Section 2 we need to be able to calculate the spectral decomposition of $T^{\rho,\tau}$ for suitable $\rho$, $\tau$ as well in another way.

**Remark 3.3.** It is clear that we can extend this to higher order recurrences. So if we assume $r$ to be a polynomial of degree $N$ and the recursion (3.1) to have $N+1$ terms, we end with a $2N+1$-recursion for the operator in Lemma 3.1 and Corollary 3.2.

### 3.2. *Example: case of little q-Jacobi polynomials*

We work out the details of the general programme of Section 3.1 for the case of the little $q$-Jacobi polynomials; cf. [11, Section 4]. Let, as usual, $0 < q < 1$, and we follow standard notation for basic hypergeometric series as in [5]; see also [9,14].

The little $q$-Jacobi polynomials are

$$p_n(x) = p_n(x; a, b; q) = {}_2\varphi_1\left(\begin{matrix} q^{-n},\ abq^{n+1} \\ aq \end{matrix}; q, qx\right) \tag{3.3}$$

with leading coefficient

$$l_n(a, b) = (-1)^n q^{-\frac{1}{2}n(n-1)} \frac{(abq^{n+1}; q)_n}{(aq; q)_n} \tag{3.4}$$

and for $0 < a < q^{-1}$, $b < q^{-1}$ the little $q$-Jacobi polynomials satisfy the orthogonality relations

$$\begin{aligned} &\sum_{k=0}^{\infty} p_n(q^k) p_m(q^k)\, w_k(a, b) = \delta_{nm} h_n(a, b), \\ &w_k(a, b) = (aq)^k \frac{(bq; q)_k\, (aq; q)_\infty}{(q; q)_k\, (abq^2; q)_\infty}, \\ &h_n(a, b) = \frac{1 - abq}{1 - abq^{2n+1}} \frac{(q, bq; q)_n}{(aq, abq; q)_n} (aq)^n \end{aligned} \tag{3.5}$$

normalizing $h_0(a, b) = 1$. The little $q$-Jacobi polynomials satisfy

$$\begin{aligned} &L^{(a,b)} p_n(\cdot; a, b; q) = \lambda_n\, p_n(\cdot; a, b; q), \\ &\lambda_n = \lambda_n(a, b) = q^{-n}(1 - q^n)(1 - abq^{n+1}) \\ &\left(L^{(a,b)} f\right)(x) = \frac{a(bqx - 1)}{x} (f(qx) - f(x)) + \frac{x - 1}{x} \left(f\left(\frac{x}{q}\right) - f(x)\right) \end{aligned} \tag{3.6}$$

In the context of Section 3.1 we take $L^2(\mu)$, respectively $L^2(\nu)$, to be the weighted $L^2$-space corresponding to the case $(aq, bq)$, respectively $(a, b)$. Note that

$$\begin{aligned} &w_k(aq, bq) = r(q^k) w_k(a, b), \qquad r(x) = K^{-1} x(1 - bqx), \\ &K = \frac{(1 - aq)(1 - bq)}{(1 - abq^2)(1 - abq^3)} > 0. \end{aligned} \tag{3.7}$$

In the context of Section 3.1 we see that we can give a five-term recursion formula for the operator $T^{\rho,\tau}$ defined by

$$\left(T^{\rho,\tau} f\right)(x) = \frac{aq}{K} (1 - bqx)(bq^2 x - 1)\, (f(qx) - f(x))$$

$$+\frac{1}{K}(1-bqx)(x-1)\,(f(x/q)-f(x))$$
$$+x\left(\frac{\rho}{K}(1-bqx)+\tau\right)f(x). \tag{3.8}$$

In order to apply the link to $2\times 2$-matrix-valued orthogonal polynomials we need to give the spectral decomposition of $T^{\rho,\tau}$ on $L^2(\nu)$ in another way.

