SPECTRAL THEORY AND SPECIAL FUNCTIONS

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Abstract. A short introduction to the use of the spectral theorem for self-adjoint operators in the theory of special functions is given. As the first example, the spectral theorem is applied to Jacobi operators, i.e. tridiagonal operators, on $\ell^2(\mathbb{Z}_{\geq 0})$, leading to a proof of Favard's theorem stating that polynomials satisfying a three-term recurrence relation are orthogonal polynomials. We discuss the link to the moment problem. In the second example, the spectral theorem is applied to Jacobi operators on $\ell^2(\mathbb{Z})$. We discuss the theorem of Masson and Repka linking the deficiency indices of a Jacobi operator on $\ell^2(\mathbb{Z})$ to those of two Jacobi operators on $\ell^2(\mathbb{Z}_{\geq 0})$. For two examples of Jacobi operators on $\ell^2(\mathbb{Z})$, namely for the Meixner, respectively Meixner-Pollaczek, functions, related to the associated Meixner, respectively Meixner-Pollaczek, polynomials, and for the second order hypergeometric q-difference operator, we calculate the spectral measure explicitly. This gives explicit (generalised) orthogonality relations for hypergeometric and basic hypergeometric series.

Contents.

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1. Introduction

In these lecture notes we give a short introduction to the use of spectral theory in the theory of special functions. Conversely, special functions can be used to determine explicitly the spectral measures of explicit operators on a Hilbert space. The main ingredient from functional analysis that we are using is the spectral theorem, both for bounded and unbounded self-adjoint operators. We recall the main results of the theory in §2, hoping that the lecture notes become more self-contained in this way. For differential operators this is a very well-known subject, and one can consult e.g. Dunford and Schwartz [7].

In §3 we discuss Jacobi operators on $\ell^2(\mathbb{Z}_{\geq 0})$, and we present the link to orthogonal polynomials. Jacobi operators on $\ell^2(\mathbb{Z}_{\geq 0})$ are symmetric tridiagonal matrices, and the link to orthogonal polynomials goes via the three-term recurrence relation for orthogonal polynomials. We prove Favard's theorem in this setting, which is more or less equivalent to the spectral decomposition of the Jacobi operator involved. We first discuss the bounded case. Next we discuss the unbounded case and its link to the classical Hamburger moment problem. This is very classical, and it can be traced back to at least Stone's book [22]. This section is much inspired by Akhiezer [1], Berezanskiĭ [2, §7.1], Deift [5, Ch. 2] and Simon [20], and it can be viewed as an introduction to [1] and [20]. Especially, Simon's paper [20] is recommended for further reading on the subject. See also the recent book [23] by Teschl on Jacobi operators and the relation to non-linear lattices, see also Deift [5, Ch. 2] for the example of the Toda lattice. We recall this material on orthogonal polynomials and Jacobi operators, since it is an important ingredient in §4.

In §4 we discuss Jacobi operators on $\ell^2(\mathbb{Z})$, and we give the link between a Jacobi operator on $\ell^2(\mathbb{Z})$ to two Jacobi operators on $\ell^2(\mathbb{Z}_{\geq 0})$ due to Masson and Repka [17], stating in particular that the Jacobi operator on $\ell^2(\mathbb{Z})$ is (essentially) self-adjoint if and only if the two Jacobi operators on $\ell^2(\mathbb{Z}_{\geq 0})$ are (essentially) self-adjoint. Next we discuss the example for the Meixner functions in detail, following Masson and Repka [17], but the spectral measure is now completely worked out. In this case the spectral measure is purely discrete. If we restrict the Jacobi operator acting on $\ell^2(\mathbb{Z})$ to a Jacobi operator on $\ell^2(\mathbb{Z}_{\geq 0})$, we obtain the Jacobi operator for the associated Meixner polynomials. The case of the Meixner-Pollaczek functions is briefly considered. As another example we discuss the second order q-hypergeometric difference operator. In this example the spectral measure has a continuous part and a discrete part. Here we follow Kakehi [10] and [13, App. A]. These operators naturally occur in the representation theory of the Lie algebra $\mathfrak{su}(1,1)$, see [17], or of the quantised universal enveloping algebra $U_q(\mathfrak{su}(1,1))$, see [13]. Here the action of certain elements from the Lie algebra or the quantised universal enveloping algebra is tridiagonal, and one needs to obtain the spectral resolution. It is precisely this interpretation that leads to the limit transition discussed in (4.5.10).

However, from the point of view of special functions, the Hilbert space $\ell^2(\mathbb{Z})$ is generally not the appropriate Hilbert space to diagonalise a second-order q-difference operator L. For the two examples in §4 this works nicely, as shown there. In particular this is true for the ${}_2\varphi_1$-series, as shown in §4, see also [4] for another example. But for natural extensions of this situation to higher levels of special functions this Hilbert space is not good enough. We refer to [12] for the case of the second order q-difference operator having ${}_3\varphi_2$-series as eigenfunctions corresponding to the big q-Jacobi functions, and to [15] for the case of the second order q-difference operator having ${}_8W_7$-series as eigenfunctions corresponding to the Askey-Wilson functions. For more references and examples of spectral analysis of second order difference equations we refer to [14].

There is a huge amount of material on orthogonal polynomials, and there is a great number of good introductions to orthogonal polynomials, the moment problem, and the functional analysis used here. For orthogonal polynomials I have used [3], [5, Ch. 2] and [24]. For the moment problem there are the classics by Shohat and Tamarkin [19] and Stone [22], see also Akhiezer [1], Simon

[20] and, of course, Stieltjes's original paper [21] that triggered the whole subject. The spectral theorem can be found in many places, e.g. Dunford and Schwartz [7] and Rudin [18].

Naturally, there are many more instances of the use of functional analytic results that can be applied to special functions. As an example of a more qualitative question you can wonder how perturbation of the coefficients in the three-term recurrence relation for orthogonal polynomials affects the orthogonality measure, i.e. the spectral measure of the associated Jacobi operator. Results of this kind can be obtained by using perturbation results from functional analysis, see e.g. Dombrowski [6] and further references given there.

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2. The spectral theorem

2.1. Hilbert spaces and bounded operators.

(2.1.1) A vector space $\mathcal{H}$ over $\mathbb{C}$ is an inner product space if there exists a mapping $\langle\cdot,\cdot\rangle\colon \mathcal{H}\times\mathcal{H}\to\mathbb{C}$ such that for all $u,v,w\in\mathcal{H}$ and for all $a,b\in\mathbb{C}$ we have (i) $\langle av+bw,u\rangle = a\langle v,u\rangle + b\langle w,u\rangle$, (ii) $\langle u,v\rangle = \overline{\langle v,u\rangle}$, and (iii) $\langle v,v\rangle \geq 0$ and $\langle v,v\rangle = 0$ if and only if $v=0$. With the inner product we associate the norm $\|v\| = \|v\|_{\mathcal{H}} = \sqrt{\langle v,v\rangle}$, and the topology from the corresponding metric $d(u,v)=\|u-v\|$. The standard inequality is the Cauchy-Schwarz inequality; $|\langle u,v\rangle|\leq \|u\|\|v\|$. A Hilbert space $\mathcal{H}$ is a complete inner product space, i.e. for any Cauchy sequence $\{x_n\}_n$ in $\mathcal{H}$, i.e. $\forall\varepsilon>0\ \exists N\in\mathbb{N}$ such that for all $n,m\geq N$ $\|x_n-x_m\|<\varepsilon$, there exists an element $x\in\mathcal{H}$ such that x_n converges to x. In these notes all Hilbert spaces are separable, i.e. there exists a denumerable set of basis vectors.

(2.1.2) *Example.* $\ell^2(\mathbb{Z})$, the space of square summable sequences $\{a_k\}_{k\in\mathbb{Z}}$, and $\ell^2(\mathbb{Z}_{\geq 0})$, the space of square summable sequences $\{a_k\}_{k\in\mathbb{Z}_{\geq 0}}$, are Hilbert spaces. The inner product is given by $\langle\{a_k\},\{b_k\}\rangle = \sum_k a_k\overline{b_k}$. An orthonormal basis is given by the sequences e_k defined by $(e_k)_l=\delta_{k,l}$, so we identify $\{a_k\}$ with $\sum_k a_k e_k$.

(2.1.3) *Example.* We consider a positive Borel measure μ on the real line $\mathbb{R}$ such that all moments exist, i.e. $\int_{\mathbb{R}}|x|^m\,d\mu(x)<\infty$ for all $m\in\mathbb{Z}_{\geq 0}$. Without loss of generality we assume that μ is a probability measure, $\int_{\mathbb{R}} d\mu(x)=1$. By $L^2(\mu)$ we denote the space of square integrable functions on $\mathbb{R}$, i.e. $\int_{\mathbb{R}}|f(x)|^2\,d\mu(x)<\infty$. Then $L^2(\mu)$ is a Hilbert space (after identifying two functions f and g for which $\int_{\mathbb{R}}|f(x)-g(x)|^2\,d\mu(x)=0$) with respect to the inner product $\langle f,g\rangle = \int_{\mathbb{R}} f(x)\overline{g(x)}\,d\mu(x)$. In case μ is a finite sum of discrete Dirac measures, we find that $L^2(\mu)$ is finite dimensional.

(2.1.4) An operator T from a Hilbert space $\mathcal{H}$ into another Hilbert space $\mathcal{K}$ is linear if for all $u,v\in\mathcal{H}$ and for all $a,b\in\mathbb{C}$ we have $T(au+bv)=aT(u)+bT(v)$. An operator T is bounded if there exists a constant M such that $\|Tu\|_{\mathcal{K}}\leq M\|u\|_{\mathcal{H}}$ for all $u\in\mathcal{H}$. The smallest M for which this holds is the norm, denoted by $\|T\|$, of T. A bounded linear operator is continuous. The adjoint of a bounded linear operator $T\colon\mathcal{H}\to\mathcal{K}$ is a map $T^*\colon\mathcal{K}\to\mathcal{H}$ with $\langle Tu,v\rangle_{\mathcal{K}} = \langle u,T^*v\rangle_{\mathcal{H}}$. We call $T\colon\mathcal{H}\to\mathcal{H}$ self-adjoint if $T^*=T$. It is unitary if $T^*T=\mathbf{1}_{\mathcal{H}}$ and $TT^*=\mathbf{1}_{\mathcal{K}}$. A projection $P\colon\mathcal{H}\to\mathcal{H}$ is a linear map such that $P^2=P$.

(2.1.5) We are also interested in unbounded linear operators. In that case we denote $(T,\mathcal{D}(T))$, where $\mathcal{D}(T)$, the domain of T, is a linear subspace of $\mathcal{H}$ and $T\colon\mathcal{D}(T)\to\mathcal{H}$. Then T is densely defined if the closure of $\mathcal{D}(T)$ equals $\mathcal{H}$. All unbounded operators that we consider in these notes are densely defined. If the operator $(T-z)$, $z\in\mathbb{C}$, has an inverse $R(z)=(T-z)^{-1}$ which is densely defined and is bounded, so that $R(z)$, the resolvent operator, extends to a bounded linear operator on $\mathcal{H}$, then we call z a regular value. The set of all regular values is the resolvent set $\rho(T)$. The complement of the resolvent set $\rho(T)$ in $\mathbb{C}$ is the spectrum $\sigma(T)$ of T. The point spectrum is the subset of the spectrum for which $T-z$ is not one-to-one. In this case there exists a vector $v\in\mathcal{H}$ such that $(T-z)v=0$, and z is an eigenvalue. The continuous spectrum consists of the points $z\in\sigma(T)$ for which $T-z$ is one-to-one, but for which $(T-z)\mathcal{H}$ is dense in $\mathcal{H}$, but not equal to $\mathcal{H}$. The remaining part of the spectrum is the residual spectrum. For self-adjoint operators, both bounded and unbounded, see (2.3.3), the spectrum only consists of the discrete and continuous spectrum.

(2.1.6) For a bounded operator T the spectrum $\sigma(T)$ is a compact subset of the disk of radius $\|T\|$. Moreover, if T is self-adjoint, then $\sigma(T)\subset\mathbb{R}$, so that $\sigma(T)\subset[-\|T\|,\|T\|]$ and the spectrum consists of the point spectrum and the continuous spectrum.

2.2. **The spectral theorem for bounded self-adjoint operators.**

(2.2.1) A resolution of the identity, say E, of a Hilbert space $\mathcal{H}$ is a projection valued Borel measure on $\mathbb{R}$ such that for all Borel sets $A, B \subseteq \mathbb{R}$ we have (i) $E(A)$ is a self-adjoint projection, (ii) $E(A\cap B) = E(A)E(B)$, (iii) $E(\emptyset) = 0$, $E(\mathbb{R}) = \mathbf{1}_{\mathcal{H}}$, (iv) $A\cap B = \emptyset$ implies $E(A\cup B) = E(A)+E(B)$, and (v) for all $u, v \in \mathcal{H}$ the map $A \mapsto E_{u,v}(A) = \langle E(A)u, v\rangle$ is a complex Borel measure.

(2.2.2) A generalisation of the spectral theorem for matrices is the following theorem for bounded self-adjoint operators, see [7, §X.2], [18, §12.22].

Theorem. (Spectral theorem) *Let $T\colon \mathcal{H} \to \mathcal{H}$ be a bounded self-adjoint linear map, then there exists a unique resolution of the identity such that $T = \int_{\mathbb{R}} t\, dE(t)$, i.e. $\langle Tu, v\rangle = \int_{\mathbb{R}} t\, dE_{u,v}(t)$. Moreover, E is supported on the spectrum $\sigma(T)$, which is contained in the interval $[-\|T\|, \|T\|]$. Moreover, any of the spectral projections $E(A)$, $A \subset \mathbb{R}$ a Borel set, commutes with T.*

A more general theorem of this kind holds for normal operators, i.e. for those operators satisfying $T^*T = TT^*$.

(2.2.3) Using the spectral theorem we define for any continuous function f on the spectrum $\sigma(T)$ the operator $f(T)$ by $f(T) = \int_{\mathbb{R}} f(t)\, dE(t)$, i.e. $\langle f(T)u, v\rangle = \int_{\mathbb{R}} f(t)\, dE_{u,v}(t)$. Then $f(T)$ is bounded operator with norm equal to the supremum norm of f on the spectrum of T, i.e. $\|f(T)\| = \sup_{x\in\sigma(T)} |f(x)|$. This is known as the functional calculus for self-adjoint operators. In particular, for $z \in \rho(T)$ we see that $f\colon x \mapsto (x - z)^{-1}$ is continuous on the spectrum, and the corresponding operator is just the resolvent operator $R(z)$ as in (2.1.5). The functional calculus can be extended to measurable functions, but then $\|f(T)\| \leq \sup_{x\in\sigma(T)} |f(x)|$.

(2.2.4) The spectral measure can be obtained from the resolvent operators by the Stieltjes-Perron inversion formula, see [7, Thm. X.6.1].

Theorem. *The spectral measure of the open interval $(a, b) \subset \mathbb{R}$ is given by*

$$E_{u,v}\big((a, b)\big) = \lim_{\delta\downarrow 0} \lim_{\varepsilon\downarrow 0} \frac{1}{2\pi i} \int_{a+\delta}^{b-\delta} \langle R(x + i\varepsilon)u, v\rangle - \langle R(x - i\varepsilon)u, v\rangle\, dx.$$

The limit holds in the strong operator topology, i.e. $T_n x \to Tx$ for all $x \in \mathcal{H}$.

2.3. **Unbounded self-adjoint operators.**

(2.3.1) Let $(T, \mathcal{D}(T))$, with $\mathcal{D}(T)$ the domain of T, be a densely defined unbounded operator on $\mathcal{H}$, see (2.1.5). We can now define the adjoint operator $(T^*, \mathcal{D}(T^*))$ as follows. First define

$$\mathcal{D}(T^*) = \{v \in \mathcal{H} \mid u \mapsto \langle Tu, v\rangle \text{ is continuous on } \mathcal{D}(T)\}.$$

By the density of $\mathcal{D}(T)$ the map $u \mapsto \langle Tu, v\rangle$ for $v \in \mathcal{D}(T^*)$ extends to a continuous linear functional $\omega\colon \mathcal{H} \to \mathbb{C}$, and by the Riesz representation theorem there exists a unique $w \in \mathcal{H}$ such that $\omega(u) = \langle u, w\rangle$ for all $u \in \mathcal{H}$. Now the adjoint T^* is defined by $T^*v = w$, so that

$$\langle Tu, v\rangle = \langle u, T^*v\rangle \qquad \forall\, u \in \mathcal{D}(T), \forall\, v \in \mathcal{D}(T^*).$$

(2.3.2) If T and S are unbounded operators on $\mathcal{H}$, then T extends S, notation $S \subset T$, if $\mathcal{D}(S) \subset \mathcal{D}(T)$ and $Sv = Tv$ for all $v \in \mathcal{D}(S)$. Two unbounded operators S and T are equal, $S = T$, if $S \subset T$ and $T \subset S$, or S and T have the same domain and act in the same way. In terms of the graph

$$\mathcal{G}(T) = \{(u, Tu) \mid u \in \mathcal{D}(T)\} \subset \mathcal{H} \times \mathcal{H}$$

we see that $S \subset T$ if and only if $\mathcal{G}(S) \subset \mathcal{G}(T)$. An operator T is closed if its graph is closed in the product topology of $\mathcal{H} \times \mathcal{H}$. The adjoint of a densely defined operator is a closed operator, since the graph of the adjoint is given as

$$\mathcal{G}(T^*) = \{(-u, Tu) \mid u \in \mathcal{D}(T)\}^{\perp},$$

for the inner product $\langle (u,v),(x,y)\rangle = \langle u,x\rangle + \langle v,y\rangle$ on $\mathcal{H}\times\mathcal{H}$, see [18, 13.8].

(2.3.3) A densely defined operator is symmetric if $T\subset T^*$, or, using the definition in (2.3.1),

$$\langle Tu,v\rangle = \langle u,Tv\rangle, \qquad \forall\ u,v\in\mathcal{D}(T).$$

A densely defined operator is self-adjoint if $T=T^*$, so that a self-adjoint operator is closed. The spectrum of an unbounded self-adjoint operator is contained in $\mathbb{R}$. Note that $\mathcal{D}(T)\subset\mathcal{D}(T^*)$, so that $\mathcal{D}(T^*)$ is a dense subspace and taking the adjoint once more gives $(T^{**},\mathcal{D}(T^{**}))$ as the minimal closed extension of $(T,\mathcal{D}(T))$, i.e. any densely defined symmetric operator has a closed extension. We have $T\subset T^{**}\subset T^*$. We say that the densely defined symmetric operator is essentially self-adjoint if its closure is self-adjoint, i.e. if $T\subset T^{**}=T^*$.

(2.3.4) In general, a densely defined symmetric operator T might not have self-adjoint extensions. This can be measured by the deficiency indices. Define for $z\in\mathbb{C}\backslash\mathbb{R}$ the eigenspace

$$N_z = \{v\in\mathcal{D}(T^*)\mid T^*v = z\,v\}.$$

Then $\dim N_z$ is constant for $\Im z>0$ and for $\Im z<0$, [7, Thm. XII.4.19], and we put $n_+=\dim N_i$ and $n_-=\dim N_{-i}$. The pair (n_+,n_-) are the deficiency indices for the densely defined symmetric operator T. Note that if T commutes with complex conjugation of the Hilbert space $\mathcal{H}$ then we automatically have $n_+=n_-$. Note furthermore that if T is self-adjoint then $n_+=n_-=0$, since a self-adjoint operator cannot have non-real eigenvalues. Now the following holds, see [7, §XII.4].