**Proposition 3.4.** *Assume $q^{-1}>b>0$. The operator $T^{\rho,\tau}$ for $\rho=(1+q\sqrt{ab})(1+q^2\sqrt{ab})$, $\tau=\frac{1}{K}\left(q\sqrt{ab}(3+2q+bq^2)-bq(1+aq)\right)$ is a bounded self-adjoint operator with explicit spectral decomposition given by $U\colon L^2(\nu)\to L^2(\sigma)$ and $UT=MU$, where $M$ is multiplication by $2x/\left(\sqrt{aq}+(1-K)/\sqrt{aq}\right)$ and $\sigma$ is the normalized orthogonality measure for the continuous dual $q$-Hahn polynomials [14] with parameters $(A,B,C)=\left(\sqrt{qb},\sqrt{qb},q\sqrt{qb}\right)$, and $U$ is given by*

$$U\colon\frac{\delta_{q^k}}{\sqrt{w_k(a,b)}}\mapsto P_k\left(\cdot;\sqrt{qb},\sqrt{qb},q\sqrt{qb}\mid q\right)$$

*using the orthonormal polynomials on the right hand side.*

**Remark 3.5.** Recall that in [11] we can introduce an additional degree of freedom, which is not possible in Proposition 3.4. On the other hand, considering more generally second-order difference operators on $L^2(\nu)$ we can introduce an additional degree of freedom in the parameters of the continuous dual Hahn polynomials, but then we have no longer a nice explicit expression for the 5-term recurrence as in Section 2.

**Proof.** Let $V\colon\ell^2(\mathbb{N})\to L^2(\nu), e_k\mapsto\delta_{q^k}/\sqrt{w_k(a,b)}$, be the unitary operator identifying the Hilbert space $\ell^2(\mathbb{N})$ with standard orthonormal basis $\{e_k\}_{k\in\mathbb{N}}$ with the weighted $L^2(\nu)$ space for the little $q$-Jacobi polynomials. Let $J^{\rho,\tau}=V^*T^{\rho,\tau}V$; then

$$\left(\sqrt{aq}+\frac{1}{\sqrt{aq}}+\frac{-K}{\sqrt{aq}}\right)J^{\rho,\tau}e_k=\tilde{\alpha}_k e_{k+1}+\tilde{\beta}_k e_k+\tilde{\alpha}_{k-1}e_{k-1}$$
$$\tilde{\alpha}_k=(1-bq^{k+1})\sqrt{(1-q^{k+1})(1-bq^{k+1})},$$
$$\tilde{\beta}_k=q^k\left(bq\sqrt{aq}(1+q)+\frac{1}{\sqrt{aq}}(1+bq)-\frac{\rho}{\sqrt{aq}}+\frac{K\tau}{\sqrt{aq}}\right)$$
$$+q^{2k}\left(\frac{bq}{\sqrt{aq}}(\rho-1)-b^2q^3\sqrt{aq}\right).$$

Comparing this Jacobi operator to the three-term recurrence relation for the orthonormal continuous dual $q$-Hahn polynomials with parameters $(A,B,C)$ as in [14, Section 3.3], we see that we need $\{AB,AC,BC\}=\{bq,bq^2,bq^2\}$ to get the right expression for $\tilde{\alpha}_k$. Since $b\neq 0$ we get $A=B$, $C=qB$, and because of symmetry we obtain $(A,B,C)=\left(\sqrt{bq},\sqrt{bq},q\sqrt{bq}\right)$.

In order to match the value of $\beta_k$ to the orthonormal continuous $q$-Hahn polynomials with these parameters we require

$$bq\sqrt{aq}(1+q)+\frac{1}{\sqrt{aq}}(1+bq)-\frac{\rho}{\sqrt{aq}}+\frac{K\tau}{\sqrt{aq}}=A+B+C+ABC,$$
$$\frac{bq}{\sqrt{aq}}(\rho-1)-b^2q^3\sqrt{aq}=ABC(1+q^{-1})$$

which determines the choice for $\rho$ and $\tau$. Then $\left(\sqrt{aq}+\frac{1}{\sqrt{aq}}+\frac{-K}{\sqrt{aq}}\right)J^{\rho,\tau}$ has continuous spectrum $[-2,2]$, which gives the statement on $U$. □