Proposition. *Let $(T,\mathcal{D}(T))$ be a densely defined symmetric operator.*
(i) *$\mathcal{D}(T^*)=\mathcal{D}(T^{**})\oplus N_i\oplus N_{-i}$, as an orthogonal direct sum with respect to the graph norm for T^* from $\langle u,v\rangle_{T^*}=\langle u,v\rangle+\langle T^*u,T^*v\rangle$. As a direct sum, $\mathcal{D}(T^*)=\mathcal{D}(T^{**})+N_z+N_{\bar z}$ for general $z\in\mathbb{C}\backslash\mathbb{R}$.*
(ii) *Let U be an isometric bijection $U\colon N_i\to N_{-i}$ and define $(S,\mathcal{D}(S))$ by*

$$\mathcal{D}(S)=\{u+v+Uv\mid u\in\mathcal{D}(T^{**}),\ v\in N_i\},\qquad Sw=T^*w,$$

then $(S,\mathcal{D}(S))$ is a self-adjoint extension of $(T,\mathcal{D}(T))$, and every self-adjoint extension of T arises in this way.

In particular, T has self-adjoint extensions if and only if the deficiency indices are equal; $n_+=n_-$. T^{**} is a closed symmetric extension of T. We can also characterise the domains of the self-adjoint extensions of T using the sesquilinear form

$$B(u,v)=\langle T^*u,v\rangle-\langle u,T^*v\rangle,\qquad u,v\in\mathcal{D}(T^*),$$

then $\mathcal{D}(S)=\{u\in\mathcal{D}(T^*)\mid B(u,v)=0,\ \forall v\in\mathcal{D}(S)\}$.

2.4. The spectral theorem for unbounded self-adjoint operators.

(2.4.1) With all the preparations of the previous subsection the Spectral Theorem (2.2.2) goes through in the unbounded setting, see [7, §XII.4], [18, Ch. 13].

Theorem. (Spectral theorem) *Let $T\colon\mathcal{D}(T)\to\mathcal{H}$ be an unbounded self-adjoint linear map, then there exists a unique resolution of the identity such that $T=\int_{\mathbb{R}} t\,dE(t)$, i.e. $\langle Tu,v\rangle=\int_{\mathbb{R}} t\,dE_{u,v}(t)$ for $u\in\mathcal{D}(T)$, $v\in\mathcal{H}$. Moreover, E is supported on the spectrum $\sigma(T)$, which is contained in $\mathbb{R}$. For any bounded operator S that satisfies $ST\subset TS$ we have $E(A)S=SE(A)$, $A\subset\mathbb{R}$ a Borel set. Moreover, the Stieltjes-Perron inversion formula* (2.2.4) *remains valid;*

$$E_{u,v}\big((a,b)\big)=\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{a+\delta}^{b-\delta}\langle R(x+i\varepsilon)u,v\rangle-\langle R(x-i\varepsilon)u,v\rangle\,dx.$$

(2.4.2) As in (2.2.3) we can now define $f(T)$ for any measurable function f by

$$\langle f(T)u, v\rangle = \int_{\mathbb{R}} f(t)\, dE_{u,v}(t), \qquad u \in \mathcal{D}(f(T)),\ v \in \mathcal{H},$$

where $\mathcal{D}(f(T)) = \{u \in \mathcal{H} \mid \int_{\mathbb{R}} |f(t)|^2\, dE_{u,u}(t) < \infty\}$ is the domain of $f(T)$. This makes $f(T)$ into a densely defined closed operator. In particular, if $f \in L^\infty(\mathbb{R})$, then $f(T)$ is a continuous operator, by the closed graph theorem. This in particular applies to $f(x) = (x-z)^{-1}$, $z \in \rho(T)$, which gives the resolvent operator.

3. Orthogonal polynomials and Jacobi operators

3.1. Orthogonal polynomials.

(3.1.1) Consider the Hilbert space $L^2(\mu)$ as in Example (2.1.3). Assume that all moments exist, so that all polynomials are integrable. In applying the Gram-Schmidt orthogonalisation process to the sequence $\{1, x, x^2, x^3, \dots\}$ we may end up in one of the following situations: (a) the polynomials are linearly dependent in $L^2(\mu)$, or (b) the polynomials are linearly independent in $L^2(\mu)$. In case (a) it follows that there is a non-zero polynomial p such that $\int_{\mathbb{R}} |p(x)|^2\, d\mu(x) = 0$. This implies that μ is a finite sum of Dirac measures at the zeros of p. From now on we exclude this case, but the reader may consider this case him/herself. In case (b) we end up with a set of orthonormal polynomials as in the following definition.

Definition. *A sequence of polynomials $\{p_n\}_{n=0}^\infty$ with $\deg(p_n) = n$ is a set of orthonormal polynomials with respect to μ if $\int_{\mathbb{R}} p_n(x)p_m(x)\, d\mu(x) = \delta_{n,m}$.*

Note that the polynomials p_n are real-valued for $x \in \mathbb{R}$, so that its coefficients are real. Moreover, from the Gram-Schmidt process it follows that the leading coefficient is positive.

(3.1.2) Note that only the moments $m_k = \int_{\mathbb{R}} x^k\, d\mu(x)$ of μ play a role in the orthogonalisation process. The Stieltjes transform of the measure μ defined by $w(z) = \int_{\mathbb{R}} (x-z)^{-1}\, d\mu(x)$, $z \in \mathbb{C}\backslash\mathbb{R}$, can be considered as a generating function for the moments of μ. Indeed, formally

$$w(z) = \frac{-1}{z}\int_{\mathbb{R}} \frac{1}{1-x/z}\, d\mu(x) = \frac{-1}{z}\sum_{k=0}^\infty \int_{\mathbb{R}} \big(\frac{x}{z}\big)^k\, d\mu(x) = -\sum_{k=0}^\infty \frac{m_k}{z^{k+1}}. \tag{3.1}$$

In case $\mathrm{supp}(\mu) \subseteq [-A, A]$ we see that $|m_k| \leq 2A^k$ implying that the series in (3.1) is absolutely convergent for $|z| > A$. In this case we see that the Stieltjes transform $w(z)$ of μ is completely determined by the moments of μ. In general, this expansion has to be interpreted as an asymptotic expansion of the Stieltjes transform $w(z)$ as $|z| \to \infty$. We now give a proof of the Stieltjes inversion formula, cf. (2.2.4).

Proposition. *Let μ be a probability measure with finite moments, and let $w(z) = \int_{\mathbb{R}} (x-z)^{-1}\, d\mu(x)$ be its Stieltjes transform, then*

$$\lim_{\varepsilon \downarrow 0} \frac{1}{\pi}\int_a^b \Im\big(w(x+i\varepsilon)\big)\, dx = \mu\big((a,b)\big) + \frac{1}{2}\mu(\{a\}) + \frac{1}{2}\mu(\{b\}).$$

Proof. Observe that

$$\begin{aligned} 2i\Im\big(w(z)\big) = w(z) - \overline{w(z)} = w(z) - w(\bar z) &= \int_{\mathbb{R}} \frac{1}{x-z} - \frac{1}{x-\bar z}\, d\mu(x) \\ &= \int_{\mathbb{R}} \frac{z-\bar z}{|x-z|^2}\, d\mu(x) = 2i\int_{\mathbb{R}} \frac{\Im z}{|x-z|^2}\, d\mu(x), \end{aligned}$$

so that

$$\Im\big(w(x+i\varepsilon)\big) = \int_{\mathbb{R}} \frac{\varepsilon}{|s-(x+i\varepsilon)|^2}\, d\mu(s) = \int_{\mathbb{R}} \frac{\varepsilon}{(s-x)^2+\varepsilon^2}\, d\mu(s).$$

Integrating this expression and interchanging integration, which is allowed since the integrand is positive, gives

$$\int_a^b \Im\big(w(x+i\varepsilon)\big)\, dx = \int_{\mathbb{R}}\int_a^b \frac{\varepsilon}{(s-x)^2+\varepsilon^2}\, dx\, d\mu(s). \tag{3.2}$$

The inner integration can be carried out easily;

$$\chi_\varepsilon(s) = \int_a^b \frac{\varepsilon}{(s-x)^2+\varepsilon^2}\, dx = \int_{(a-s)/\varepsilon}^{(b-s)/\varepsilon} \frac{1}{1+y^2}\, dy = \arctan y\Big|_{(a-s)/\varepsilon}^{(b-s)/\varepsilon}$$

by $y = (x-s)/\varepsilon$. It follows that $0 \le \chi_\varepsilon(s) \le \pi$, and

$$\lim_{\varepsilon\downarrow 0} \chi_\varepsilon(s) = \begin{cases} \pi, & \text{for } a < s < b, \\ \frac{1}{2}\pi, & \text{for } s = a \text{ or } s = b. \end{cases}$$

It suffices to show that we can interchange integration and the limit $\varepsilon \downarrow 0$ in (3.2). This follows from Lebesgue's dominated convergence theorem since μ is a probability measure and $0 \le \chi_\varepsilon(s) \le \pi$. □

As a corollary to the proof we get, cf. (2.2.4), (2.4.1),

$$\lim_{\varepsilon\downarrow 0}\lim_{\delta\downarrow 0} \frac{1}{\pi}\int_{a+\delta}^{b-\delta} \Im\big(w(x+i\varepsilon)\big)\,dx = \mu\big((a,b)\big).$$

We need the following extension of this inversion formula in (3.3.10). For a polynomial p with real coefficients we have

$$\lim_{\varepsilon\downarrow 0} \frac{1}{\pi}\int_a^b \Im\big(p(x+i\varepsilon)w(x+i\varepsilon)\big)\,dx = \int_{(a,b)} p(x)\,d\mu(x) + \frac{1}{2}p(a)\mu(\{a\}) + \frac{1}{2}p(b)\mu(\{b\}). \tag{3.3}$$

We indicate how the proof of the proposition can be extended to obtain (3.3). Start with

$$\Im\big(p(x+i\varepsilon)w(x+i\varepsilon)\big) = \int_{\mathbb{R}} \frac{(s-x)\Im\big(p(x+i\varepsilon)\big) + \varepsilon\Re\big(p(x-i\varepsilon)\big)}{(s-x)^2+\varepsilon^2}\,d\mu(s).$$

Integrate this expression with respect to x and interchange summations, which is justified since $\Im\big(p(x+i\varepsilon)\big)$ and $\Re\big(p(x-i\varepsilon)\big)$ are bounded on (a,b). This time we have to evaluate two integrals. The first integral

$$\int_a^b \frac{(s-x)\Im\big(p(x+i\varepsilon)\big)}{(s-x)^2+\varepsilon^2}\,dx = \int_{(a-s)/\varepsilon}^{(b-s)/\varepsilon} \frac{-y\,\Im\big(p(\varepsilon y+s+i\varepsilon)\big)}{y^2+1}\,dy$$

can be estimated, using $\Im\big(p(x+i\varepsilon)\big) = \mathcal{O}(\varepsilon)$ uniformly on $[a,b]$, by

$$\varepsilon\,M \int_{(a-s)/\varepsilon}^{(b-s)/\varepsilon} \frac{y}{y^2+1}\,dy = \varepsilon M \ln\sqrt{y^2+1}\Big|_{(a-s)/\varepsilon}^{(b-s)/\varepsilon}.$$

This term tends to zero independently of a, b and s, since $\varepsilon\ln(\frac{A^2}{\varepsilon^2}+1) = -2\varepsilon\ln\varepsilon + \varepsilon\ln(A^2+\varepsilon^2)$ which can be estimated by $\mathcal{O}(\varepsilon\ln\varepsilon)$ with a constant independent of A. The other integral can be dealt with as in the proof of the proposition. Next Lebesgue's dominated convergence theorem can be applied and (3.3) follows.

(3.1.3) The following theorem describes the fundamental property of orthogonal polynomials in these notes.

Theorem. (Three term recurrence relation) *Let $\{p_k\}_{k=0}^\infty$ be a set of orthonormal polynomials in $L^2(\mu)$, then there exist sequences $\{a_k\}_{k=0}^\infty$, $\{b_k\}_{k=0}^\infty$, with $a_k > 0$ and $b_k \in \mathbb{R}$, such that*

$$x\,p_k(x) = a_k p_{k+1}(x) + b_k p_k(x) + a_{k-1}p_{k-1}(x), \qquad k \ge 1, \tag{3.4}$$

$$x\,p_0(x) = a_0 p_1(x) + b_0 p_0(x). \tag{3.5}$$

Moreover, if μ is compactly supported, then the coefficients a_k and b_k are bounded.

Note that (3.4), (3.5) together with the initial condition $p_0(x) = 1$ completely determine the polynomials $p_k(x)$ for all $k \in \mathbb{N}$.

Proof. The degree of $xp_k(x)$ is $k+1$, so there exist constants c_i such that $x\,p_k(x) = \sum_{i=0}^{k+1} c_i\,p_i(x)$. By the orthonormality properties of p_k it follows that

$$c_i = \int_{\mathbb{R}} p_i(x)xp_k(x)\,d\mu(x).$$

Since the degree of $xp_i(x)$ is $i+1$, we see that $c_i = 0$ for $i+1 < k$. Then

$$b_k = c_k = \int_{\mathbb{R}} x\big(p_k(x)\big)^2\, d\mu(x) \in \mathbb{R}.$$

Moreover, $c_{k+1} = \int_{\mathbb{R}} p_{k+1}(x) x p_k(x)\, d\mu(x)$ and $c_{k-1} = \int_{\mathbb{R}} p_{k-1}(x) x p_k(x)\, d\mu(x)$ display the required structure for the other coefficients. The positivity of a_k follows by considering the leading coefficient.

For the last statement we observe that

$$\begin{aligned}|a_k| = \Big|\int_{\mathbb{R}} x p_{k+1}(x) p_k(x)\, d\mu(x)\Big| &\leq \int_{\mathbb{R}} |p_{k+1}(x)||p_k(x)|\, d\mu(x) \sup_{x\in\mathrm{supp}(\mu)} |x| \\ &\leq \|p_{k+1}\|_{L^2(\mu)} \|p_k\|_{L^2(\mu)} \sup_{x\in\mathrm{supp}(\mu)} |x| = \sup_{x\in\mathrm{supp}(\mu)} |x| < \infty,\end{aligned}$$

since $\|p_k\|_{L^2(\mu)} = 1$ and $\mathrm{supp}(\mu)$ is compact. In the second inequality we have used the Cauchy-Schwarz inequality (2.1.1). Similarly,

$$|b_k| \leq \|p_k\|^2_{L^2(\mu)} \sup_{x\in\mathrm{supp}(\mu)} |x| = \sup_{x\in\mathrm{supp}(\mu)} |x| < \infty$$

gives the estimate on the coefficients b_k. □

(3.1.4) We observed that (3.4) and (3.5) together with an initial condition for the degree zero component completely determines a solution for the recurrence (3.4), (3.5). We can also generate solutions of (3.4) by specifying the initial values for $k = 0$ and $k = 1$. From now on we let $r_k(x)$ be the sequence of polynomials generated by (3.4) subject to the initial conditions $r_0(x) = 0$ and $r_1(x) = a_0^{-1}$. Then r_k is a polynomial of degree $k-1$, and (3.5) is not valid. The polynomials $\{r_k\}_{k=0}^{\infty}$ are the associated polynomials.

Lemma. *The associated polynomial r_k is given by*

$$r_k(x) = \int_{\mathbb{R}} \frac{p_k(x) - p_k(y)}{x-y}\, d\mu(y).$$

Proof. It suffices to show that the right hand side, denoted temporarily by $q_k(x)$, satisfies the recurrence (3.4) together with the initial conditions. Using Theorem (3.1.3) for $p_k(x)$ and the definition of $q_k(x)$ we obtain

$$\begin{aligned} x\, q_k(x) =& a_k q_{k+1}(x) + b_k q_k(x) + a_{k-1} q_{k-1} \\ &+ \int_{\mathbb{R}} \frac{a_k p_{k+1}(y) + b_k p_k(y) + a_{k-1} p_{k-1}(y) - x p_k(y)}{x-y}\, d\mu(y).\end{aligned}$$

Using Theorem (3.1.3) again shows that the integral equals $-\int_{\mathbb{R}} p_k(y)\, d\mu(y)$, which is zero for $k \geq 1$ and -1 for $k = 0$ by the orthogonality properties. Hence, (3.4) is satisfied. Using $p_0(x) = 1$ we find $q_0(x) = 0$ and using $p_1(x) = a_0^{-1}(x - b_0)$ gives $q_1(x) = a_0^{-1}$. □

Considering

$$\int_{\mathbb{R}} \frac{p_k(x)}{x-z}\, d\mu(x) = \int_{\mathbb{R}} \frac{p_k(x) - p_k(z)}{x-z}\, d\mu(x) + p_k(z) \int_{\mathbb{R}} \frac{1}{x-z}\, d\mu(x)$$

immediately proves the following corollary.

Corollary. *Let $z \in \mathbb{C}\backslash\mathbb{R}$ be fixed. The k-th coefficient with respect to the orthonormal set $\{p_k\}_{k=0}^{\infty}$ in $L^2(\mu)$ of $x \mapsto (x-z)^{-1}$ is given by $w(z)p_k(z) + r_k(z)$. Hence,*

$$\sum_{k=0}^{\infty} |w(z)p_k(z) + r_k(z)|^2 \leq \int_{\mathbb{R}} |x-z|^{-2}\, d\mu(x) < \infty.$$

The inequality follows from the Bessel inequality. If the $\{p_n\}_{n=0}^{\infty}$ is an orthonormal basis of $L^2(\mu)$ then we can write an equality by Parseval's identity.

(3.1.5) Since $r_k(y)$ is another solution to (3.4), multiplying (3.4) by $r_k(y)$ and (3.4) for $r_k(y)$ by $p_k(x)$, subtracting leads to

$$\begin{aligned}(x-y)p_k(x)r_k(y) =& a_k\bigl(p_{k+1}(x)r_k(y)-p_k(x)r_{k+1}(y)\bigr)\\ &- a_{k-1}\bigl(p_k(x)r_{k-1}(y)-p_{k-1}(x)r_k(y)\bigr)\end{aligned} \tag{3.6}$$

for $k\geq 1$. Taking $x=y$ in (3.6), we see that the Wronskian, or Casorati determinant,

$$[p,r]_k(x) = a_k\bigl(p_{k+1}(x)r_k(x)-p_k(x)r_{k+1}(x)\bigr) \tag{3.7}$$

is independent of $k\in\mathbb{Z}_{\geq 0}$, and taking $k=0$ gives $[p,r]_k(x)=[p,r]=-1$. This also shows that p_k and r_k are linearly independent solutions to (3.4).

On the other hand, replacing r_k by p_k and summing we get the Christoffel-Darboux formula

$$(x-y)\sum_{k=0}^{n-1}p_k(x)p_k(y) = a_{n-1}\bigl(p_n(x)p_{n-1}(y)-p_{n-1}(x)p_n(y)\bigr). \tag{3.8}$$

The case $x=y$ is obtained after dividing by $x-y$ and in the right hand side letting $y\to x$. This gives

$$\sum_{k=0}^{n-1}p_k(x)^2 = a_{n-1}\bigl(p_n'(x)p_{n-1}(x)-p_{n-1}'(x)p_n(x)\bigr).$$

3.2. **Moment problems.**

(3.2.1) The moment problem consists of the following two questions:

1. Given a sequence $\{m_0,m_1,m_2,\ldots\}$, does there exist a positive Borel measure μ on $\mathbb{R}$ such that $m_k=\int x^k\,d\mu(x)$?
2. If the answer to problem 1 is yes, is the measure obtained unique?

Note that we can assume without loss of generality that $m_0=1$. This is always assumed.

(3.2.2) In case $\mathrm{supp}(\mu)$ is required to be contained in a finite interval we speak of the Haussdorf moment problem (1920). In case $\mathrm{supp}(\mu)$ is to be contained in $[0,\infty)$ we speak of the Stieltjes moment problem (1894). Finally, without a condition on the support, we speak of the Hamburger moment problem (1922). Here, a moment problem is always a Hamburger moment problem. The answer to question 1 can be given completely in terms of positivity requirements of matrices composed of the m_i's, see Akhiezer [1], Shohat and Tamarkin [19], Simon [20], Stieltjes [21], Stone [22]. In these notes we only discuss an answer to question 2, see §3.4.

In case the answer to question 2 is affirmative, we speak of a determinate moment problem and otherwise of an indeterminate moment problem. So for an indeterminate moment problem we have a convex set of probability measures on $\mathbb{R}$ solving the same moment problem. The fact that this may happen has been observed first by Stieltjes [21]. The Haussdorf moment problem is always determinate as follows from (3.1.2) and the Stieltjes-Perron inversion formula, see Proposition (3.1.2).

For a nice overview of the early history of the moment problem, see Kjeldsen [11].

3.3. **Jacobi operators.**

(3.3.1) A tridiagonal matrix of the form

$$J = \begin{pmatrix} b_0 & a_0 & 0 & 0 & 0 & 0 & \dots \\ a_0 & b_1 & a_1 & 0 & 0 & 0 & \dots \\ 0 & a_1 & b_2 & a_2 & 0 & 0 & \dots \\ 0 & 0 & a_2 & b_3 & a_3 & 0 & \dots \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \end{pmatrix}$$

is a Jacobi operator, or an infinite Jacobi matrix, if $b_i \in \mathbb{R}$ and $a_i > 0$. If $a_i = 0$ for some i, the Jacobi matrix splits as the direct sum of two Jacobi matrices, of which the first is an $(i+1)\times(i+1)$-matrix.

We consider J as an operator defined on the Hilbert space $\ell^2(\mathbb{Z}_{\geq 0})$, see Example (2.1.2). So with respect to the standard orthonormal basis $\{e_k\}_{k\in\mathbb{Z}_{\geq 0}}$ of $\ell^2(\mathbb{Z}_{\geq 0})$ the Jacobi operator is defined as

$$J\, e_k = \begin{cases} a_k\, e_{k+1} + b_k\, e_k + a_{k-1}\, e_{k-1}, & k \geq 1, \\ a_0\, e_1 + b_0\, e_0, & k = 0. \end{cases} \tag{3.9}$$

Note the similarity with Theorem (3.1.3). So to each probability measure on $\mathbb{R}$ with finite moments we associate a Jacobi operator on the Hilbert space $\ell^2(\mathbb{Z}_{\geq 0})$ from the three-term recurrence relation for the corresponding orthonormal polynomials. However, some care is necessary, since (3.9) might not define a bounded operator on $\ell^2(\mathbb{Z}_{\geq 0})$.

From (3.9) we extend J to an operator defined on $\mathcal{D}(\mathbb{Z}_{\geq 0})$, the set of finite linear combinations of the elements e_k of the orthonormal basis of $\ell^2(\mathbb{Z}_{\geq 0})$. The linear subspace $\mathcal{D}(\mathbb{Z}_{\geq 0})$ is dense in $\ell^2(\mathbb{Z}_{\geq 0})$. From (3.9) it follows that

$$\langle J\, v, w\rangle = \langle v, J\, w\rangle, \qquad \forall\, v, w \in \mathcal{D}(\mathbb{Z}_{\geq 0}), \tag{3.10}$$

so that J is a densely defined symmetric operator, see (2.3.3). In particular, if J is bounded on $\mathcal{D}(\mathbb{Z}_{\geq 0})$, J extends to a bounded self-adjoint operator by continuity.

Lemma. (3.3.2) *$e_k = P_k(J)e_0$ for some polynomial P_k of degree k with real coefficients. In particular, e_0 is a cyclic vector for the action of J, i.e. the linear subspace $\{J^k e_0 \mid k \in \mathbb{Z}_{\geq 0}\}$ is dense in $\ell^2(\mathbb{Z}_{\geq 0})$.*

Proof. It suffices to show that $e_k = P_k(J)e_0$ for some polynomial of degree k, which follows easily from (3.9) and $a_i > 0$ using induction on k. □

Lemma. (3.3.3) *If the sequences $\{a_k\}$ and $\{b_k\}$ are bounded, say $\sup_k |a_k| + \sup_k |b_k| \leq M < \infty$, then J extends to a bounded self-adjoint operator with $\|J\| \leq 2M$. On the other hand, if J is bounded, then the sequences $\{a_k\}$ and $\{b_k\}$ are bounded.*

Proof. If $\{a_k\}$, $\{b_k\}$ are bounded, then, with $v = \sum_{k=0}^\infty v_k e_k \in \mathcal{D}(\mathbb{Z}_{\geq 0})$, $\|v\| = 1$,

$$\|Jv\|^2 = \sum_{k=0}^\infty |a_k v_{k-1} + b_k v_k + a_{k-1} v_{k+1}|^2.$$

Let $\sup_k |a_k| = A$, $\sup_k |b_k| = B$ with $A + B \leq M$, then each summand can be written as

$$\begin{aligned} & a_k^2|v_{k-1}|^2 + b_k^2|v_k|^2 + a_{k-1}^2|v_{k+1}|^2 + 2a_k b_k \Re(v_{k-1}\overline{v_k}) + 2a_k a_{k-1}\Re(v_{k-1}\overline{v_{k+1}}) + 2b_k a_k \Re(v_{k+1}\overline{v_k}) \\ \leq & A^2(|v_{k-1}|^2 + |v_{k+1}|^2) + B^2|v_k|^2 + 2A^2|\Re(v_{k-1}\overline{v_{k+1}})| + 2AB|\Re(v_{k-1}\overline{v_k})| + 2AB|\Re(v_{k+1}\overline{v_k})|. \end{aligned}$$

Using the bounded shift operator $S\colon e_k \mapsto e_{k+1}$ we have, using the Cauchy-Schwarz inequality (2.1.1) and $\|S\| = 1$,

$$\begin{aligned}\|Jv\|^2 &\leq 2A^2 + B^2 + 2A^2|\langle S^2 v, v\rangle| + 4AB|\langle Sv, v\rangle| \leq 4A^2 + B^2 + 4AB \\ &= (A+B)^2 + 2AB + 3A^2 = 2(A+B)^2 + 2A^2 - B^2 \leq 4M^2.\end{aligned}$$

By continuity J extends to a bounded operator on $\ell^2(\mathbb{Z}_{\geq 0})$.

To prove the reverse statement, we have $|\langle J\, e_k, e_l\rangle| \leq \|J\|$ implying that $|a_k| \leq \|J\|$ (take $l = k+1$) and $|b_k| \leq \|J\|$ (take $l = k$). □

(3.3.4) Assume J is bounded, then J is self-adjoint and we can apply the spectral theorem for bounded self-adjoint operators, see Theorem (2.2.2). Thus

$$\langle J\, v, w\rangle = \int_{\mathbb{R}} t\, dE_{v,w}(t), \qquad \forall\, v, w \in \ell^2(\mathbb{Z}_{\geq 0}).$$

In particular, we define the measure $\mu(A) = E_{e_0,e_0}(A) = \langle E(A)e_0, e_0\rangle$. Since E is a resolution of the identity, $E(A)$ is an orthogonal projection implying that μ is a positive Borel measure. Indeed, $\mu(A) = \langle E(A)^2 e_0, e_0\rangle = \langle E(A)e_0, E(A)e_0\rangle \geq 0$ for any Borel set A. Moreover, $E(\mathbb{R}) = I$, so that μ is a probability measure. The support of μ is contained in the interval $[-\|J\|, \|J\|]$, since J is a bounded self-adjoint operator. In particular, μ has finite moments. Hence the spectral theorem associates to a bounded Jacobi operator J a compactly supported probability measure μ. Moreover, the spectral measure E is completely determined by μ. Indeed,

$$\begin{aligned}\langle E(A)e_k, e_l\rangle &= \langle E(A)P_k(J)e_0, P_l(J)e_0\rangle \\ &= \langle P_l(J)P_k(J)E(A)e_0, e_0\rangle = \int_A P_k(x)P_l(x)\, d\mu(x),\end{aligned} \tag{3.11}$$

where the polynomials P_k are as in Lemma (3.3.2) using the self-adjointness of J and the fact that the spectral projections commute with J.

Theorem. (3.3.5) *Let J be a bounded Jacobi operator, then there exists a unique compactly supported probability measure μ such that for any polynomial P the map $U\colon P(J)e_0 \mapsto P$ extends to a unitary operator $\ell^2(\mathbb{Z}_{\geq 0}) \to L^2(\mu)$ with $UJ = MU$, where $M\colon L^2(\mu) \to L^2(\mu)$ is the multiplication operator $(Mf)(x) = xf(x)$. Moreover, let $p_k = Ue_k$, then the set $\{p_k\}_{k=0}^{\infty}$ is the set of orthonormal polynomials with respect to μ;*

$$\int_{\mathbb{R}} p_k(x)p_l(x)\, d\mu(x) = \delta_{k,l}.$$

Proof. By Lemma (3.3.2) we see that U maps a dense subspace of $\ell^2(\mathbb{Z}_{\geq 0})$ onto a dense subspace of $L^2(\mu)$, since the polynomials are dense in $L^2(\mu)$ because μ is compactly supported. Using (3.11) we see that for any two polynomials P, Q we have

$$\begin{aligned}\langle P(J)e_0, Q(J)e_0\rangle &= \langle \bar{Q}(J)P(J)e_0, e_0\rangle = \int_{\mathbb{R}} \bar{Q}(x)P(x)\, d\mu(x) \\ &= \langle P, Q\rangle_{L^2(\mu)} = \langle UP(J)e_0, UQ(J)e_0\rangle_{L^2(\mu)},\end{aligned}$$

or U is unitary, and it extends uniquely to a unitary operator.

To show that U intertwines the Jacobi operator J with the multiplication operator we show that $UJ\, e_k = MU\, e_k$ for all $k \in \mathbb{Z}_{\geq 0}$. Define $p_k = Ue_k$, then $p_k \in L^2(\mu)$ is a polynomial of degree k and the set $\{p_k\}_{k=0}^{\infty}$ is the set of orthonormal polynomials with respect to μ;

$$\int_{\mathbb{R}} p_k(x)p_l(x)\, d\mu(x) = \langle Ue_k, Ue_l\rangle_{L^2(\mu)} = \langle e_k, e_l\rangle = \delta_{k,l}$$

by the unitarity of U. It now suffices to show that the coefficients in the three-term recurrence relation for the orthogonal polynomials as in Theorem (3.1.3) correspond to the matrix coefficients of J. This is immediate using the functional calculus of (2.2.3), (3.11) and the explicit expressions for the coefficients in the three-term recurrence relation given in the proof of Theorem (3.1.3);

$$a_k = \langle J\, e_k, e_{k+1}\rangle = \int_{\mathbb{R}} x\, dE_{e_k,e_{k+1}}(x) = \int_{\mathbb{R}} x p_k(x) p_{k+1}(x)\, d\mu(x),$$
$$b_k = \langle J\, e_k, e_k\rangle = \int_{\mathbb{R}} x\, dE_{e_k,e_k}(x) = \int_{\mathbb{R}} x\big(p_k(x)\big)^2\, d\mu(x).$$

To show uniqueness, we observe that the moments of μ are uniquely determined by the fact that $\{p_k\}_{k=0}^{\infty}$ is a set of orthonormal polynomials for $L^2(\mu)$. Since the measure is compactly supported its Stieltjes transform is analytic in a neighbourhood of ∞. Using the Stieltjes inversion formula of Proposition (3.1.2), we see that the compactly supported measure is uniquely determined by its moments. □

Theorem (3.3.5) is called Favard's theorem restricted to the case of bounded coefficients in the three-term recurrence operator. It states that any set $\{p_k\}_{k=0}^{\infty}$ of polynomials generated by (3.4), (3.5) with the initial condition $p_0(x) = 1$ with $a_k > 0$, $b_k \in \mathbb{R}$ are orthonormal polynomials with respect to some, see §3.2, positive probability measure μ.

Corollary. *The moment generating function for μ is in terms of the resolvent $R(z)$ for the Jacobi operator J;*

$$\int_{\mathbb{R}} \frac{d\mu(x)}{x-z} = \langle R(z)e_0, e_0\rangle = \langle (J-z)^{-1}e_0, e_0\rangle, \qquad z \in \mathbb{C}\backslash\mathbb{R}.$$

(3.3.6) The asymptotically free solution to $J\, f(z) = z\, f(z)$ for $z \in \mathbb{C}\backslash\mathbb{R}$, is the element $f(z) = \{f_k(z)\}_{k=0}^{\infty}$ satisfying $\big(Jf(z)\big)_k = z\, f_k(z)$ for $k \geq 1$ (and in general not for $k = 0$) and $\sum_{k=0}^{\infty} |f_k(z)|^2 < \infty$. The asymptotically free solution encodes the spectral measure of J, hence the probability measure μ of Theorem (3.3.5).

Proposition. *Let J be a bounded Jacobi matrix. Take $z \in \mathbb{C}\backslash\mathbb{R}$ fixed. Then $f(z) = (J-z)^{-1}e_0$ is the asymptotically free solution for the Jacobi operator J. There exists a unique $w(z) \in \mathbb{C}\backslash\mathbb{R}$ such that $f_k(z) = w(z)p_k(z) + r_k(z)$, with p_k, r_k the polynomials as in* (3.1.3), (3.1.4). *Moreover, w is the Stieltjes transform of the measure μ.*

Proof. We have already observed in Corollary (3.1.4) that $\{w(z)p_k(z) + r_k(z)\}_{k=0}^{\infty} \in \ell^2(\mathbb{Z}_{\geq 0})$. Next we consider

$$f_k(z) = \langle (J-z)^{-1}e_0, e_k\rangle = \int_{\mathbb{R}} \frac{p_k(x)}{x-z}\, d\mu(x) = w(z)p_k(z) + r_k(z)$$

again by (3.1.4). Hence, $\big(Jf(z)\big)_k = z\, f_k(z)$ for $k \geq 1$.

It remains to show uniqueness. If not, then there would be two linearly independent solutions, so that we could combine to get $\sum_{k=0}^{\infty} |p_k(z)|^2 < \infty$ for $z \in \mathbb{C}\backslash\mathbb{R}$, so that J would have a non-real eigenvalue z contradicting the self-adjointness of J. □

(3.3.7) Note that we need $\lim_{K\to\infty} w(z)p_k(z) + r_k(z) = 0$ in order to have $\{f_k(z)\}_{k=0}^{\infty} \in \ell^2(\mathbb{Z}_{\geq 0})$. This implies

$$w(z) = -\lim_{k\to\infty} \frac{r_k(z)}{p_k(z)}, \qquad z \in \mathbb{C}\backslash\mathbb{R},$$

assuming that the limit in the right hand side exists. The fraction $\frac{r_k(z)}{p_k(z)}$ has no non-real poles due to the following lemma.

Lemma. *The zeroes of $p_k(x)$ are real and simple.*

Proof. Define

$$J_N = \begin{pmatrix} b_0 & a_0 & 0 & 0 & \dots & 0 \\ a_0 & b_1 & a_1 & 0 & \dots & 0 \\ \vdots & & \ddots & \ddots & & \vdots \\ 0 & \dots & & a_{N-2} & b_{N-1} & a_{N-1} \\ 0 & \dots & & 0 & a_{N-1} & b_N \end{pmatrix},$$

i.e. a tridiagonal matrix that is obtained from J by keeping only the first $(N+1)\times(N+1)$ block matrix. Then $J_N = J_N^*$, and it follows that its spectrum is real. Moreover, its spectrum is simple. Indeed, $(J_N - \lambda)f = 0$ and $f_0 = 0$ implies $f_1 = 0$ and hence $f_k = 0$. So if the multiplicity of the eigenspace is more than one, we could construct a non-zero eigenvector with $f_0 = 0$, a contradiction.

On the other hand we have, from Theorem (3.3.5),

$$(J_N - z)\begin{pmatrix} p_0(z) \\ p_1(z) \\ \vdots \\ p_N(z) \end{pmatrix} = -a_N \begin{pmatrix} 0 \\ \vdots \\ 0 \\ p_{N+1}(z) \end{pmatrix},$$

so that the eigenvalues of J_N are the zeroes of p_{N+1}. □

(3.3.8) The norm of the asymptotically free solution for fixed $z \in \mathbb{C}\backslash\mathbb{R}$ can be expressed in terms of the Stieltjes transform of μ;

$$\begin{aligned} \sum_{k=0}^{\infty} |w(z)p_k(z) + r_k(z)|^2 &= \langle (J-z)^{-1}e_0, (J-z)^{-1}e_0\rangle \\ = \frac{1}{z-\bar z}\big(\langle (J-z)^{-1}e_0, e_0\rangle - \langle (J-\bar z)^{-1}e_0, e_0\rangle\big) &= \frac{w(z) - \overline{w(z)}}{z - \bar z}. \end{aligned} \tag{3.12}$$

For z fixed and $w = w(z)$ a complex parameter (3.12) gives rise to an equation in the complex w-plane, which is in general a circle or a point. The radius of this circle is $\big(|z-\bar z| \sum_{k=0}^{\infty} |p_k(z)|^2\big)^{-1}$. Proposition (3.3.6) shows that it is a point for a bounded Jacobi operator, see [1], [20] for a discussion of limit points and limit circles.

(3.3.9) We now introduce the Green kernel for $z \in \mathbb{C}\backslash\mathbb{R}$,

$$G_{k,l}(z) = \begin{cases} f_l(z)p_k(z), & k \le l, \\ f_k(z)p_l(z), & k > l. \end{cases}$$

Hence $\{G_{k,l}(z)\}_{k=0}^{\infty}, \{G_{k,l}(z)\}_{l=0}^{\infty} \in \ell^2(\mathbb{Z}_{\ge 0})$ by Proposition (3.3.6), and the map

$$\ell^2(\mathbb{Z}_{\ge0}) \ni v \mapsto (Gz)v, \qquad \big(G(z)v\big)_k = \sum_{l=0}^{\infty} v_l G_{k,l}(z) = \langle v, \overline{G_{k,\cdot}(z)}\rangle$$

is a well-defined map. A priori it is not clear that $G(z)$ is a bounded map, but it is densely defined, e.g. on $\mathcal{D}(\mathbb{Z}_{\ge0})$. The next proposition states that G is bounded.