Now that we have determined for which values of $(\rho,\tau)$ we have an explicit spectral decomposition in Proposition 3.4, we have to work out the coefficients in Corollary 3.2 in this case. We start with (3.1) in this case, or equivalently

$$p_n(x;a,b;q) = a_{n,n}p_n(x;aq,bq;q) + a_{n,n-1}p_{n-1}(x;aq,bq;q) + a_{n,n-2}p_{n-2}(x;aq,bq;q). \tag{3.9}$$

By comparing leading coefficients in (3.9) we obtain

$$a_{n,n} = \frac{(1-aq^{n+1})(1-abq^{n+1})(1-abq^{n+2})}{(1-aq)(1-abq^{2n+1})(1-abq^{2n+2})}. \tag{3.10}$$

Using the orthogonality and (3.7) we obtain

$$\begin{aligned} a_{n-2,n}h_{n-2}(aq,bq) &= \sum_{k=0}^{\infty} p_n(q^k;a,b;q)p_{n-2}(q^k;aq,bq;q)r(q^k)w_k(a,b) \\ &= \mathrm{lc}(r)\frac{l_{n-2}(aq,bq)}{l_n(a,b)}\,h_n(a,b) \end{aligned}$$

using the expansion of $p_{n-2}(\cdot;aq,bq;q)r(\cdot)$ in terms of little $q$-Jacobi polynomials with parameters $(a,b)$. This gives

$$a_{n,n-2} = \frac{-bq^{n+2}}{K}\frac{(1-q^{n-1})(1-q^n)(1-bq)(1-bq^n)}{(1-abq^2)(1-abq^3)(1-abq^{2n-1})(1-abq^{2n})}. \tag{3.11}$$

Note that (3.11) is not clear from the general connection coefficient formula for little $q$-Jacobi polynomials due to Andrews and Askey; see [5, Ex. 1.33]. The coefficient $a_{n,n-1}$ can be obtained by comparing coefficients of $x^{n-1}$ on both sides. This gives, after a straightforward calculation,

$$a_{n,n-1} = q^{1-n}\frac{(1-q^n)(1-abq^{n+1})}{(1-q)(1-aq)}\left(\frac{1-aq^n}{1-abq^{2n}} - \frac{1-aq^{n+1}}{1-abq^{2n+2}}\right) \tag{3.12}$$

Using the orthonormal version we find that in this example the coefficients in (3.1) are

$$\begin{aligned} \alpha_n &= \frac{q^{\frac{1}{2}n}(1-abq^{n+2})\sqrt{(1-abq^2)(1-abq^3)(1-abq^{n+1})(1-aq^{n+1})(1-bq^{n+1})}}{(1-abq^{2n+1})(1-abq^{2n+2})\sqrt{(1-abq^{n+4})(1-aq)(1-bq)}} \\ \beta_n &= q^{-\frac{1}{2}n}a^{-\frac{1}{2}}\frac{\sqrt{(1-abq^2)(1-abq^3)(1-q^n)(1-abq^{n+1})(1-abq^{n+2})}}{(1-q)\sqrt{(1-abq^{n+3})(1-aq)(1-bq)}} \\ &\quad\times\left(\frac{1-aq^n}{1-abq^{2n}} - \frac{1-aq^{n+1}}{1-abq^{2n+2}}\right) \\ \gamma_n &= \frac{-bq^{\frac{3}{2}n}}{aK}\frac{\sqrt{(1-q^{n-1})(1-q^n)(1-aq)(1-aq^n)(1-bq)(1-bq^n)}}{(1-abq^{2n-1})(1-abq^{2n})}. \end{aligned} \tag{3.13}$$

Finally, we need the three-term recurrence relation for the orthonormal little $q$-Jacobi polynomials, which corresponds to (3.2) with explicit values

$$\begin{aligned}\theta_n &= q^n \frac{\sqrt{aq(1-aq^{n+1})(1-bq^{n+1})(1-q^{n+1})(1-abq^{n+1})(1-abq^{n+2})}}{(1-abq^{2n+1})(1-abq^{2n+2})\sqrt{1-abq^{n+3}}}\\ \xi_n &= \frac{q^n\,(1-aq^{n+1})(1-abq^{n+1})}{(1-abq^{2n+1})(1-abq^{2n+2})} + \frac{aq^n\,(1-q^n)(1-bq^n)}{(1-abq^{2n})(1-abq^{2n+1})}.\end{aligned} \tag{3.14}$$