Proposition. *The resolvent of J is given by $(J-z)^{-1} = G(z)$ for $z \in \mathbb{C}\backslash\mathbb{R}$.*

Proof. Since $z \in \mathbb{C}\backslash\mathbb{R} \subset \rho(J)$ we know that $(J-z)^{-1}$ is a bounded operator, so it suffices to check $(J-z)G(z) = \mathbf{1}_{\ell^2(\mathbb{Z}_{\geq 0})}$ on a dense subspace $\mathcal{D}(\mathbb{Z}_{\geq 0})$ of $\ell^2(\mathbb{Z}_{\geq 0})$. Now

$$\begin{aligned}
\big((J-z)G(z)v\big)_k &= \sum_{l=0}^{\infty} v_l\big(a_k G_{k+1,l}(z) + (b_k - z)G_{k,l}(z) + a_{k-1}G_{k-1,l}(z)\big) \\
&= \sum_{l=0}^{k-1} v_l p_l(z)\big(a_k f_{k+1}(z) + (b_k - z) f_k(z) + a_{k-1} f_{k-1}(z)\big) \\
&\quad + \sum_{l=k+1}^{\infty} v_l f_l(z)\big(a_k p_{k+1}(z) + (b_k - z)p_k(z) + a_{k-1}p_{k-1}(z)\big) \\
&\quad + v_k\big(a_k f_{k+1}(z)p_k(z) + (b_k - z) f_k(z)p_k(z) + a_{k-1} f_k(z)p_{k-1}(z)\big) \\
&= v_k\big(a_k f_{k+1}(z)p_k(z) + (b_k - z) f_k(z)p_k(z) + a_{k-1} f_k(z)p_{k-1}(z)\big) \\
&= v_k a_k\big(f_{k+1}(z)p_k(z) - f_k(z)p_{k+1}(z)\big)
\end{aligned}$$

using that $f_k(z)$ and $p_k(z)$ are solutions to $Jf = zf$ for $k \geq 1$. The term at the right hand side involves the Wronskian, see (3.1.5). Since $[p,p] = 0$, and $[p,r] = -1$ and $f_k(z) = w(z)p_k(z) + r_k(z)$, it follows that $[f,p] = a_k\big(f_{k+1}(z)p_k(z) - f_k(z)p_{k+1}(z)\big) = 1$. ◻

(3.3.10) We can now find the spectral measure of J from the resolvent, see the Stieltjes-Perron inversion formula (2.2.4);

$$E_{u,v}\big((a,b)\big) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0} \frac{1}{2\pi i}\int_{a+\delta}^{b-\delta} \langle G(x+i\varepsilon)u, v\rangle - \langle G(x-i\varepsilon)u, v\rangle\, dx.$$

First observe that

$$\begin{aligned}
\langle G(z)u, v\rangle = \sum_{k,l=0}^{\infty} G_{k,l}(z)u_l\bar{v}_k &= \sum_{k\leq l} f_l(z)p_k(z)u_l\bar{v}_k + \sum_{k>l} f_k(z)p_l(z)u_l\bar{v}_k \\
&= \sum_{k\leq l} f_l(z)p_k(z)(u_l\bar{v}_k + u_k\bar{v}_l)(1 - \frac{1}{2}\delta_{k,l}),
\end{aligned}$$

by splitting the sum and renaming summation variables. The factor $(1-\frac{1}{2}\delta_{k,l})$ is introduced in order to avoid doubling in the case $k = l$. Since $f_l(z) = w(z)p_l(z) + r_l(z)$, with p_l and r_l polynomials, the only term contributing to $\langle G(x+i\varepsilon)u, v\rangle - \langle G(x-i\varepsilon)u, v\rangle$ as $\varepsilon \downarrow 0$ comes from $w(z)$, cf. (3.1.2). Hence,

$$\begin{aligned}
&E_{u,v}\big((a,b)\big) = \\
&\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0} \frac{1}{2\pi i}\int_{a+\delta}^{b-\delta} \Big(w(x+i\varepsilon) - w(x-i\varepsilon)\Big) \sum_{k\leq l} p_l(x)p_k(x)(u_l\bar{v}_k + u_k\bar{v}_l)(1 - \frac{1}{2}\delta_{k,l})\, dx
\end{aligned}$$

and using Proposition (3.1.2) and symmetrising the sum gives

$$E_{u,v}\big((a,b)\big) = \int_{(a,b)} \big(Uu\big)(x)\overline{\big(Uv\big)(x)}\, d\mu(x), \tag{3.13}$$

where $U\colon \ell^2(\mathbb{Z}_{\geq 0}) \to L^2(\mu)$ is the unitary operator U of Theorem (3.3.5). Note that (3.13) proves that U is a unitary operator by letting $a \to -\infty$ and $b \to \infty$, so that

$$\langle u, v\rangle = \int_{\mathbb{R}} \big(Uu\big)(x)\overline{\big(Uv\big)(x)}\, d\mu(x) = \langle Uu, Uv\rangle_{L^2(\mu)}.$$

We can think of U as the Fourier transform;

$$u_k = \int_{\mathbb{R}} (Uu)(x) p_k(x)\, d\mu(x),$$

so that $u \in \ell^2(\mathbb{Z}_{\geq 0})$ is expanded in terms of (generalised) eigenvectors $\{p_k(x)\}_{k=0}^{\infty}$ of the Jacobi operator J.

Theorem. (3.3.11) *There is one-to-one correspondence between bounded Jacobi operators and probability measures on* $\mathbb{R}$ *with compact support.*

Proof. Since a probability measure μ of compact support has finite moments, we can build the corresponding orthonormal polynomials and write down the three-term recurrence relation by Theorem (3.1.3). This gives a map $\mu \mapsto J$. Using the moment generating function, analytic at ∞, and the Stieltjes inversion formula, cf. proof of Theorem (3.3.5), we see that the map is injective. In Theorem (3.3.5) the inverse map has been constructed. □

3.4. **Unbounded Jacobi operators.**

(3.4.1) We now no longer assume that J is bounded. This occurs for example in the following case.

Lemma. *Let* μ *be a probablity measure with finite moments. Consider the three-term recurrence relation of Theorem* (3.1.3) *and the corresponding densely defined Jacobi operator* J*. If* $\operatorname{supp}(\mu)$ *is unbounded, then* J *is unbounded.*

Proof. Suppose not, so we assume that J is bounded. Using the Cauchy-Schwarz inequality and (3.11) we obtain

$$\begin{aligned}\|J\|^{2k} &\geq |\langle J^{2k} e_0, e_0\rangle| = \Big|\int_{\mathbb{R}} x^{2k}\, d\mu(x)\Big| \\ &\geq \int_{|x|\geq \|J\|+1} x^{2k}\, d\mu(x) \geq \big(|J\| + 1\big)^{2k} \int_{|x|\geq \|J\|+1} d\mu(x).\end{aligned}$$

This implies

$$\Big(\frac{\|J\|}{\|J\|+1}\Big)^{2k} \geq \int_{|x|\geq\|J\|+1} d\mu(x)$$

and by the assumption on μ the right hand side is strictly positive. The left hand side tends to 0 as $k \to \infty$, so that we obtain the required contradiction. □

(3.4.2) We use the notions as recalled in §2.3. Recall from (3.10) that J is a densely defined symmetric operator. Let us extend J to an arbitrary vector $v = \sum_{k=0}^{\infty} v_k e_k \in \ell^2(\mathbb{Z}_{\geq 0})$ by formally putting

$$J^*\, v = (a_0 v_1 + b_0 v_0)\, e_0 + \sum_{k=1}^{\infty} \big(a_k v_{k+1} + b_k v_k + a_{k-1} v_{k-1}\big)\, e_k, \tag{3.14}$$

which, in general, is not an element of $\ell^2(\mathbb{Z}_{\geq 0})$.

Proposition. *The adjoint of* $(J, \mathcal{D}(\mathbb{Z}_{\geq 0}))$ *is* $(J^*, \mathcal{D}^*)$*, where*

$$\mathcal{D}^* = \{v \in \ell^2(\mathbb{Z}_{\geq 0}) \mid J^* v \in \ell^2(\mathbb{Z}_{\geq 0})\}$$

and J^* *is given by* (3.14)*.*

Proposition (3.4.2) says that the adjoint of J is its natural extension to its maximal domain. In case J is essentially self-adjoint we have that $(J^*, \mathcal{D}^*)$ is self-adjoint and that $(J^*, \mathcal{D}^*)$ is the closure of J.

Proof. To determine the domain of J^* we have to consider for which $v \in \ell^2(\mathbb{Z}_{\geq 0})$ the map $w \mapsto \langle Jw, v\rangle$, $\mathcal{D}(\mathbb{Z}_{\geq 0}) \to \mathbb{C}$ is continuous, see (2.3.1). Now, with the convention $e_{-1} = 0$,

$$\begin{aligned}|\langle Jw, v\rangle| &= \big|\sum_k w_k \langle a_k e_{k+1} + b_k e_k + a_{k-1} e_{k-1}, v\rangle\big| \\ &= \big|\sum_k w_k (a_k \bar{v}_{k+1} + b_k \bar{v}_k + a_{k-1}\bar{v}_{k-1})\big| \\ &\leq \|w\| \Big(\sum_k |a_k v_{k+1} + b_k v_k + a_{k-1} v_{k-1}|^2\Big)^{\frac{1}{2}} = \|w\| \|J^* v\|,\end{aligned}$$

where the sums are finite since $w \in \mathcal{D}(\mathbb{Z}_{\geq 0})$ and where we have used the Cauchy-Schwarz inequality. This proves $w \mapsto \langle Jw, v\rangle$ is continuous for $v \in \mathcal{D}^*$. Hence, we have proved $\mathcal{D}^* \subseteq \mathcal{D}(J^*)$.

For the other inclusion, we observe that for $v \in \mathcal{D}(J^*)$ we have

$$\big|\sum_k w_k (a_k \bar{v}_{k+1} + b_k \bar{v}_k + a_{k-1}\bar{v}_{k-1})\big| \leq C\|w\|$$

for some constant C independent of $w \in \mathcal{D}(\mathbb{Z}_{\geq 0})$. Specialise to $w_k = (Jv)_k$ for $0 \leq k \leq N$ and $w_k = 0$ for $k > N$, to find $\|w\|^2 \leq C\|w\|$, or

$$\Big(\sum_{k=0}^N |a_k v_{k+1} + b_k v_k + a_{k-1} v_{k-1}|^2\Big)^{\frac{1}{2}} \leq C$$

and since C is independent of w, C is independent of N. Letting $N \to \infty$ we find $\|J^* v\| \leq C$, or $v \in \mathcal{D}^*$. □

Since the coefficients are real, J^* commutes with complex conjugation. This implies that the deficiency indices are equal. Since a solution of $J^* f = z f$ is completely determined by $f_0 = \langle f, e_0\rangle$, it follows that the deficiency spaces are either zero-dimensional or one-dimensional. In the first case we see that J with domain $\mathcal{D}(\mathbb{Z}_{\geq 0})$ is essentially self-adjoint, and in the second case there exists a one-parameter family of self-adjoint extensions of $(J, \mathcal{D}(\mathbb{Z}_{\geq 0}))$. Since the only possible element in N_z is $\{p_k(z)\}_{k=0}^\infty$ we obtain the following corollary to Proposition (2.3.4).

Corollary. *$(J, \mathcal{D}(\mathbb{Z}_{\geq 0}))$ is essentially self-adjoint if and only if $\sum_{k=0}^\infty |p_k(z)|^2 = \infty$ for all $z \in \mathbb{C}\backslash\mathbb{R}$ if and only if $\sum_{k=0}^\infty |p_k(z)|^2 = \infty$ for some $z \in \mathbb{C}\backslash\mathbb{R}$.*

(3.4.3) In case J has deficiency indices $(1,1)$ every self-adjoint extension, say $(J_1, \mathcal{D}_1)$, satisfies $(J, \mathcal{D}(\mathbb{Z}_{\geq 0})) \subsetneq (J_1, \mathcal{D}_1) \subsetneq (J^*, \mathcal{D}^*)$, and by Proposition (3.4.2) $(J_1, \mathcal{D}_1)$ is the restriction of J^* to a domain $\mathcal{D}_1$. Since the polynomials p_k and r_k are generated from the restriction to $\mathcal{D}(\mathbb{Z}_{\geq 0})$, these polynomials are independent of the choice of the self-adjoint extension. To describe the domains of the self-adjoint extensions we rewrite the sesquilinear form B of (2.3.4) in terms of the Wronskian; using the convention $u_{-1} = 0 = v_{-1}$

$$\begin{aligned}&\sum_{k=0}^N (J^*u)_k \bar{v}_k - u_k \overline{(J^*v)_k} \\ &= \sum_{k=0}^N (a_k u_{k+1} + b_k u_k + a_{k-1} u_{k-1})\bar{v}_k - u_k (a_k \bar{v}_{k+1} + b_k \bar{v}_k + a_{k-1}\bar{v}_{k-1}) \\ &= [u, \bar{v}]_0 + \sum_{k=1}^N \Big([u,\bar{v}]_k - [u,\bar{v}]_{k-1}\Big) = [u,\bar{v}]_N,\end{aligned}$$

where $[u, v]_k = a_k(u_{k+1} v_k - v_{k+1} u_k)$ is the Wronskian, cf. (3.7). So for $u, v \in \mathcal{D}^*$ we have $B(u, v) = \lim_{N\to\infty} [u, v]_N$. Note that the limit exists, since $u, v \in \mathcal{D}^*$.

Lemma. *Assume that J has deficiency indices $(1,1)$, then the self-adjoint extensions are in one-to-one correspondence with $(J^*, \mathcal{D}_\theta)$, $\theta \in [0, 2\pi)$, where*

$$\mathcal{D}_\theta = \{v \in \mathcal{D}^* \mid \lim_{N\to\infty} [v, e^{i\theta}\psi_i + e^{-i\theta}\psi_{-i}]_N = 0\}$$

where $J^*\psi_{\pm i} = \pm i\, \psi_{\pm i}$, $\overline{(\psi_i)_k} = (\psi_{-i})_k$ and $\|\psi_{\pm i}\| = 1$.

So $(\psi_{\pm i})_k = C\, p_k(\pm i)$ with $C^{-2} = \sum_{k=0}^\infty |p_k(i)|^2 < \infty$ by Corollary (3.4.2).

Proof. Since $n_+ = n_- = 1$, Proposition (2.3.4) gives that the domain of a self-adjoint extension is of the form $u + c(\psi_i + e^{-2i\theta}\psi_{-i})$ with $u \in \mathcal{D}(J^{**})$, $c \in \mathbb{C}$. Using $B(\psi_i, \psi_i) = 2i$, $B(\psi_{-i}, \psi_{-i}) = -2i$ and $B(\psi_i, \psi_{-i}) = 0$ shows that

$$\begin{aligned} &B(u + c(\psi_i + e^{-2i\theta}\psi_{-i}), e^{i\theta}\psi_i + e^{-i\theta}\psi_{-i}) = B(u, e^{i\theta}\psi_i + e^{-i\theta}\psi_{-i}) \\ &= \langle J^*u, e^{i\theta}\psi_i + e^{-i\theta}\psi_{-i}\rangle - \langle u, e^{i\theta}J^*\psi_i + e^{-i\theta}J^*\psi_{-i}\rangle. \end{aligned}$$

Now observe that for $v \in N_{\pm i}$ we have $B(u, v) = \pm i\langle u, v\rangle_{J^*} = 0$, $u \in \mathcal{D}(J^{**})$, using the graph norm as in Proposition (2.3.4). □

The condition $\overline{(\psi_i)_k} = (\psi_{-i})_k$ in Lemma (3.4.3) is meaningful, since J^* commutes with complex conjuagtion. It is needed to ensure the one-to-one correspondence.

(3.4.4) The results of §3.3 go through in the setting of unbounded operators up to minor changes. Lemma (3.3.2) remains valid, as it has nothing to do with the unboundedness of J. Lemma (3.3.3) implies that for an unbounded Jacobi matrix we have to deal with unbounded sequences $\{a_k\}$, $\{b_k\}$, or at least one of them is unbounded. (3.3.4) goes through, using Theorem (2.4.1), after choosing a self-adjoint extension of J. This operator is uniquely determined if $(n_+, n_-) = (0, 0)$ and is labeled by one real parameter if $(n_+, n_-) = (1, 1)$. For this self-adjoint extension (3.3.4) and Theorem (3.3.5) remain valid, except that μ is no longer compactly supported. In this case we observe that μ has finite moments, since $\int_{\mathbb{R}} x^k\, d\mu(x) = \langle J^k e_0, e_0\rangle < \infty$. From the unicity statement in Theorem (2.4.1) we deduce that the polynomials are dense in $L^2(\mu)$, which is needed to obtain the unitarity of U in Theorem (3.3.5). The results of §3.3 until Theorem (3.3.11) remain valid after replacing J by a self-adjoint extension. Observe that f as in Proposition (3.3.6) is contained in the domain of a self-adjoint extension, so that the calculation in Proposition (3.3.9) remains valid. In the unbounded case it is no longer true that (3.12) in the complex w-plane describes a point. Theorem (3.4.5) and Corollary (3.4.2) show that in the general case (3.12) describes a circle (with positive radius) if and only if the Jacobi operator has deficiency indices $(1, 1)$ if and only if the corresponding (Hamburger) moment problem is indeterminate. Finally, Theorem (3.3.11) cannot be extended to unbounded self-adjoint Jacobi operators.

(3.4.5) There is a nice direct link between the moment problem in §3.2 and the Jacobi operators. It gives an answer to question 2 of (3.2.1).

Theorem. *The (Hamburger) moment problem is determinate if and only if the corresponding Jacobi operator is essentially self-adjoint.*

Proof. Assume first that the corresponding Jacobi operator is essentially self-adjoint. Then $(J - z)\big(\mathcal{D}(\mathbb{Z}_{\geq 0})\big)$ is dense in $\ell^2(\mathbb{Z}_{\geq 0})$ by Proposition (2.3.4), $z \in \mathbb{C}\backslash\mathbb{R}$. The density and Lemma (3.3.2) say that we can find polynomials $R_k(x; z)$ such that $\|(J - z)R_k(J; z)e_0 - e_0\| \to 0$ as $k \to \infty$. Let μ be any solution to the moment problem, so that J is realised as the multiplication operator on the closure of the span of the polynomials in $L^2(\mu)$. Then

$$\lim_{k\to\infty} \int_{\mathbb{R}} |(x - z)R_k(x; z) - 1|^2\, d\mu(x) = 0.$$

Since $z \in \mathbb{C}\backslash\mathbb{R}$ we see that $x \mapsto (x-z)^{-1}$ is bounded for $x \in \mathbb{R}$, hence

$$\lim_{k\to\infty} \int_{\mathbb{R}} |R_k(x;z) - \frac{1}{x-z}|^2 \, d\mu(x) = 0.$$

Since μ is a probability measure $L^2(\mu) \hookrightarrow L^1(\mu)$, so the Stieltjes transform of μ is given by

$$\int_{\mathbb{R}} \frac{d\mu(x)}{x-z} = \lim_{k\to\infty} \int_{\mathbb{R}} R_k(x;z)\, d\mu(x),$$

but the right hand side only involves integration of polynomials, hence only the moments, so it is independent of the choice of the solution of the moment problem. By the Stieltjes inversion of Proposition (3.1.2) this determines μ uniquely.

For the converse statement, we assume that J has deficiency indices $(1,1)$. Let J_1 and J_2 be two different self-adjoint extensions of $(J, \mathcal{D}(\mathbb{Z}_{\geq 0}))$. We have to show that they give rise to different solutions of the moment problem. By the Stieltjes inversion of Proposition (3.1.2) it suffices to show that the Stieltjes transforms $\langle (J_1-z)^{-1}e_0, e_0\rangle$ and $\langle (J_2-z)^{-1}e_0, e_0\rangle$ are different.

Let us first observe that $e_0 \notin \mathrm{Ran}(J^{**}-z)$. Indeed, suppose not, then there exists $u \in \mathcal{D}(J^{**})$ such that $(J^{**}-z)u = e_0$, and taking the inner product with $0 \neq v \in N_{\bar z}$ gives $\langle e_0, v\rangle = \langle (J^{**}-z)u, v\rangle = \langle u, (J^* - \bar z)v\rangle = 0$, since $u \in \mathcal{D}(J^{**})$ and $v \in \mathcal{D}(J^*)$ and $v \in N_{\bar z}$. So v is an eigenvector of J^* with $v_0 = 0$, so that $v = 0$ by (3.4.2). This contradicts the fact that J has deficiency indices $(1,1)$.