We next want to use Theorem 2.1 with the spectral decomposition $U$ given by Proposition 3.4, so that we assume the situation of Proposition 3.4. The spectrum is simple, so that $\Omega_2 = \emptyset$. It remains to calculate $U\phi_0$ and $U\phi_1$. Keeping track of normalization we have

$$\begin{aligned}(U\phi_n)(\cos t) = &\frac{\sqrt{a(aq,bq,q;q)_\infty}}{\sqrt{(abq^2;q)_\infty}}(bq^2;q)_\infty\\ &\times \sum_{k=0}^{\infty} \frac{q^{\frac{1}{2}k}\, p_n(q^k;a,b;q)}{(q,bq^2;q)_k}\, p_k\left(\cos t; \sqrt{qb}, \sqrt{qb}, q\sqrt{qb} \mid q\right)\end{aligned}$$

where we have used the standard notation, see [14], for the continuous dual $q$-Hahn polynomials. Using one of the standard generating functions, see [14, (3.3.15)], and $p_1(q^k;a,b;q) = 1 - q^k \frac{(1-abq)}{(1-aq)}$ we find

$$\begin{aligned}F_0(\cos t) &= (U\phi_0)(\cos t)\\ &= \frac{\sqrt{a(aq,bq,q;q)_\infty}}{\sqrt{(abq^2;q)_\infty}} \frac{(bq^2;q)_\infty \left(q\sqrt{b};q\right)_\infty}{\left(e^{it}\sqrt{q};q\right)_\infty}\\ &\quad\times {}_2\varphi_1\left(\begin{matrix}\sqrt{qb}e^{it}, q\sqrt{qb}e^{it}\\ bq^2\end{matrix}; q, \sqrt{q}e^{-it}\right)\\ F_1(\cos t) &= (U\phi_1)(\cos t) = \frac{\sqrt{a(aq,bq,q;q)_\infty}}{\sqrt{(abq^2;q)_\infty}}(bq^2;q)_\infty\\ &\quad\times\left(\frac{\left(q\sqrt{b};q\right)_\infty}{\left(e^{it}\sqrt{q};q\right)_\infty}\, {}_2\varphi_1\left(\begin{matrix}\sqrt{qb}e^{it}, q\sqrt{qb}e^{it}\\ bq^2\end{matrix}; q, \sqrt{q}e^{-it}\right)\right.\\ &\quad\left. - \frac{(1-abq)}{(1-aq)} \frac{\left(q^2\sqrt{b};q\right)_\infty}{\left(e^{it}q\sqrt{q};q\right)_\infty}\, {}_2\varphi_1\left(\begin{matrix}\sqrt{qb}e^{it}, q\sqrt{qb}e^{it}\\ bq^2\end{matrix}; q, q^{\frac{3}{2}}e^{-it}\right)\right).\end{aligned} \tag{3.15}$$

We summarize this situation in the following Proposition 3.6, using the explicit expression for the orthogonality measure $d\sigma$ of the continuous dual $q$-Hahn polynomials; see [14, Section 3.3].

**Proposition 3.6.** *Define the coefficients $a_n$, $b_n$ and $c_n$ as in Corollary 3.2 with the explicit values for $\alpha_n, \beta_n, \gamma_n$ as in (3.13), $\lambda_n$ as (3.6), $\theta_n, \xi_n$ as in (3.14) and $\rho$ and $\tau$ as in Proposition 3.4. The $2 \times 2$-matrix-valued orthogonal polynomials generated by the three-term recurrence relation (2.3) with initial conditions $P_{-1}(\lambda) = 0$, $P_0(\lambda) = I$ satisfy the orthogonality relations*

$$\int_0^\pi P_n(\cos t)W_1(\cos t)P_m(\cos t)^* \frac{(e^{\pm 2it};q)_\infty}{\left(\sqrt{qb}e^{\pm it},\sqrt{qb}e^{\pm it},q\sqrt{qb}e^{\pm it};q\right)_\infty}dt$$
$$= \frac{2\pi\delta_{nm}I}{(q,qb,q^2b,q^2b;q)_\infty}$$