From the previous paragraph we conclude that $(J_i - z)^{-1}e_0 \in \mathcal{D}(J^*)\backslash\mathcal{D}(J^{**})$, $i = 1,2$, by Proposition (2.3.4). Now the $\dim\big(\mathcal{D}(J_i)\backslash\mathcal{D}(J^{**})\big) = 1$, so that $(J_1-z)^{-1}e_0 = (J_1-z)^{-1}e_0$ implies $\mathcal{D}(J_1) = \mathcal{D}(J_2)$ and hence $J_1 = J_2$ by Proposition (2.3.4). So the vectors $(J_i-z)^{-1}e_0$ are different. To finish the proof we need to show that the zero-components are also different. Let $u = (J_1 - z)^{-1}e_0 - (J_2-z)^{-1}e_0 \neq 0$, then

$$(J^*-z)u = (J^*-z)(J_1-z)^{-1}e_0 - (J^*-z)(J_2-z)^{-1}e_0 = e_0 - e_0 = 0,$$

or $u \in N_z$. By (3.4.2) $\langle u, e_0\rangle = 0$ implies $u = 0$, so $\langle u, e_0\rangle \neq 0$. Hence, J_1 and J_2 give rise to two different Stieltjes transforms, hence to two different solutions of the moment problem. □

(3.4.6) From Lemma (3.3.3) we see that boundedness of the coefficients in the three-term recurrence relation of Theorem (3.1.3) for the orthonormal polynomials implies that J extends to a bounded self-adjoint operator. For unbounded coefficients there are several conditions on the sequences $\{a_k\}$, $\{b_k\}$ that ensure that the Jacobi operator J is essentially self-adjoint, and hence, by Theorem (3.4.5), the corresponding moment problem is determinate. We give three examples.

Proposition. (i) *If* $\sum_{k=0}^\infty \frac{1}{a_k} = \infty$, *then* J *is essentially self-adjoint.*
(ii) *If* $a_k + b_k + a_{k-1} \leq M < \infty$ *for* $k \in \mathbb{N}$, *or if* $a_k - b_k + a_{k-1} \leq M < \infty$ *for* $k \in \mathbb{N}$, *then* J *is essentially self-adjoint.*
(iii) *If* $\sum_{k=0}^\infty m_{2k}^{-1/2k} = \infty$, *where* m_j *is the* j*-th moment* $m_j = \int_{\mathbb{R}} x^j\, d\mu(x)$, *then* J *is essentially self-adjoint.*

Proof. To prove (i), we use the Christoffel-Darboux formula (3.8) with $x = z$, $y = \bar z$, and using that the polynomials have real coefficients, we find for $z \in \mathbb{C}\backslash\mathbb{R}$,

$$\sum_{k=0}^N |p_k(z)|^2 = \frac{a_N}{z - \bar z}\big(p_{N+1}(z)\bar p_N(z) - p_N(z)\bar p_{N+1}(z)\big).$$

Since the left hand side is at least $1 = p_0(z)$, we obtain

$$1 \leq \frac{a_N}{|z-\bar z|}\big(|p_{N+1}(z)||p_N(z)| + |p_N(z)||p_{N+1}(z)|\big) = \frac{2a_N}{|z-\bar z|}|p_N(z)||p_{N+1}(z)|.$$

For non-real z we have $C = 2/|z-\bar{z}| > 0$ and so

$$\sum_{k=0}^{\infty} \frac{1}{a_k} \leq C \sum_{k=0}^{\infty} |p_k(z)||p_{k+1}(z)| \leq C \sum_{k=0}^{\infty} |p_k(z)|^2 \tag{3.15}$$

by the Cauchy-Schwarz inequality (2.1.1) in $\ell^2(\mathbb{Z}_{\geq 0})$. So, if $\sum_{k=0}^{\infty} \frac{1}{a_k}$ diverges, we see from Corollary (3.4.2) and (3.15) that J is essentially self-adjoint.

The cases in (ii) are equivalent, by switching to the orthonormal polynomials $(-1)^n p_n(-x)$ for the measure $\tilde{\mu}(A) = \mu(-A)$ for any Borel set $A \subset \mathbb{R}$. We start with an expression for $p_n(x)$ in terms of the lower degree orthonormal polynomials;

$$p_n(x) = 1 + \sum_{k=0}^{n-1} \frac{1}{a_k} \sum_{j=0}^{k} (x - b_j - a_j - a_{j-1}) p_j(x), \tag{3.16}$$

with the convention $a_{-1} = 0$ and $p_{-1}(x) = 0$. In order to prove (3.16) we start with the telescoping series

$$\begin{aligned} a_{n-1}(p_n(x) - p_{n-1}(x)) &= \sum_{j=0}^{n-1} \big(a_j(p_{j+1}(x) - p_j(x)) - a_{j-1}(p_j(x) - p_{j-1}(x)) \big) \\ &= \sum_{j=0}^{n-1} (x - b_j - a_j - a_{j-1})\, p_j(x) \end{aligned}$$

by (3.4), (3.5). This gives

$$p_n(x) = p_{n-1}(x) + \frac{1}{a_{n-1}} \sum_{j=0}^{n-1} (x - b_j - a_j - a_{j-1})\, p_j(x)$$

and iterating this expression gives (3.16).

Now take $x > M$ in (3.16) to obtain inductively $p_0(x) = 1$, $p_k(x) \geq 1$ for $k \in \mathbb{N}$, so that $\sum_{k=0}^{\infty} |p_k(x)|^2$ is divergent. Since the polynomials p_k have real zeroes, see Lemma (3.3.7), we have $p_k(x) = C_k \prod_{i=1}^{k} (x - x_i)$ with $x_i \in \mathbb{R}$ which implies that $|p_k(x+iy)| \geq |p_k(x)|$. Hence, $\sum_{k=0}^{\infty} |p_k(x+iy)|^2 = \infty$ and Corollary (3.4.2) shows J is essentially self-adjoint.

Finally for (iii) we note that

$$1 = \|p_k\|_{L^2(\mu)} \leq \|\mathrm{lc}(p_k)\, x^k\| = \mathrm{lc}(p_k)\sqrt{m_{2k}} = \frac{\sqrt{m_{2k}}}{a_0 a_1 a_2 \ldots a_{k-1}}$$

by the triangle inequality, where $\mathrm{lc}(p_k)$ denotes the leading coefficient of the polynomial p_k. Hence

$$m_{2k}^{-1/2k} \leq \Big(\frac{1}{a_0}\frac{1}{a_1}\frac{1}{a_2}\cdots\frac{1}{a_{k-1}}\Big)^{1/k} \Longrightarrow \sum_{k=0}^{\infty} m_{2k}^{-1/2k} \leq \sum_{k=0}^{\infty} \Big(\prod_{i=0}^{k-1} \frac{1}{a_i} \Big)^{1/k}.$$

Using the geometric-arithmetic mean inequality,

$$\prod_{i=1}^{n} a_i^{p_i} \leq \sum_{i=1}^{n} p_i a_i, \qquad \sum_{i=1}^{n} p_i = 1,$$

we find

$$\Big(\prod_{i=0}^{k-1} \frac{1}{a_i} \Big)^{1/k} = (k!)^{-1/k} \Big(\prod_{i=0}^{k-1} \frac{i+1}{a_i} \Big)^{1/k} \leq (k!)^{-1/k} \frac{1}{k} \sum_{i=0}^{k-1} \frac{i+1}{a_i}.$$

Next use $k^k \leq e^k k!$, which can be proved by induction on k and $(1+\frac{1}{k})^k \leq e$, to see that we can estimate

$$\sum_{k=0}^{\infty} m_{2k}^{-1/2k} \leq \sum_{k=0}^{\infty} \frac{e}{k^2} \sum_{i=0}^{k-1} \frac{i+1}{a_i} = e \sum_{i=0}^{\infty} \frac{1}{a_i} \sum_{k=i}^{\infty} \frac{i+1}{k^2}$$

and the inner sum over k can be estimated independent of i. Now the result follows from (i). □

(3.4.7) A famous example of an indeterminate moment problem has been given by Stieltjes in his posthumously published memoir [21]. Consider for $\gamma > 0$ —Stieltjes considered the case $\gamma = 1$—

$$\int_0^{\infty} x^n \, e^{-\gamma^2 \ln^2 x} \sin(2\pi\gamma^2 \ln x)\, dx = e^{\frac{(n+1)^2}{4\gamma^2}} \int_0^{\infty} e^{-(\gamma \ln x - \frac{n+1}{2\gamma})^2} \sin(2\pi\gamma^2 \ln x)\, \frac{dx}{x}$$

and put $y = \gamma \ln x - \frac{n+1}{2\gamma}$, $x^{-1}dx = \gamma^{-1}dy$ to see that the integral equals

$$\gamma^{-1} e^{\frac{(n+1)^2}{4\gamma^2}} \int_{-\infty}^{\infty} e^{-y^2} \sin(2\pi\gamma y + \pi(n+1))\, dy = 0,$$

since the integrand is odd. In the same way we can calculate the same integral without the sine-term and we find that for any $-1 \leq r \leq 1$ we have

$$\int_0^{\infty} x^n \, e^{-\gamma^2 \ln^2 x} \big(1 + r \sin(2\pi\gamma^2 \ln x)\big)\, dx = \frac{\sqrt{\pi}}{\gamma} \exp\Big(\frac{(n+1)^2}{4\gamma^2}\Big),$$

so that the probablity measure

$$d\mu(x) = \frac{\gamma}{\sqrt{\pi}} e^{\frac{-1}{4\gamma^2}} \, e^{-\gamma^2 \ln^2 x}\, dx, \qquad x > 0,$$

corresponds to an indeterminate moment problem. The corresponding orthogonal polynomials are known as the Stieltjes-Wigert polynomials. Put $q = \exp(-1/2\gamma^2)$ or $\gamma^{-2} = -2\ln q$, then the orthonormal Stieltjes-Wigert polynomials satisfy (3.4), (3.5) with $a_k = q^{-2k-\frac{3}{2}}\sqrt{1-q^{k+1}}$ and $b_k = q^{-2k}(1+q^{-1}-q^k)$, see e.g. [3, §VI.2]. Note that $0 < q < 1$, and that a_k and b_k are exponentially increasing.

(3.4.8) Another example is to consider the following measure on $\mathbb{R}$

$$d\mu(x) = C_{\alpha,\gamma}\, e^{-\gamma|x|^{\alpha}}\, dx, \qquad \alpha, \gamma > 0.$$

The moments and the explicit value for $C_{\alpha,\gamma}$ can be calculated using the Γ-function;

$$\int_0^{\infty} x^{c-1} e^{-bx}\, dx = b^{-c}\Gamma(c), \qquad c > 0,\ \Re b > 0. \tag{3.17}$$

For $0 < \alpha < 1$ the (Hamburger) moment problem is indeterminate as we can see from the following observations. Note that all odd moments vanish. Put $x = y^{\alpha}$ and $c = (2n+1)/\alpha$ to find from (3.17), after doubling the interval,

$$\frac{\alpha}{2} \int_{-\infty}^{\infty} y^{2n} e^{-b|y|^{\alpha}}\, dy = b^{-\frac{2n+1}{\alpha}} \Gamma\Big(\frac{2n+1}{\alpha}\Big).$$

By taking the real parts we obtain

$$\frac{\alpha}{2} \int_{-\infty}^{\infty} y^{2n} e^{-\Re b|y|^{\alpha}} \cos(-\Im b|y|^{\alpha})\, dy = \Gamma\Big(\frac{2n+1}{\alpha}\Big)|b|^{-\frac{2n+1}{\alpha}} \cos\Big(-\arg(b)\frac{2n+1}{\alpha}\Big),$$

so that the right hand side is zero for all $n \in \mathbb{Z}_{\geq 0}$ if $\arg(b) = \frac{1}{2}\alpha\pi$. Since we need $\Re b > 0$ this is possible if $|\alpha| < 1$. So for $0 < \alpha < 1$ the (Hamburger) moment problem is indeterminate, since we obtain more solutions in the same way as for the Stieltjes-Wigert polynomials in (3.4.7).

The (Hamburger) moment problem is determinate for $\alpha \geq 1$, which follows using Proposition (3.4.6)(iii). See also Deift [5, p. 34] for another proof, in which the essentially self-adjointness of the corresponding Jacobi operator is established.

Restricting the measure $d\mu(x)$ to $[0,\infty)$ gives a Stieltjes moment problem, see §3.2, and for the Stieltjes moment problem this is an indeterminate moment problem if and only if $0 < \alpha < \frac{1}{2}$, see [19, Ch. 1, §8]. In particular, for $\frac{1}{2} \leq \alpha < 1$, the Hamburger moment problem is indeterminate, whereas the Stieltjes moment problem is determinate. In terms of Jacobi operators, this means that the corresponding Jacobi operator J has deficiency indices $(1,1)$, but that J has a unique positive self-adjoint extension, see Simon [20].

(3.4.9) A great number of results exist for the description of the solutions to an indeterminate moment problem. A nice way to describe all solutions is due to Nevannlina; see e.g. [1], [20]. There exist four entire functions A, B, C and D, that can be described using the polynomials p_k and r_k, such that the Stieltjes transform of any solution μ to the indeterminate moment problem is given by

$$\int_{\mathbb{R}} \frac{d\mu(x)}{x-z} = -\frac{A(z)\phi(z) - C(z)}{B(z)\phi(z) - D(z)}$$

where ϕ is any function that is analytic in the upper half plane having non-negative imaginary part, or $\phi = \infty$.

Now the solutions to the moment problem corresponding to $\phi(z) = t \in \mathbb{R} \cup \{\infty\}$ are precisely the measures that can be obtained from the spectral measure of a self-adjoint extension of the Jacobi operator J. In particular, this implies that these orthogonality measures are discrete with support at the zeroes of an entire function $B(z)t - D(z)$, so that there is no accumulation point. According to a theorem of M. Riesz (1923) these are precisely the measures for which the polynomials are dense in the corresponding L^2-space, cf. Theorem (3.3.5) for the unbounded case. See Akhiezer [1] and Simon [20] for more information.

4. Doubly infinite Jacobi operators

4.1. **Doubly infinite Jacobi operators.**

(4.1.1) We consider an operator on the Hilbert space $\ell^2(\mathbb{Z})$, see (2.1.2), of the form

$$L\, e_k = a_k\, e_{k+1} + b_k\, e_k + a_{k-1}\, e_{k-1}, \qquad a_k > 0,\ b_k \in \mathbb{R},$$

where $\{e_k\}_{k\in\mathbb{Z}}$ is the standard orthonormal basis of $\ell^2(\mathbb{Z})$ as in (2.1.2). If $a_i = 0$ for some $i \in \mathbb{Z}$, then L splits as the direct sum of two Jacobi operators as defined in (3.3.1). We call L a Jacobi operator on $\ell^2(\mathbb{Z})$ or a doubly infinite Jacobi operator.

The domain $\mathcal{D}(L)$ of L is the dense subspace $\mathcal{D}(\mathbb{Z})$ of finite linear combinations of the basis elements e_k. This makes L a densely defined symmetric operator.

(4.1.2) We extend the action of L to an arbitrary vector $v = \sum_{k=-\infty}^{\infty} v_k e_k \in \ell^2(\mathbb{Z})$ by

$$L^*\, v = \sum_{k=-\infty}^{\infty} (a_k\, v_{k+1} + b_k\, v_k + a_{k-1}\, v_{k-1})\, e_k,$$

which is not an element of $\ell^2(\mathbb{Z})$ in general. Define

$$\mathcal{D}^* = \{v \in \ell^2(\mathbb{Z}) \mid L^* v \in \ell^2(\mathbb{Z})\}.$$

Lemma. *$(L^*, \mathcal{D}^*)$ is the adjoint of $(L, \mathcal{D}(\mathbb{Z}))$.*

The proof of this Lemma is the same as the proof of Proposition (3.4.2).

(4.1.3) In particular, L^* commutes with complex conjugation, so its deficiency indices are equal. The solution space of $L^* v = z\, v$ is two-dimensional, since v is completely determined by any initial data (v_{n-1}, v_n) for any fixed $n \in \mathbb{Z}$. So the deficiency indices are equal to (i,i) with $i \in \{0,1,2\}$. From §2.3 we conclude that L has self-adjoint extensions.

4.2. **Relation to Jacobi operators.**

(4.2.1) To the operator L we associate two Jacobi operators J^+ and J^- acting on $\ell^2(\mathbb{Z}_{\geq 0})$ with orthonormal basis denoted by $\{f_k\}_{k\in\mathbb{Z}_{\geq 0}}$ in order to avoid confusion. Define

$$J^+\, f_k = \begin{cases} a_k\, f_{k+1} + b_k\, f_k + a_{k-1}\, f_{k-1}, & \text{for } k \geq 1,\\ a_0\, f_1 + b_0\, f_0, & \text{for } k = 0, \end{cases}$$

$$J^-\, f_k = \begin{cases} a_{-k-2}\, f_{k+1} + b_{-k-1}\, f_k + a_{-k-1}\, f_{k-1}, & \text{for } k \geq 1,\\ a_{-2}\, f_1 + b_{-1}\, f_0, & \text{for } k = 0, \end{cases}$$

and extend by linearity to $\mathcal{D}(\mathbb{Z}_{\geq 0})$, the space of finite linear combinations of the basis vectors $\{f_k\}_{k=0}^{\infty}$ of $\ell^2(\mathbb{Z}_{\geq 0})$. Then $J^\pm$ are densely defined symmetric operators with deficiency indices $(0,0)$ or $(1,1)$ corresponding to whether the associated Hamburger moment problems is determinate or indeterminate, see §3. The following theorem, due to Masson and Repka [17], relates the deficiency indices of L and $J^\pm$.

Theorem. (4.2.2) (Masson and Repka) *The deficiency indices of L are obtained by summing the deficiency indices of J^+ and the deficiency indices of J^-.*

Proof. Let $P_k(z)$, $Q_k(z)$ be generated by the recursion

$$z\, p_k(z) = a_k\, p_{k+1}(z) + b_k\, p_k(z) + a_{k-1}\, p_{k-1}(z), \tag{4.1}$$

subject to the initial conditions $P_0(z) = 1$, $P_{-1}(z) = 0$ and $Q_0(z) = 0$, $Q_{-1} = 1$. Then, see (4.1.3), any solution of $L^* v = z\, v$ can be written as $v_k = v_0 P_k(z) + v_{-1} Q_k(z)$. Note that $\{p_k^+\}_{k=0}^{\infty}$, $p_k^+(z) = P_k(z)$, are the orthonormal polynomials corresponding to the Jacobi operator J^+ and that $\{p_k^-\}_{k=0}^{\infty}$, $p_k^-(z) = Q_{-k-1}(z)$, are the orthonormal polynomials corresponding to J^-.

Introduce the spaces

$$
\begin{aligned}
S_z^- &= \{\{f_k\}_{k=-\infty}^\infty \mid L^*f = z\,f \text{ and } \sum_{k=-\infty}^{-1} |f_k|^2 < \infty\},\\
S_z^+ &= \{\{f_k\}_{k=-\infty}^\infty \mid L^*f = z\,f \text{ and } \sum_{k=0}^{\infty} |f_k|^2 < \infty\}.
\end{aligned}
\tag{4.2}
$$

From (4.1.3) we find $\dim S_z^\pm \leq 2$. The deficiency space for L is precisely $S_z^+ \cap S_z^-$.

From the results in §3, in particular Corollary (3.1.4), Proposition (3.3.6), Corollary (3.4.2) and (3.4.4), we have for $z \in \mathbb{C}\backslash\mathbb{R}$ that $\dim S_z^\pm = 1$ if and only if $J^\pm$ has deficiency indices $(0,0)$ and $\dim S_z^\pm = 2$ if and only if $J^\pm$ has deficiency indices $(1,1)$.

Let us now consider the four possible cases. Case 1: J^+ and J^- have deficiency indices $(1,1)$. Then $\dim S_z^\pm = 2$ and by (4.1.3) we get $S_z^+ = S_z^-$, so that L has deficiency indices $(2,2)$. Case 2: one of $J^\pm$ is essentially self-adjoint. We can assume that J^+ has deficiency indices $(0,0)$ and that J^- has deficiency indices $(1,1)$. Then $\dim S_z^+ = 1$, $\dim S_z^- = 2$ and by (2.1.6) S_z^- coincides with the solution space of $L^*v = z\,v$, i.e. every solution of $L^*v = z\,v$ is square summable at $-\infty$. So (4.2) shows that $S_z^+ \subset S_z^-$ and hence $\dim S_z^+ \cap S_z^- = 1$. So L has deficiency indices $(1,1)$ in this case. Case 3: J^+ and J^- have deficiency indices $(0,0)$. Then $\dim S_z^\pm = 1$ and we have to show that $S_z^+ \cap S_z^- = \{0\}$. Let $v^\pm = \{v_k^\pm\}_{k=-\infty}^\infty$ span the space $S_z^\pm$, and we have to show that v^+ is not a multiple of v^-. Let $v_k^\pm = C_\pm^P P_k(z) + C_\pm^Q Q_k(z)$. We calculate $C_\pm^P$ and $C_\pm^Q$ explicitly in terms of the Stieltjes transform $w^\pm(z) = \int_\mathbb{R} (x-z)^{-1}\,d\mu^\pm(x)$ of the spectral measures $\mu^\pm$ for $J^\pm$. Since J^+ and J^- are both essentially self-adjoint, the spaces $S_z^\pm$ are described in Proposition (3.3.6). It follows from the recursion (4.1) that the associated polynomials $r_k^\pm(z)$ for $J^\pm$, see (3.1.4), satisfy $r_k^+(z) = -a_1^{-1} Q_k(z)$, $k \geq 0$, and $r_k^-(z) = -a_{-1}^{-1} P_{-k-1}(z)$, $k \geq 0$. By Proposition (3.3.6) $v_k^+ = f_k^+(z) = w^+(z) P_k(z) - a_1^{-1} Q_k(z)$, $k \geq 0$, and $v_k^- = f_{-k-1}^-(z) = w^-(z) p_{-k-1}^-(z) + r_{-k-1}^-(z) = w^-(z) Q_k(z) - a_{-1}^{-1} P_k(z)$. So $C_+^P = w^+(z)$, $C_+^Q = \frac{-1}{a_1}$, $C_-^P = \frac{-1}{a_{-1}}$ and $C_-^Q = w^-(z)$, and consequently

$$
\frac{C_+^P}{C_+^Q} = -a_1\, w^+(z) = \mathcal{O}(\frac{1}{z}), \quad |z| \to \infty, \qquad \frac{C_-^P}{C_-^Q} = \frac{-1}{a_{-1} w^-(z)} = \mathcal{O}(z), \quad |z| \to \infty.
$$

In case v^+ is a non-zero multiple of v^- the quotients have to be equal. Since they are also independent of z we find the required contradiction. This implies $S_z^+ \cap S_z^- = \{0\}$ or L has deficiency indices $(0,0)$. □

(4.2.3) As in (3.4.3) we can describe the sesquilinear form B as introduced in (2.3.4) in terms of the Wronskian $[u,v]_k = a_k(u_{k+1}v_k - u_k v_{k+1})$. Note that, as in §3, the Wronskian $[u,v] = [u,v]_k$ is independent of k for $L^*u = z\,u$, $L^*v = z\,v$, and then $[u,v] \neq 0$ if and only if u and v are linearly independent solutions. Now, as in (3.4.3),

$$
\begin{aligned}
&\sum_{k=M}^N (L^*u)_k \bar v_k - u_k \overline{(L^*v)_k}\\
&= \sum_{k=M}^N (a_k u_{k+1} + b_k u_k + a_{k-1} u_{k-1}) \bar v_k - u_k (a_k \bar v_{k+1} + b_k \bar v_k + a_{k-1} \bar v_{k-1})\\
&= \sum_{k=M}^N [u, \bar v]_k - [u, \bar v]_{k-1} = [u, \bar v]_N - [u, \bar v]_{M-1},
\end{aligned}
$$

so that

$$B(u,v) = \lim_{N\to\infty} [u,\bar v]_N - \lim_{M\to-\infty} [u,\bar v]_M, \qquad u,v\in\mathcal{D}^*.$$

In particular, if J^- is essentially self-adjoint, we have $\lim_{M\to-\infty}[u,\bar v]_M = 0$, so that in this case the sesquilinear form B is as in §3. In case J^+ has deficiency indices $(1,1)$ we see as in Lemma (3.4.3) that the same formula for the domains of self-adjoint extensions of L are valid.

Lemma. *Let J^-, respectively J^+, have deficiency indices $(0,0)$, respectively $(1,1)$, so that L has deficiency indices $(1,1)$. Then the self-adjoint extensions of L are given by $(L^*,\mathcal{D}_\theta)$, $\theta\in[0,2\pi)$, with*

$$\mathcal{D}_\theta = \{v\in\mathcal{D}^* \mid \lim_{N\to\infty} [v, e^{i\theta}\Phi_i + e^{-i\theta}\Phi_{-i}]_N = 0\}$$

where $L^*\Phi_{\pm i} = \pm i\Phi_{\pm i}$, $\overline{(\Phi_i)_k} = (\Phi_{-i})_k$ and $\|\Phi_{\pm i}\| = 1$.

The proof of Lemma (4.2.3) mimics the proof of Lemma (3.4.3).

4.3. **The Green kernel.**

(4.3.1) From on we assume that J^- has deficiency indices $(0,0)$, so that J^- is essentially self-adjoint and by Theorem (4.2.2) the deficiency indices of L are $(0,0)$ or $(1,1)$. (The reason for the restriction to this case is that in case L has deficiency indices $(2,2)$ the restriction of the domain of a self-adjoint extension of L to the Jacobi operator $J^\pm$ does not in general correspond to a self-adjoint extension of $J^\pm$, cf. [7, Thm. XII.4.31].) Let $z\in\mathbb{C}\backslash\mathbb{R}$ and choose $\Phi_z\in S_z^-$, so that Φ_z is determined up to a constant. We assume $\overline{(\Phi_z)_k} = (\Phi_{\bar z})_k$, cf. Lemma (4.2.3).

(4.3.2) Let $\phi_z\in S_z^+$, such that $\overline{(\phi_z)_k} = (\phi_{\bar z})_k$. We now show that we may assume

1. $[\phi_z,\Phi_z]\neq 0$,
2. $\tilde\phi_z$, defined by $(\tilde\phi_z)_k = 0$ for $k<0$ and $(\tilde\phi_z)_k = (\phi_z)_k$ for $k\geq 0$, is contained in the domain of a self-adjoint extension of L.

First observe $L^*\tilde\phi_z = z\tilde\phi_z + a_{-1}((\phi_z)_0 e_{-1} - (\phi_z)_{-1}e_0)$, so that $\tilde\phi_z\in\mathcal{D}^*$. In case L is essentially self-adjoint, $(L^*,\mathcal{D}^*)$ is the unique self-adjoint extension and (2) is valid. In this case (1) follows from case 3 in the proof of Theorem (4.2.2).

In case L has deficiency indices $(1,1)$, we have $S_z^-\subset S_z^+$ and (2) implies (1). Indeed, if (2) holds and (1) not, then $\Phi_z\in\ell^2(\mathbb{Z})$ and $\Phi_z = C\phi_z$ is in the domain of a self-adjoint extension. Since $L^*\Phi_z = z\,\Phi_z$ this shows that the self-adjoint extension would have a non-real eigenvalue; a contradiction. To show that we can assume (2) we observe that

$$\lim_{N\to\infty} [\tilde\phi_z, e^{i\theta}\Phi_i + e^{-i\theta}\Phi_{-i}]_N = \lim_{N\to\infty} [\phi_z, e^{i\theta}\Phi_i + e^{-i\theta}\Phi_{-i}]_N,$$

which exists since $\tilde\phi_z,\Phi_{\pm i}\in\mathcal{D}^*$. If the limit is non-zero, say K, we use that

$$\begin{aligned} A(z,\theta) &= \lim_{N\to\infty} [\Phi_z, e^{i\theta}\Phi_i + e^{-i\theta}\Phi_{-i}]_N \\ &= \langle L^*\Phi_z, e^{i\theta}\Phi_i + e^{-i\theta}\Phi_{-i}\rangle - \langle \Phi_z, L^*(e^{i\theta}\Phi_i + e^{-i\theta}\Phi_{-i})\rangle \\ &= e^{-i\theta}(z+i)\langle\Phi_z,\Phi_i\rangle + e^{i\theta}(z-i)\langle\Phi_z,\Phi_{-i}\rangle \neq 0. \end{aligned}$$

Otherwise, as before, Φ_z would be in the domain of a self-adjoint extension of L by Lemma (4.2.3). So that replacing ϕ_z by $\phi_z - \frac{K}{A(z,\theta)}\Phi_z$ gives the desired result, since $S_z^-\subset S_z^+$.

(4.3.3) Let $(L',\mathcal{D}')$ be a self-adjoint extension of L, assuming, as before, that J^- has deficiency indices $(0,0)$. Let $\phi_z\in S_z^+$, $\Phi_z\in S_z^-$ as in (4.3.2). We define the Green kernel for $z\in\mathbb{C}\backslash\mathbb{R}$ by

$$G_{k,l}(z) = \frac{1}{[\phi_z,\Phi_z]} \begin{cases} (\Phi_z)_k\,(\phi_z)_l, & k\leq l, \\ (\Phi_z)_l\,(\phi_z)_k, & k>l. \end{cases}$$

So $\{G_{k,l}(z)\}_{k=-\infty}^{\infty}, \{G_{k,l}(z)\}_{l=-\infty}^{\infty} \in \ell^2(\mathbb{Z})$ and $\ell^2(\mathbb{Z}) \ni v \mapsto G(z)v$ given by

$$(G(z)v)_k = \sum_{l=-\infty}^{\infty} v_l G(z)_{k,l} = \langle v, \overline{G_{k,\cdot}(z)}\rangle$$

is well-defined. For $v \in \mathcal{D}(\mathbb{Z})$ we have $G(z)v \in \mathcal{D}'$.

Proposition. *The resolvent of $(L', \mathcal{D}')$ is given by $(L'-z)^{-1} = G(z)$ for $z \in \mathbb{C}\backslash\mathbb{R}$.*

Proof. Note $\mathbb{C}\backslash\mathbb{R} \subset \rho(L')$, because L' is self-adjoint. Hence $(L'-z)^{-1}$ is a bounded operator mapping $\ell^2(\mathbb{Z})$ onto $\mathcal{D}'$. So $v \mapsto ((L'-z)^{-1}v)_k$ is a continuous map, hence, by the Riesz representation theorem, $((L'-z)^{-1}v)_k = \langle v, \overline{G_{k,\cdot}(z)}\rangle$ for some $G_{k,\cdot}(z) \in \ell^2(\mathbb{Z})$. So it suffices to check $(L'-z)G(z)v = v$ for v in the dense subspace $\mathcal{D}(\mathbb{Z})$. As in the proof of Proposition (3.3.9) we have

$$\begin{aligned}
[\phi_z, \Phi_z]\big((L'-z)G(z)v\big)_k =& \sum_{l=-\infty}^{k-1} v_l\big(a_k(\phi_z)_{k+1} + (b_k - z)(\phi_z)_k + a_{k-1}(\phi_z)_{k-1}\big)(\Phi_z)_l \\
&+ \sum_{l=k+1}^{\infty} v_l\big(a_k(\Phi_z)_{k+1} + (b_k - z)(\Phi_z)_k + a_{k-1}(\Phi_z)_{k-1}\big)(\phi_z)_l \\
&+ v_k\big(a_k(\Phi_z)_k(\phi_z)_{k+1} + (b_k - z)(\Phi_z)_k(\phi_z)_k + a_{k-1}(\Phi_z)_{k-1}(\phi_z)_k\big) \\
=& v_k a_k\big((\Phi_z)_k(\phi_z)_{k+1} - (\Phi_z)_{k+1}(\phi_z)_k\big) = v_k[\phi_z, \Phi_z]
\end{aligned}$$

and canceling the Wronskian gives the result. □

(4.3.4) As in (3.3.10) we can calculate

$$\langle G(z)u, v\rangle = \sum_{k,l=-\infty}^{\infty} G_{k,l}(z)u_l\bar{v}_k = \frac{1}{[\phi_z, \Phi_z]}\sum_{k\leq l}(\Phi_z)_k(\phi_z)_l\big(u_l\bar{v}_k + u_k\bar{v}_l\big)(1 - \frac{1}{2}\delta_{k,l}), \tag{4.3}$$

but in general we cannot pin down the terms of (4.3) that will contribute to the spectral measure of L' in the Stieltjes-Perron inversion formula of (2.2.4), (2.4.1). We now consider some examples.

4.4. **Example: the Meixner functions.** This subsection is based on Masson and Repka [17], see also Masson [16]. We extend to the results of [17] by calculating explicitly the spectral measure of the Jacobi operator.

(4.4.1) In this example we take for the coefficients of L in (4.1.1) the following;

$$a_k = a_k(a, \lambda, \varepsilon) = \sqrt{(\lambda + k + \varepsilon + 1)(k + \varepsilon - \lambda)}, \qquad b_k = b_k(a, \lambda, \varepsilon) = 2a(k + \varepsilon).$$

Without loss of generality we may assume that $0 \leq \varepsilon < 1$ and $a > 0$ by changing to the orthonormal basis $f_k = (-1)^k e_k$ and the operator $-L$. We will do not so in order to retain symmetry properties. The conditions $a_k > 0$ and $b_k \in \mathbb{R}$ are met if we require $a \in \mathbb{R}$, $\varepsilon \in \mathbb{R}$ for $b_k \in \mathbb{R}$ and either $\lambda = -\frac{1}{2} + ib$, $b \geq 0$ or $\varepsilon \in [0, \frac{1}{2})$ and $-\frac{1}{2} \leq \lambda < -\varepsilon$ or $\varepsilon \in (\frac{1}{2}, 1)$ and $\lambda \in (-\frac{1}{2}, \varepsilon - 1)$ for $a_k > 0$. Now L is essentially self-adjoint by Theorem (4.2.2), since $J^{\pm}$ are essentially self-adjoint by (i) of Proposition (3.4.6).

(4.4.2) In case we choose λ, ε in such a way that $a_i = 0$ for some $i \in \mathbb{Z}$, the corresponding Jacobi operator on the $\mathbb{C}$-span of e_k, $k > i$, can be identified with the three-term recurrence relation for the Meixner-Pollaczek, Meixner or Laguerre polynomials depending on the size of a. In case $a_i \neq 0$, we can still consider the corresponding Jacobi operator on $\ell^2(\mathbb{Z}_{\geq 0})$ by putting $a_{-1} = 0$. Then the corresponding orthogonal polynomials are the associated Meixner-Pollaczek, Meixner or Laguerre polynomials.

(4.4.3) First note that if we find a solution $u_k(z) = u_k(z; a, \lambda, \varepsilon)$ to

$$z\, u_k(z) = a_k(a, \lambda, \varepsilon)\, u_{k+1}(z) + b_k(a, \lambda, \varepsilon)\, u_k(z) + a_{k-1}(a, \lambda, \varepsilon)\, u_{k-1}(z) \tag{4.4}$$

then $v_k(z) = (-1)^k u_k(-z)$ satisfies

$$z\, v_k(z) = a_k(-a, \lambda, \varepsilon)\, v_{k+1}(z) + b_k(-a, \lambda, \varepsilon)\, v_k(z) + a_{k-1}(-a, \lambda, \varepsilon)\, v_{k-1}(z)$$

and $w_k(z) = u_{-k}(z; -a, \lambda, -\varepsilon)$ also satisfies (4.4). Indeed, introducing a new orthonormal basis $f_k = e_{-k}$ of $\ell^2(\mathbb{Z})$ we see that L is given by

$$L\, f_k = a_{-k-1}\, f_{k+1} + b_{-k}\, f_k + a_{-k}\, f_{k-1}$$

and

$$a_{-k-1}(\lambda, \varepsilon, a) = a_k(\lambda, -\varepsilon, -a), \qquad b_{-k}(\lambda, \varepsilon, a) = b_k(\lambda, -\varepsilon, -a).$$

(4.4.4) In order to find explicit solutions to $L^* v = z\, v$ we need the hypergeometric function. Recall

$$ {}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix}; x\right) = \sum_{k=0}^{\infty} \frac{(a)_k\, (b)_k}{(c)_k\, k!} x^k,$$
$$(a)_k = a(a+1)\ldots(a+k-1) = \frac{\Gamma(a+k)}{\Gamma(a)},$$

where the series is absolutely convergent for $|x| < 1$. The hypergeometric function has a unique analytic continuation to $\mathbb{C}\backslash[1, \infty)$. It can also be extended non-uniquely to the cut $[1, \infty)$. See e.g. [8, Ch. II] for all the necessary material on hypergeometric functions.

Lemma. *Let $a^2 > 1$. The functions*

$$\begin{aligned} u_k^{\pm}(z) =& (\pm 2)^{-k} \big(\sqrt{a^2-1}\big)^{-k} \frac{\sqrt{\Gamma(k+\lambda+\varepsilon+1)\, \Gamma(k+\varepsilon-\lambda)}}{\Gamma(k+1+\varepsilon \pm z/2\sqrt{a^2-1})} \\ & \times\ {}_2F_1\left(\begin{matrix} k+\varepsilon+1+\lambda, k+\varepsilon-\lambda \\ k+\varepsilon+1 \pm z/2\sqrt{a^2-1} \end{matrix}; \frac{1}{2} \pm \frac{a}{2\sqrt{a^2-1}}\right) \end{aligned}$$

and

$$\begin{aligned} v_k^{\pm}(z) =& (\pm 2)^{k} \big(\sqrt{a^2-1}\big)^{k} \frac{\sqrt{\Gamma(-k+\lambda-\varepsilon+1)\, \Gamma(-k-\varepsilon-\lambda)}}{\Gamma(-k+1-\varepsilon \pm z/2\sqrt{a^2-1})} \\ & \times\ {}_2F_1\left(\begin{matrix} -k-\varepsilon+1+\lambda, -k-\varepsilon-\lambda \\ -k-\varepsilon+1 \pm z/2\sqrt{a^2-1} \end{matrix}; \frac{1}{2} \mp \frac{a}{2\sqrt{a^2-1}}\right) \end{aligned}$$

satisfy the recursion (4.4)*.*

Proof. The hypergeometric function is a solution to the hypergeometric differential equation;

$$x(1-x)y'' + (c - (a+b+1)x)y' - aby = 0.$$

Now $f(x; a, b, c) = \frac{\Gamma(a)\Gamma(b)}{\Gamma(c)} {}_2F_1(a, b; c; x)$ satisfies $f'(x; a, b, c) = f(x; a+1, b+1, c+1)$. Hence,

$$\begin{aligned} & r_k = f(x; k+1+\varepsilon+\lambda, k+\varepsilon-\lambda, k+1+\varepsilon-y), \\ & x(1-x)r_{k+1} + (k+\varepsilon-y-2(k+\varepsilon)x)r_k - (k+\varepsilon+\lambda)(k+\varepsilon-\lambda-1)r_{k-1} = 0. \end{aligned}$$

Replace $x = \frac{1}{2} - \frac{a}{2\sqrt{a^2-1}}$ and $y = z/2\sqrt{a^2-1}$. Let

$$r_k = (-2)^k (a^2-1)^{\frac{1}{2}k} \sqrt{\Gamma(k+\varepsilon+1+\lambda)\Gamma(k+\varepsilon-\lambda)} p_k$$

then p_k satisfies (4.4).

This proves the lemma for $u_k^-(z)$. The case $u_k^+(z)$ follows by replacing a by $-a$, and applying (4.4.3). Replacing k by $-k$, a by $-a$ and ε by $-\varepsilon$ and using (4.4.3) gives the other sets of solutions to (4.4). □

From now on we assume that $a^2 > 1$ in order not to complicate matters. The case $a^2 = 1$ corresponds to the Laguerre functions, and the case $0 \leq a^2 < 1$ corresponds to the Meixner-Pollaczek functions, see [17] and (4.4.11).