*with*

$$W_1(\cos t) = \begin{pmatrix} |F_0(\cos t)|^2 & F_0(\cos t)F_1(\cos t) \\ F_0(\cos t)F_1(\cos t) & |F_1(\cos t)|^2 \end{pmatrix}.$$

In view of [11, Section 4] we view the $2 \times 2$-matrix-valued polynomials of Proposition 3.6 as matrix-valued analogue of (a subfamily) Askey–Wilson polynomials. The case $b \leq 0$ can be dealt with similarly, where the case $b = 0$ allows for additional degrees of freedom.

## 4. Example: spectral decomposition of an operator arising from quantum groups

In an influential paper [18] Koornwinder has introduced a special element $\rho_{\tau,\sigma}$ in the quantum $SU(2)$ group. In this context it is important to have the action of this element in an infinite dimensional representation as an explicit 5-term recurrence relation. On the other hand, the spectral decomposition of the corresponding operator has been solved in [17] exploiting the special case $\sigma \to \infty$ as an intermediate step. So the spectral decomposition of the 5-term recurrence is completely known, and by the set-up of Theorem 2.1 we obtain orthogonality relations for $2 \times 2$-matrix-valued orthogonal polynomials with explicit coefficients for the three-term recurrence relation. The resulting Proposition 4.1 describes the weight function explicitly in terms of ${}_2\varphi_1$-series.

Throughout this section we assume $\sigma, \tau \in \mathbb{R}$. In this case the Hilbert space is $\mathcal{H} = \ell^2(\mathbb{N})$ with standard orthonormal basis $\{f_n\}_{n=0}^\infty$. The operator $T$ corresponds to the operator $\pi_\phi(\rho_{\tau,\sigma})$ of [17, Section 6]; explicitly in the notation of (2.1) we have in this case

$$\begin{aligned} a_n &= \frac{1}{2}\sqrt{(1-q^{2n+2})(1-q^{2n+4})}, \\ b_n &= \frac{1}{2}iq^{n+1}\sqrt{1-q^{2n+2}}\left(e^{i\phi}(q^{-\sigma}-q^{\sigma}) + e^{-i\phi}(q^{-\tau}-q^{\tau})\right) \\ c_n &= q^{1+2n}\left(\cos(2\phi) - \frac{1}{2}(q^{-\sigma}-q^{\sigma})(q^{-\tau}-q^{\tau})\right). \end{aligned} \tag{4.1}$$

Note that $a_{-1} = a_{-2} = b_{-1} = 0$. Moreover, we have a symmetry $(\sigma,\tau,\phi) \leftrightarrow (\tau,\sigma,-\phi)$ and $(\sigma,\tau,\phi) \leftrightarrow (-\sigma,-\tau,\phi+\pi)$. So we can assume $\sigma \geq \tau$ and $\sigma \geq -\tau$. From [17, Section 6] we deduce that $T$ has absolutely continuous spectrum $[-1,1]$ of multiplicity 2 and discrete spectrum (possibly empty) of multiplicity 1 at $\Sigma_- \cup \Sigma_+$, where, using the notation $\mu(x) = \frac{1}{2}(x + x^{-1})$,

$$\begin{aligned} \Sigma_- &= \{\mu(-q^{1-\sigma-\tau+2k}) \mid k \in \mathbb{N},\ q^{1-\sigma-\tau+2k} > 1\} \\ \Sigma_+ &= \{\mu(q^{1-\sigma+\tau+2k}) \mid k \in \mathbb{N},\ q^{1-\sigma+\tau+2k} > 1\}. \end{aligned} \tag{4.2}$$

From [17, Section 6] we can read off $L^2(\mathcal{V})$. Assume that $\sigma + \tau \leq 1, \sigma - \tau \leq 1$, so that there is no discrete spectrum. Then $V$ is a diagonal matrix with the orthonormal measure for the Al-Salam–Chihara polynomials with parameters $(q^{1+\sigma-\tau}, -q^{1-\sigma-\tau})$, respectively