(4.4.5) In order to find the asymptotic behaviour of the solutions in Lemma (4.4.4) we first use

$$ {}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix}; x\right) = (1-x)^{c-a-b} {}_2F_1\left(\begin{matrix} c-a, c-b \\ c \end{matrix}; x\right), $$

so that

$$ \begin{aligned} &{}_2F_1\left(\begin{matrix} k+\varepsilon+1+\lambda, k+\varepsilon-\lambda \\ k+\varepsilon+1 \pm z/2\sqrt{a^2-1} \end{matrix}; \frac{1}{2} \pm \frac{a}{2\sqrt{a^2-1}}\right) \\ &= (\frac{1}{2} \mp \frac{a}{2\sqrt{a^2-1}})^{-k-\varepsilon\pm z/2\sqrt{a^2-1}} \big(1+\mathcal{O}(\frac{1}{k})\big), \qquad k\to\infty. \end{aligned} $$

Use

$$ \frac{\Gamma(z+a)}{\Gamma(z+b)} = z^{a-b}\big(1+\mathcal{O}(\frac{1}{z})\big), \qquad z\to\infty,\ |\arg(z)|<\pi, $$

to find

$$ \frac{\sqrt{\Gamma(k+\lambda+\varepsilon+1)\,\Gamma(k+\varepsilon-\lambda)}}{|\Gamma(k+1+\varepsilon+y)|} = k^{-\Re y-\frac{1}{2}}\Big(1+\mathcal{O}(\frac{1}{k})\Big), \qquad k\to\infty, $$

so that we find the asymptotic behaviour

$$ |u_k^{\pm}(z)| = (\frac{1}{2} \mp \frac{a}{2\sqrt{a^2-1}})^{-\varepsilon\pm\Re z/2\sqrt{a^2-1}} k^{-\frac{1}{2}\mp\Re z/2\sqrt{a^2-1}} \,|-a\pm\sqrt{a^2-1}|^{-k}\big(1+\mathcal{O}(\frac{1}{k})\big), $$

as $k\to\infty$. This implies that $u^+(z)\in S_z^+$ if $a<-1$ and $u^-(z)\in S_z^+$ if $a>1$.

Similarly we obtain the asymptotic behaviour

$$ |v_{-k}^{\pm}(z)| = (\frac{1}{2} \pm \frac{a}{2\sqrt{a^2-1}})^{\varepsilon\pm\Re z/2\sqrt{a^2-1}} k^{-\frac{1}{2}\mp\Re z/2\sqrt{a^2-1}} (a\pm\sqrt{a^2-1})^{-k}\big(1+\mathcal{O}(\frac{1}{k})\big), $$

as $k\to\infty$, so that $v^-(z)\in S_z^-$ if $a<-1$ and $v^+(z)\in S_z^-$ if $a>1$.

Note that we have completely determined $S_z^{\pm}$, hence ϕ_z and Φ_z, since these spaces are one-dimensional.

(4.4.6) If we reparametrise the parameter $a=\frac{1}{2}(s+s^{-1})$, then

$$ \{s, s^{-1}\} = \{a+\sqrt{a^2-1}, a-\sqrt{a^2-1}\}. $$

Note that $a^2-1=\frac{1}{4}(s-s^{-1})^2$. In this case we can let $u^{\pm}(z)$ and $v^{\pm}(z)$ correspond to hypergeometric series with only $s^{\pm 1}$-dependence. The results can be written somewhat nicer after transforming Lemma (4.4.4) by

$$ {}_2F_1\left(\begin{matrix} a, b \\ c \end{matrix}; x\right) = (1-x)^{-a} {}_2F_1\left(\begin{matrix} a, c-b \\ c \end{matrix}; \frac{x}{x-1}\right). $$

We leave this to the reader.

(4.4.7) Note that $v^{\pm}(z)$ are linearly independent solutions to (4.4), because they display different asymptotic behaviour. Since the solution space to (4.4) is two-dimensional, we see that there exist constants such that

$$ u_k^+(z) = A^+(z)v_k^+(z) + B^+(z)v_k^-(z), \qquad u_k^-(z) = A^-(z)v_k^+(z) + B^-(z)v_k^-(z). $$

Or stated differently, relations between hypergeometric series of argument x and $1-x$. Relations connecting hypergeometric series are very classical. We use

$$
\begin{aligned}
&{}_2F_1\left(\begin{matrix}a,b\\ a+b+1-c\end{matrix};1-x\right)=A\,{}_2F_1\left(\begin{matrix}a,b\\ c\end{matrix};x\right)+Bx^{1-c}(1-x)^{c-a-b}{}_2F_1\left(\begin{matrix}1-a,1-b\\ 2-c\end{matrix};x\right),\\
&A=\frac{\Gamma(a+b+1-c)\Gamma(1-c)}{\Gamma(a+1-c)\Gamma(b+1-c)},\qquad B=\frac{\Gamma(a+b+1-c)\Gamma(c-1)}{\Gamma(a)\,\Gamma(b)}
\end{aligned}
$$

with $a\mapsto -k-\varepsilon+1+\lambda$, $b\mapsto -k-\varepsilon-\lambda$, $c\mapsto -k-\varepsilon+1+y$, $x\mapsto \frac12-\frac{a}{2\sqrt{a^2-1}}$. Then the first ${}_2F_1$ is as in $v_k^-(z)$, the second one as in $v_k^+(z)$, and the third one as in $u_k^-(z)$. This gives, using $y=z/2\sqrt{a^2-1}$,

$$
\begin{aligned}
B^-(z)=&(-2)^{-k}\big(\sqrt{a^2-1}\big)^{-k}\frac{\Gamma(-k+1-\varepsilon-y)}{\sqrt{\Gamma(-k+\lambda-\varepsilon+1)\Gamma(-k-\varepsilon-\lambda)}}\\
&\hfill\text{from factor of } v_k^-(z)\\
&\times\frac{\Gamma(-k-\varepsilon+1+\lambda)\Gamma(-k-\varepsilon-\lambda)}{\Gamma(1-k-\varepsilon-y)\Gamma(-k-\varepsilon+y)}\big(\frac12-\frac{a}{2\sqrt{a^2-1}}\big)^{y-k-\varepsilon}\big(\frac12+\frac{a}{2\sqrt{a^2-1}}\big)^{-y-k-\varepsilon}\\
&\hfill\text{from } B\\
&\times(-2)^{-k}\big(\sqrt{a^2-1}\big)^{-k}\frac{\sqrt{\Gamma(k+\lambda+\varepsilon+1)\Gamma(k+\varepsilon-\lambda)}}{\Gamma(k+1+\varepsilon-y)}\\
&\hfill\text{from factor of } u_k^-(z).
\end{aligned}
$$

Now $B^-(z)$ has to be independent of k. After canceling common factors we use $\Gamma(z)\Gamma(1-z)=\pi/\sin\pi z$, $z\notin\mathbb{Z}$, to obtain

$$
B^-(z)=\Big(\frac{\sqrt{a^2-1}-a}{\sqrt{a^2-1}+a}\Big)^y(4(1-a^2))^{\varepsilon}\frac{\sin(\pi(y-\varepsilon))}{\sqrt{\sin(\pi(\varepsilon-\lambda))\,\sin(\pi(-\varepsilon-\lambda))}}.
$$

Similarly, also using $\Gamma(z+1)=z\Gamma(z)$, we find

$$
A^-(z)=\frac{\pi}{\Gamma(1+\lambda-y)\Gamma(-\lambda-y)}\Big(\frac{\sqrt{a^2-1}-a}{\sqrt{a^2-1}+a}\Big)^y\frac{(4(1-a^2))^{\varepsilon}}{\sqrt{\sin(\pi(\varepsilon-\lambda))\,\sin(\pi(-\varepsilon-\lambda))}}.
$$

(4.4.8) Next we calculate the Wronskians $[v^-(z),v^+(z)]$ and $[u^-(z),v^+(z)]$. To calculate the first Wronskian observe that we can take the limit $k\to\infty$ in

$$
[v^-(z),v^+(z)]=a_{-k}\big(v^-_{-k+1}(z)v^+_{-k}(z)-v^-_{-k}(z)v^+_{-k+1}(z)\big)
$$

using the asymptotic behaviour of (4.4.5). This gives, using $y=z/2\sqrt{a^2-1}$,

$$
\begin{aligned}
[v^-(z),v^+(z)]=&a_{-k}\big(\frac12-\frac{a}{2\sqrt{a^2-1}}\big)^{\varepsilon-y}\big(\frac12+\frac{a}{2\sqrt{a^2-1}}\big)^{\varepsilon+y}\\
&\times\Big((k-1)^{y-\frac12}(a-\sqrt{a^2-1})^{1-k}k^{-\frac12-y}(a+\sqrt{a^2-1})^{-k}\\
&\qquad-k^{y-\frac12}(a-\sqrt{a^2-1})^{-k}(k-1)^{-\frac12-y}(a+\sqrt{a^2-1})^{1-k}\Big)
\end{aligned}
$$

and taking out common factors and using that $a_{-k}=k(1+\mathcal{O}(\frac1k))$ gives

$$
[v^-(z),v^+(z)]=-2\sqrt{a^2-1}(4(1-a^2))^{-\varepsilon}\Big(\frac{\sqrt{a^2-1}+a}{\sqrt{a^2-1}-a}\Big)^y.
$$

From (4.4.7) it follows that, $y = z/2\sqrt{a^2-1}$,

$$[u^-(z), v^+(z)] = B^-(z)[v^-(z), v^+(z)] = -2\sqrt{a^2-1}\frac{\sin(\pi(y-\varepsilon))}{\sqrt{\sin(\pi(\varepsilon-\lambda))\,\sin(\pi(-\varepsilon-\lambda))}}.$$

We see that the Wronskian $[u^-(z), v^+(z)]$, as a function of z, has no poles and it has zeroes at $z = 2(\varepsilon + l)\sqrt{a^2-1}$, $l \in \mathbb{Z}$.

(4.4.9) With all these preparations we can calculate the spectral measure for the doubly infinite Jacobi operator L with coefficients as in (4.4.1), where we assume $a > 1$. So we can take $\phi_z = u^-(z)$ and $\Phi_z = v^+(z)$. And we see that these solutions are analytic in z, since $\Gamma(c)^{-1}\,{}_2F_1(a, b; c; z)$ is analytic in c. Hence, the only contribution in the spectral measure, cf. (4.3.4), comes from the zeroes of the Wronskian, so that the spectrum is purely discrete.

Theorem. *The operator L on $\ell^2(\mathbb{Z})$ defined by* (4.1.1), (4.4.1) *is essentially self-adjoint. For $a > 1$ its self-adjoint extension has completely discrete spectrum $\{2(\varepsilon + l)\sqrt{a^2-1}\}_{l\in\mathbb{Z}}$, and in particular the set*

$$\bigl\{u^-(2(\varepsilon + l)\sqrt{a^2-1}) \mid l \in \mathbb{Z}\bigr\}$$

constitutes a complete orthogonal basis of $\ell^2(\mathbb{Z})$. Moreover,

$$\|u^-(2(\varepsilon + l)\sqrt{a^2-1})\|^2 = \Bigl(\frac{4(a^2-1)(a-\sqrt{a^2-1})}{a+\sqrt{a^2-1}}\Bigr)^{\varepsilon}\Bigl(\frac{a-\sqrt{a^2-1}}{a+\sqrt{a^2-1}}\Bigr)^{l}\Gamma(\varepsilon + l - \lambda)\Gamma(1 + \varepsilon + l + \lambda).$$

Remark (i) Note that hypergeometric expression for u^- as in Lemma (4.4.4) displays Bessel coefficient behaviour, and we can think of the orthogonality relations as a natural extension of the Hansen-Lommel orthogonality relations $\sum_{k=-\infty}^{\infty} J_{k+n}(z)J_k(z) = \delta_{n,0}$ for the Bessel functions, see (4.4.10).
(ii) Note that the spectrum is independent of λ.

Proof. Put $\phi_z = u^-(z)$ and $\Phi_z = v^+(z)$, then we see that, see (4.3),

$$\langle G(z)u, v\rangle = \sum_{k,l=-\infty}^{\infty} G_{k,l}(z)u_l\bar{v}_k = \frac{1}{[\phi_z, \Phi_z]}\sum_{k\le l}(\Phi_z)_k(\phi_z)_l\bigl(u_l\bar{v}_k + u_k\bar{v}_l\bigr)(1 - \frac{1}{2}\delta_{k,l}).$$

Hence, the only contribution in

$$E_{u,v}\bigl((a, b)\bigr) = \lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\frac{1}{2\pi i}\int_{a+\delta}^{b-\delta}\langle G(x + i\varepsilon)u, v\rangle - \langle G(x - i\varepsilon)u, v\rangle\, dx$$

can come from the zeroes of the Wronskian. Put $x_l = 2(\varepsilon + l)\sqrt{a^2-1}$, then for (a, b) containing precisely one of the x_l's we find

$$E_{u,v}\bigl((a, b)\bigr) = E_{u,v}\bigl(\{x_l\}\bigr) = -\frac{1}{2\pi i}\oint_{(x_l)}\langle G(z)u, v\rangle\, dz.$$

Note that the minus sign comes from the clockwise orientation of the rectangle with upper side $x + i\varepsilon$, $x \in [a, b]$, and lower side $x - i\varepsilon$, $x \in [a, b]$. This residue can be calculated and we find

$$\begin{aligned}\mathrm{Res}_{z=x_l}\frac{1}{[\phi_z, \Phi_z]} &= \frac{-\sqrt{\sin(\pi(\varepsilon-\lambda))\,\sin(\pi(-\varepsilon-\lambda))}}{2\sqrt{a^2-1}}\mathrm{Res}_{z=x_l}\frac{1}{\sin(-\varepsilon\pi + \pi z/2\sqrt{a^2-1})}\\ &= \frac{(-1)^{l+1}}{\pi}\sqrt{\sin(\pi(\varepsilon-\lambda))\,\sin(\pi(-\varepsilon-\lambda))}\end{aligned}$$

Since $u_k^-(x_l) = A^-(x_l)v_k^+(x_l)$, because the zeroes of the Wronskian $[u^-(z), v^+(z)]$ correspond to the zeroes of $B^-(z)$, see (4.4.8), we see that ϕ_z and Φ_z are multiples of each other for $z = x_l$. So we can symmetrise the sum in $\langle G(z)u, v\rangle$ again, and we find

$$E_{u,v}\big(\{x_l\}\big) = \frac{(-1)^l}{\pi A^-(x_l)}\sqrt{\sin(\pi(\varepsilon-\lambda))\,\sin(\pi(-\varepsilon-\lambda))}\langle u, \phi_{x_l}\rangle\langle v, \phi_{x_l}\rangle.$$

Using the explicit expression for $A^-(x_l)$ of (4.4.7) and the reflection identity for the Γ-function we arrive at

$$E_{u,v}\big(\{x_l\}\big) = \Big(\frac{4(a^2-1)(a-\sqrt{a^2-1})}{a+\sqrt{a^2-1}}\Big)^{-\varepsilon}\Big(\frac{a+\sqrt{a^2-1}}{a-\sqrt{a^2-1}}\Big)^l \frac{\langle u, \phi_{x_l}\rangle\langle v, \phi_{x_l}\rangle}{\Gamma(\varepsilon+l-\lambda)\Gamma(1+\varepsilon+l+\lambda)}.$$

Note that in particular, ϕ_{x_l} are eigenvectors of L for the eigenvalue x_l, and moreover these eigenspaces are 1-dimensional. Hence $E(\{x_l\})\phi_{x_l} = \phi_{x_l}$. Recall $E_{u,v}\big(\{x_l\}\big) = \langle E\big(\{x_l\}\big)u, v\rangle$, and take $u = v = \phi_{x_l}$ to find

$$\|\phi_{x_l}\|^2 = \Big(\frac{4(a^2-1)(a-\sqrt{a^2-1})}{a+\sqrt{a^2-1}}\Big)^{-\varepsilon}\Big(\frac{a+\sqrt{a^2-1}}{a-\sqrt{a^2-1}}\Big)^l \frac{\|\phi_{x_l}\|^4}{\Gamma(\varepsilon+l-\lambda)\Gamma(1+\varepsilon+l+\lambda)}$$

from which the squared norm follows. Using $E(\{x_l\})E(\{x_m\}) = \delta_{l,m}E(\{x_l\})$ and self-adjointness of E gives

$$\begin{aligned}\langle \phi_{x_l}, \phi_{x_m}\rangle &= \langle E(\{x_l\})\phi_{x_l}, E(\{x_m\})\phi_{x_m}\rangle = \langle E(\{x_m\})E(\{x_l\})\phi_{x_l}, \phi_{x_m}\rangle \\ &= \delta_{l,m}\langle E(\{x_l\})\phi_{x_l}, \phi_{x_m}\rangle = \delta_{l,m}\langle \phi_{x_l}, \phi_{x_m}\rangle\end{aligned}$$

which proves the orthogonality. □

(4.4.10) The orthogonality relations arising from Theorem (4.4.9) can be worked out and they give

$$\begin{aligned}\sum_{k=-\infty}^{\infty} &\frac{\Gamma(k+\lambda+\varepsilon+1)\Gamma(k+\varepsilon-\lambda)}{(4(a^2-1))^k} \\ &\times \frac{1}{\Gamma(k+1-l)}\,{}_2F_1\left(\begin{matrix}k+\varepsilon+\lambda+1, k+\varepsilon-\lambda\\ k+1-l\end{matrix};\frac12-\frac{a}{2\sqrt{a^2-1}}\right) \\ &\times \frac{1}{\Gamma(k+1-p)}\,{}_2F_1\left(\begin{matrix}k+\varepsilon+\lambda+1, k+\varepsilon-\lambda\\ k+1-p\end{matrix};\frac12-\frac{a}{2\sqrt{a^2-1}}\right) \\ &= \delta_{p,l}\Big(\frac{4(a^2-1)(a-\sqrt{a^2-1})}{a+\sqrt{a^2-1}}\Big)^{\varepsilon}\Big(\frac{a-\sqrt{a^2-1}}{a+\sqrt{a^2-1}}\Big)^l\Gamma(\varepsilon+l-\lambda)\Gamma(1+\varepsilon+l+\lambda).\end{aligned}$$

Since Theorem (4.4.9) also gives the completeness of this set of vectors, the dual orthogonality relations also hold, i.e.

$$\begin{aligned}\sum_{l=-\infty}^{\infty} &\Big(\frac{a+\sqrt{a^2-1}}{a-\sqrt{a^2-1}}\Big)^l\frac{1}{\Gamma(\varepsilon+l-\lambda)\Gamma(1+\varepsilon+l+\lambda)} \\ &\times \frac{1}{\Gamma(k+1-l)}\,{}_2F_1\left(\begin{matrix}k+\varepsilon+\lambda+1, k+\varepsilon-\lambda\\ k+1-l\end{matrix};\frac12-\frac{a}{2\sqrt{a^2-1}}\right) \\ &\times \frac{1}{\Gamma(m+1-l)}\,{}_2F_1\left(\begin{matrix}m+\varepsilon+\lambda+1, m+\varepsilon-\lambda\\ m+1-l\end{matrix};\frac12-\frac{a}{2\sqrt{a^2-1}}\right) \\ &= \delta_{k,m}\frac{(4(a^2-1))^k}{\Gamma(k+\lambda+\varepsilon+1)\Gamma(k+\varepsilon-\lambda)}\Big(\frac{4(a^2-1)(a-\sqrt{a^2-1})}{a+\sqrt{a^2-1}}\Big)^{\varepsilon}.\end{aligned}$$

(4.4.11) *Exercise.* Use the results of [17] in order to calculate explicitly the spectral measures for the case $|a| \leq 1$. In this case the spaces $S_z^{\pm}$ are spanned by different solutions depending on the sign of $\Im z$.