$(q^{1-\sigma+\tau}, -q^{1+\sigma+\tau})$, on the (1, 1)-entry, respectively the (2, 2)-entry. Explicitly, $f:[-1,1]\to\mathbb{C}^2$ is in $L^2(\mathcal{V})$ if

$$\int_0^\pi |f_1(\cos t)|^2 v_{11}(\cos t) + |f_2(\cos t)|^2 v_{22}(\cos t)\,dt < \infty \tag{4.3}$$

with

$$\begin{aligned} v_{11}(\cos t) &= v_{11}(\cos t; q^\tau, q^\sigma \mid q^2) \\ &= \frac{(q^2, -q^{2-2\tau}; q^2)_\infty (e^{\pm 2it}; q^2)_\infty}{2\pi(-q^{2\tau}; q^2)_\infty (q^{1+\sigma-\tau}e^{\pm it}, -q^{1-\sigma-\tau}e^{\pm it}; q^2)_\infty} \\ v_{22}(\cos t) &= v_{11}(\cos t; q^{-\tau}, q^{-\sigma} \mid q^2) \end{aligned} \tag{4.4}$$

and so $v_{12}(\cos t) = 0 = v_{21}(\cos t)$.

In order to write down the orthogonality measure for the $2\times 2$-matrix-valued orthogonal polynomials from Theorem 2.1 we need to calculate $Uf_k$ for $k = 0$ and $k = 1$. Expanding the standard orthonormal basis into the basis $\{w_m^\phi, u_m^\phi\}_{m=0}^\infty$ as in [17, p. 410], and applying $U$, which is given by $(\Lambda_1, \Lambda_2)$ as in [17, p. 411], we get after a straightforward calculation that $Uf_k(\lambda) = (U_1 f_k(\lambda), U_2 f_k(\lambda))^t$ with

$$\begin{aligned} U_1 f_k(\lambda) &= \sum_{m=0}^\infty \frac{i^{-k} e^{-ik\phi} p_k(-q^{2m})}{\| v^\phi_{-q^{2m}} \|} e^{2im\phi}\, h_m(\lambda; q^\tau, q^\sigma \mid q^2) \\ U_2 f_k(\lambda) &= \sum_{m=0}^\infty \frac{i^{-k} e^{-ik\phi} p_k(q^{2\tau+2m})}{\| v^\phi_{q^{2m+2\tau}} \|} e^{2im\phi}\, h_m(\lambda; q^{-\tau}, q^{-\sigma} \mid q^2) \end{aligned} \tag{4.5}$$

where we have used the notation as in [17, Prop. 5.2, p. 410] for the length of the vector, the Al-Salam–Carlitz polynomials $p_k(\cdot)$ and the Al-Salam–Chihara polynomials $h_m(\cdot)$.

For $k = 0$ we can use the generating function, see e.g. [14, (3.8.14)], directly to find

$$\begin{aligned} &F_{1,0}(\cos t; q^\tau, q^\sigma \mid q^2) = (U_1 f_0)(\cos t) \\ &\quad = \frac{1}{(-q^{2\tau}; q^2)_\infty^{\frac12} (q e^{i(t+2\phi)}; q^2)_\infty} {}_2\varphi_1\left( \begin{matrix} q^{1+\sigma-\tau}e^{it}, -q^{1-\sigma-\tau}e^{it} \\ -q^{2-2\tau} \end{matrix} ; q^2, q e^{i(2\phi - t)} \right) \end{aligned} \tag{4.6}$$

and $(U_2 f_0)(\cos t) = F_{1,0}(\cos t; q^{-\tau}, q^{-\sigma} \mid q^2)$ is obtained from $(U_1 f_0)(\cos t)$ by replacing $(\sigma,\tau)$ by $(-\sigma,-\tau)$.

For $k = 1$ we have to take a linear combination. First, note, in the notation of [17, Prop. 5.2], $p_1(x) = q^{-\tau}(1-q^2)^{-\frac12}(x + 1 - q^{2\tau})$, so that $p_1(-q^{2m}) = -p_1(q^{2m+2\tau})$. In particular, we obtain, also using [17, Prop. 5.2], that $(U_2 f_1)(\cos t)$ is obtained from $(U_1 f_1)(\cos t)$ by switching $(\sigma,\tau)$ to $(-\sigma,-\tau)$ and multiplying by $-1$. Using the same generating function for the Al-Salam–Chihara polynomials twice we obtain

$$\begin{aligned} &F_{1,1}(\cos t; q^\tau, q^\sigma \mid q^2) = (U_1 f_1)(\cos t) \\ &\quad = \frac{-i e^{-i\phi} q^{-\tau}}{\sqrt{(1-q^2)(-q^{2\tau}; q^2)_\infty}} \\ &\quad\quad \times \left( \frac{-1}{(q^3 e^{i(t+2\phi)}; q^2)_\infty} {}_2\varphi_1\left( \begin{matrix} q^{1+\sigma-\tau}e^{it}, -q^{1-\sigma-\tau}e^{it} \\ -q^{2-2\tau} \end{matrix} ; q^2, q^3 e^{i(2\phi - t)} \right) \right. \end{aligned}$$

$$+\frac{(1-q^{2\tau})}{(qe^{i(t+2\phi)};q^2)_\infty}{}_2\varphi_1\left(\begin{matrix} q^{1+\sigma-\tau}e^{it}, -q^{1-\sigma-\tau}e^{it} \\ -q^{2-2\tau}\end{matrix}; q^2, qe^{i(2\phi-t)}\right)\Bigg) \tag{4.7}$$

and $(U_2 f_1)(\cos t) = -F_{1,1}(\cos t; q^{-\tau}, q^{-\sigma} \mid q^2)$.

**Proposition 4.1.** *Consider the matrix-valued polynomials $P_n$ generated by (2.3) with initial conditions $P_{-1}(\lambda) = 0$, $P_0(\lambda) = I$ and where the entries of the matrices $A_n$ and $B_n$ are given by (4.1) with $\sigma \geq \tau, \sigma \geq -\tau$. Assume moreover $\sigma + \tau \leq 1, \sigma - \tau \leq 1$; then the matrix-valued polynomials $P_n$ satisfy the orthogonality relations*

$$\int_0^\pi P_n(\cos t) W_2(\cos t) P_m(\cos t)^* \, dt = \delta_{nm} I,$$

$$W_2(\cos t)_{11} = |F_{1,0}(\cos t; q^\tau, q^\sigma \mid q^2)|^2 v_{11}(\cos t; q^\tau, q^\sigma) + ((\sigma,\tau) \leftrightarrow (-\sigma,-\tau))$$

$$\begin{aligned} W_2(\cos t)_{21} &= W_2(\cos t)_{12} \\ &= F_{1,0}(\cos t; q^\tau, q^\sigma \mid q^2) v_{11}(\cos t; q^\tau, q^\sigma) F_{1,1}(\cos t; q^\tau, q^\sigma \mid q^2) \\ &\quad - ((\sigma,\tau) \leftrightarrow (-\sigma,-\tau)) \end{aligned}$$

$$W_2(\cos t)_{22} = |F_{1,1}(\cos t; q^\tau, q^\sigma \mid q^2)|^2 v_{11}(\cos t; q^\tau, q^\sigma) + ((\sigma,\tau) \leftrightarrow (-\sigma,-\tau))$$

*where the functions on the right hand side are defined by (4.6), (4.7) and the notation $((\sigma,\tau) \leftrightarrow (-\sigma,-\tau))$ means that we have to add the same term but with parameters $(\sigma,\tau)$ replaced by $(-\sigma,-\tau)$.*

Note that $W_2(\cos t)_{ij}$ is explicit as a sum of $i + j$ terms, each term being a product of two ${}_2\varphi_1$-series.

In case the assumption $\sigma + \tau \leq 1, \sigma - \tau \leq 1$ is dropped we obtain a finite discrete set of mass points in the orthogonality relations of Proposition 4.1, and the weight $W_1$ at these points can be calculated in the same way from Theorem 2.1. Alternatively, they can be obtained from writing the integral of Proposition 4.1 as a contour integral, and then shifting contours which leads to discrete masses at the poles with weights given in terms of residues analogous to the case of the Askey–Wilson polynomials; see [1].

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