In case $|a| \leq 1$ the situation changes considerably, and let us state briefly some of the results needed for the Meizner-Pollaczek case, i.e. $|a| < 1$. The analogue of Lemma (4.4.4) is proved in entirely the same way, and we find that

$$\begin{aligned} U_k^{\pm}(z) &= (\pm 1)^k (2i\sin\psi)^{-k} \frac{\sqrt{\Gamma(k+1+\lambda+\varepsilon)\Gamma(k+\varepsilon-\lambda)}}{\Gamma(k+1+\varepsilon \mp iz)} \\ &\quad \times {}_2F_1\left(\begin{matrix} k+1+\lambda+\varepsilon, k+\varepsilon-\lambda \\ k+1+\varepsilon\mp iz \end{matrix}; \frac{1}{1-e^{\pm 2i\psi}}\right), \\ V_k^{\pm}(z) &= (\pm 1)^k (2i\sin\psi)^{k} \frac{\sqrt{\Gamma(1-k+\lambda-\varepsilon)\Gamma(-k-\varepsilon-\lambda)}}{\Gamma(1-k-\varepsilon \mp iz)} \\ &\quad \times {}_2F_1\left(\begin{matrix} 1-k+\lambda-\varepsilon, -k-\varepsilon-\lambda \\ 1-k-\varepsilon\mp iz \end{matrix}; \frac{1}{1-e^{\mp 2i\psi}}\right), \end{aligned}$$

satisfy the recurrence relation

$$(2\sin\psi)\, z\, u_k(z) = a_k(\cos\psi,\lambda,\varepsilon)\, u_{k+1}(z) + b_k(\cos\psi,\lambda,\varepsilon)\, u_k(z) + a_{k-1}(\cos\psi,\lambda,\varepsilon)\, u_{k-1}(z)$$

with the explicit values for a_k and b_k of (4.4.1) with $a = \cos\psi$, $0 < \psi < \pi$. This gives four linearly independent solutions of the recurrence relation. The connection formulae for these four solutions are given by

$$U_k^+(z) = A^+(z)\, V_k^+(z) + B^+(z)\, V_k^-(z), \qquad U_k^-(z) = A^-(z)\, V_k^+(z) + B^-(z)\, V_k^-(z)$$

and it follows easily from the explicit expressions and the assumptions on λ and ε of (4.4.1) that $\overline{U_k^+(z)} = U_k^-(\bar z)$ and $\overline{V_k^+(z)} = V_k^-(\bar z)$, implying that $A^-(z) = \overline{B^+(\bar z)}$ and $B^-(z) = \overline{A^+(\bar z)}$. The same formula for hypergeometric series as in (4.4.7) can be used to find the connection coefficients;

$$\begin{aligned} A^+(z) &= (2\sin\psi)^{2\varepsilon} e^{2z(\psi-\frac{\pi}{2})} \frac{\sqrt{\Gamma(-\varepsilon-\lambda)\Gamma(1+\lambda-\varepsilon)\Gamma(1+\lambda+\varepsilon)\Gamma(\varepsilon-\lambda)}}{\Gamma(iz-\varepsilon)\Gamma(1+\varepsilon-iz)}, \\ B^+(z) &= (2\sin\psi)^{2\varepsilon} e^{2z(\psi-\frac{\pi}{2})} \frac{\sqrt{\Gamma(-\varepsilon-\lambda)\Gamma(1+\lambda-\varepsilon)\Gamma(1+\lambda+\varepsilon)\Gamma(\varepsilon-\lambda)}}{\Gamma(\lambda+1-iz)\Gamma(-\lambda-iz)}. \end{aligned}$$

The asymptotic behaviour can be determined as in (4.4.5), and we find that $\phi_z = U^+(z)$ for $\Im z > 0$ and $\phi_z = U^-(z)$ for $\Im z < 0$ and $\Phi_z = V^+(z)$ for $\Im z > 0$ and $\Phi_z = V^-(z)$ for $\Im z < 0$. The explicit asymptotic behaviour can be used as in (4.4.8) to find the Wronskian

$$[V^-(z), V^+(z)] = -i\,(2\sin\psi)^{1-2\varepsilon} e^{-2z(\psi-\frac{\pi}{2})},$$

and from this expression and the connection coefficients we can calculate all Wronskians needed. In order to find the spectral measure we have to investigate the limit $\varepsilon \downarrow 0$ of $\langle G(x+i\varepsilon)u, v\rangle - \langle G(x-i\varepsilon)u, v\rangle$, $x \in \mathbb{R}$, and for this we consider, using the connection formulae,

$$\begin{aligned} &\frac{V_k^+(x)U_l^+(x)}{B^+(x)[V^-(x),V^+(x)]} - \frac{V_k^-(x)U_l^-(x)}{A^-(x)[V^+(x),V^-(x)]} = \\ &\frac{V_k^+(x)V_l^-(x) + V_k^-(x)V_l^+(x)}{[V^-(x),V^+(x)]} + \frac{A^+(x)A^-(x)V_l^+(x)V_k^+(x) + B^-(x)B^+(x)V_k^-(x)V_l^-(x)}{A^-(x)B^+(x)[V^-(x),V^+(x)]}, \end{aligned}$$

which is obviously symmetric in k and l. Hence we can antisymmetrise the sum for the spectral measure and we find for $u,v\in\ell^2(\mathbb{Z})$

$$\begin{aligned}2\pi i\langle u,v\rangle &= \int_{\mathbb{R}}\Big(A^-(x)B^+(x)\langle u,V^+(x)\rangle\langle V^+(x),v\rangle + A^-(x)B^+(x)\langle u,V^-(x)\rangle\langle V^-(x),v\rangle \\ &\qquad + A^+(x)A^-(x)\langle u,V^-(x)\rangle\langle V^+(x),v\rangle + B^+(x)B^-(x)\langle u,V^+(x)\rangle\langle V^-(x),v\rangle\Big) \\ &\qquad \times\frac{dx}{A^-(x)B^+(x)[V^-(x),V^+(x)]} \\ &= \int_{\mathbb{R}}\Big(\langle u,U^-(x)\rangle\langle U^-(x),v\rangle + (A^-(x)B^+(x)-A^+(x)B^-(x))\langle u,V^-(x)\rangle\langle V^-(x),v\rangle\Big) \\ &\qquad \times\frac{dx}{A^-(x)B^+(x)[V^-(x),V^+(x)]}\end{aligned}$$

describing the spectral measure, where we have used the relations between $U_k^\pm(z)$ and $V_k^\pm(x)$ for the second equality. So we see that the spectrum of the corresponding operator is $\mathbb{R}$, and by inserting the values for the Wronskian and the connection coefficients we see that the spectral measure is described by the following integral;

$$\begin{aligned}&\langle u,v\rangle = \\ &\frac{1}{2\pi}\int_{\mathbb{R}}\frac{|\Gamma(\lambda+1-ix)\Gamma(-\lambda-ix)|^2}{\Gamma(-\varepsilon-\lambda)\Gamma(1+\lambda-\varepsilon)\Gamma(1+\lambda+\varepsilon)\Gamma(\varepsilon-\lambda)}(2\sin\psi)^{-1-2\varepsilon}e^{-2x(\psi-\frac{\pi}{2})}\langle u,U^-(x)\rangle\langle U^-(x),v\rangle \\ &\quad + \Big(1-\frac{|\Gamma(\lambda+1-ix)\Gamma(-\lambda-ix)|^2}{|\Gamma(ix-\varepsilon)\Gamma(1+\varepsilon-ix)|^2}\Big)(2\sin\psi)^{-1+2\varepsilon}e^{2x(\psi-\frac{\pi}{2})}\langle u,V^-(x)\rangle\langle V^-(x),v\rangle\,dx.\end{aligned}$$

We see that the spectral projection is on a two-dimensional space of generalised eigenvectors. Note that the general theory ensures the positivity of the measure in case $u=v$, and we can also check directly that, under the conditions on λ and ε as in (4.4.1), the second term in the integrand is indeed positive.

4.5. **Example: the basic hypergeometric difference equation.** This example is based on Appendix A in [13], which was greatly motivated by Kakehi [10] and unpublished notes by Koornwinder. The transform described in this section has been obtained from its quantum $SU(1,1)$ group theoretic interpretation, see [10], [13] for references. On a formal level the result can be obtained as a limit case of the orthogonality of the Askey-Wilson polynomials, see [14] for a precise formulation. The limit transition descibed in (4.5.10) is motivated from the fact that the Jacobi operators in this example and the previous example play the same role.

(4.5.1) We take the coefficients as

$$a_k=\frac{1}{2}\sqrt{(1-\frac{q^{-k}}{r})(1-\frac{cq^{-k}}{d^2r})},\qquad b_k=\frac{q^{-k}(c+q)}{2dr},$$

where we assume $0<q<1$, and $r<0$, $c>0$, $d\in\mathbb{R}$. This assumption is made in order to get the expression under the square root sign positive. There are more possible choices in order to achieve this, see [13, App. A]. Note that a_k and b_k are bounded for $k<0$, so that J^- is self-adjoint. Hence, the deficiency indices of L are $(0,0)$ or $(1,1)$ by Theorem (4.2.2).

(4.5.2) In order to write down solutions of $Lu = z\,u$ we need the basic hypergeometric series. Define

$$(a;q)_k = \prod_{i=0}^{k-1}(1-aq^i), \qquad k \in \mathbb{Z}_{\geq 0} \cup \{\infty\}, \qquad (a_1,\ldots,a_n;q)_k = \prod_{j=1}^{n}(a_j;q)_k,$$

and the basic hypergeometric series

$${}_2\varphi_1\left(\begin{matrix} a,b \\ c \end{matrix};q,x\right) = \sum_{k=0}^{\infty}\frac{(a,b;q)_k}{(q,c;q)_k}x^k.$$

The radius of convergence is 1, and there exists a unique analytic continuation to $\mathbb{C}\backslash[1,\infty)$. See Gasper and Rahman [9] for all the necessary information on basic hypergeometric series.

Lemma. *Put*

$$w_k^2 = d^{2k}\frac{(cq^{1-k}/d^2r;q)_\infty}{(q^{1-k}/r;q)_\infty},$$

$$f_k(\mu(y)) = {}_2\varphi_1\left(\begin{matrix} dy, d/y \\ c \end{matrix};q,rq^k\right), \qquad c \notin q^{-\mathbb{Z}_{\geq 0}}, \quad \mu(y) = \frac{1}{2}(y+y^{-1}),$$

$$g_k(\mu(y)) = q^k c^{-k}\,{}_2\varphi_1\left(\begin{matrix} qdy/c, qd/cy \\ q^2/c \end{matrix};q,rq^k\right), \quad \mu(y) = \frac{1}{2}(y+y^{-1}),$$

$$F_k(y) = (dy)^{-k}\,{}_2\varphi_1\left(\begin{matrix} dy, qdy/c \\ qy^2 \end{matrix};q,\frac{q^{1-k}c}{d^2r}\right), \qquad y^2 \notin q^{-\mathbb{N}},$$

then, with $z=\mu(y)$, we have that $u_k(z) = w_k f_k(\mu(y))$, $u_k(z) = w_k g_k(\mu(y))$, $u_k(z) = w_k F_k(y)$ and $u_k(z) = w_k F_k(y^{-1})$ define solutions to

$$z\,u_k(z) = a_k\,u_{k+1}(z) + b_k\,u_k(z) + a_{k-1}\,u_{k-1}(z).$$

Proof. Put $u_k(z) = w_k v_k(z)$, then $v_k(z)$ satisfies

$$2z\,v_k(z) = (d - \frac{cq^{-k}}{dr})\,v_{k+1}(z) + q^{-k}\frac{c+q}{dr}\,v_k(z) + (d^{-1} - \frac{q^{1-k}}{dr})\,v_{k-1}(z)$$

and this is precisely the second order q-difference equation that has the solutions given, see [9, exerc. 1.13]. □

(4.5.3) The asymptotics of the solutions of Lemma (4.5.2) can be given as follows. First observe that $w_{-k} = d^{-k}$ as $k\to\infty$, and using

$$w_k^2 = c^k\frac{(rq^k, d^2r/c, cq/d^2r;q)_\infty}{(d^2rq^k/c, r, q/r;q)_\infty} \Rightarrow w_k = \mathcal{O}(c^{\frac{1}{2}k}),\ k\to\infty.$$

Now $f_k(\mu(y)) = \mathcal{O}(1)$ as $k\to\infty$, and $g_k(\mu(y)) = \mathcal{O}((q/c)^k)$ as $k\to\infty$. Similarly, $F_{-k}(y) = \mathcal{O}((dy)^k)$ as $k\to\infty$.

Proposition. *The operator L is essentially self-adjoint for $0 < c \leq q^2$, and L has deficiency indices $(1,1)$ for $q^2 < c < 1$. Moreover, for $z \in \mathbb{C}\backslash\mathbb{R}$ the one-dimensional space S_z^- is spanned by $wF(y)$ with $\mu(y) = z$ and $|y| < 1$. For $0 < c \leq q^2$ the one-dimensional space S_z^+ is spanned by $wf(z)$, and for $q^2 < c < 1$ the two-dimensional space S_z^+ is spanned by $wf(z)$ and $wg(z)$.*

Proof. In (4.5.1) we have already observed that the deficiency indices of L are $(0,0)$ or $(1,1)$. Now $2a_k = q^{-k}\sqrt{c/d^2r^2} - \frac{1}{2}(r + d^2r/c) + \mathcal{O}(q^k)$, $k\to\infty$, shows that the boundedness condition of Proposition (3.4.6)(ii) is satisfied if the coefficient of q^{-k} in $a_k + a_{k-1} \pm b_k$ is non-positive. Since $c > 0$, $dr \in \mathbb{R}$, this is the case when $(1+q)\sqrt{c} \leq c + q$. For $0 < c \leq q^2$ the inequality holds, so that by Proposition (3.4.6)(ii) also J^+, and hence L by Theorem (4.2.2), is essentially self-adjoint.

From the asymptotic behaviour we see that $wf(z)$ and $wg(z)$ are linearly independent solutions of the recurrence in Lemma (4.5.3), and moreover that they both belong to S_z^+ for $q^2 < c < 1$. The other statements follow easily from the asymptotics described above. □

(4.5.4) The Wronskian

$$[wF(y), wF(y^{-1})] = \lim_{k\to-\infty} a_k w_{k+1} w_k \big(F_{k+1}(y)F_k(y^{-1}) - F_k(y)F_{k+1}(y^{-1})\big) = \frac{1}{2}(y^{-1} - y)$$

using $a_k \to \frac{1}{2}$ as $k \to -\infty$ and the asymptotics of (4.5.3). Note that the Wronskian is non-zero for $y \neq \pm 1$ or $z \neq \pm 1$. Since $wF(y)$ and $wF(y^{-1})$ are linearly independent solutions to the recurrence in Lemma (4.5.2) for $z \in \mathbb{C}\backslash\mathbb{R}$, we see that we can express $f_k(\mu(y))$ in terms of $F_k(y)$ and $F_k(y^{-1})$. These solutions are related by the expansion

$$\begin{aligned} f_k(\mu(y)) &= c(y)F_k(y) + c(y^{-1})F_k(y^{-1}), \\ c(y) &= \frac{(c/dy, d/y, dry, q/dry; q)_\infty}{(y^{-2}, c, r, q/r; q)_\infty}, \end{aligned} \tag{4.5}$$

for $c \notin q^{-\mathbb{Z}_{\geq 0}}$, $y^2 \notin q^{\mathbb{Z}}$, see [9, (4.3.2)]. This shows that we have

$$[wf(\mu(y)), wF(y)] = \frac{1}{2}c(y^{-1})(y - y^{-1}).$$

(4.5.5) Let us assume first that $0 < c \leq q^2$, so that L is essentially self-adjoint. Then for $z \in \mathbb{C}\backslash\mathbb{R}$ we have $\phi_z = wf(z)$ and $\Phi_z = wF(y)$, where $z = \mu(y)$ and $|y| < 1$. In particular, it follows that $\phi_{x\pm i\varepsilon} \to \phi_x$ as $\varepsilon \downarrow 0$. For the asymptotic solution Φ_z we have to be more careful in computing the limit of z to the real axis. For $x \in \mathbb{R}$ satisfying $|x| > 1$ we have $\Phi_{x\pm i\varepsilon} \to wF_y$ as $\varepsilon \downarrow 0$, where $y \in (-1,1)\backslash\{0\}$ is such that $\mu(y) = x$. If $x \in [-1,1]$, then we put $x = \cos\chi = \mu(e^{i\chi})$ with $\chi \in [0,\pi]$, and then $\Phi_{x-i\varepsilon} \to wF_{e^{i\chi}}$ and $\Phi_{x+i\varepsilon} \to wF_{e^{-i\chi}}$ as $\varepsilon \downarrow 0$.

(4.5.6) We calculate the integrand in the Stieltjes-Perron inversion formula of (2.3.4) using Proposition (4.3.3) and (4.3) in the case $|x| < 1$, where $x = \cos\chi = \mu(e^{i\chi})$. For $u, v \in \mathcal{D}(\mathbb{Z})$ we have

$$\begin{aligned}
&\lim_{\varepsilon\downarrow 0} \langle G(x+i\varepsilon)u, v\rangle - \langle G(x-i\varepsilon)u, v\rangle = \\
&\lim_{\varepsilon\downarrow 0} \sum_{k\leq l} \Big(\frac{(\Phi_{x+i\varepsilon})_k (\phi_{x+i\varepsilon})_l}{[\phi_{x+i\varepsilon}, \Phi_{x+i\varepsilon}]} - \frac{(\Phi_{x-i\varepsilon})_k (\phi_{x-i\varepsilon})_l}{[\phi_{x-i\varepsilon}, \Phi_{x-i\varepsilon}]} \Big) (u_l \bar v_k + u_k \bar v_l)(1 - \frac{1}{2}\delta_{k,l}) = \\
&2\sum_{k\leq l} \Big(\frac{w_k F_k(e^{-i\chi}) w_l f_l(\cos\chi)}{c(e^{i\chi})(e^{-i\chi} - e^{i\chi})} - \frac{w_k F_k(e^{i\chi}) w_l f_l(\cos\chi)}{c(e^{-i\chi})(e^{i\chi} - e^{-i\chi})} \Big) (u_l \bar v_k + u_k \bar v_l)(1 - \frac{1}{2}\delta_{k,l}) = \\
&2\sum_{k\leq l} \Big(w_k w_l f_l(\cos\chi) \frac{c(e^{-i\chi})F_k(e^{-i\chi}) + c(e^{i\chi})F_k(e^{i\chi})}{c(e^{i\chi})c(e^{-i\chi})(e^{-i\chi} - e^{i\chi})} \big(u_l \bar v_k + u_k \bar v_l\big)(1 - \frac{1}{2}\delta_{k,l}) = \\
&2\sum_{k\leq l} \Big(\frac{w_k w_l f_l(\cos\chi) f_k(\cos\chi)}{c(e^{i\chi})c(e^{-i\chi})(e^{-i\chi} - e^{i\chi})} \big(u_l \bar v_k + u_k \bar v_l\big)(1 - \frac{1}{2}\delta_{k,l}) = \\
&\frac{2}{c(e^{i\chi})c(e^{-i\chi})(e^{-i\chi} - e^{i\chi})} \sum_{l=-\infty}^{\infty} w_l f_l(\cos\chi) u_l \sum_{k=-\infty}^{\infty} w_k f_k(\cos\chi) \bar v_k
\end{aligned}$$

using the expansion (4.5) and the Wronskian in (4.5.4). Now integrate over the interval (a,b) with $-1 \leq a < b \leq 1$ and replacing x by $\cos\chi$, so that $\frac{1}{2\pi i}dx = (e^{i\chi} - e^{-i\chi})d\chi/4\pi$ we obtain, with

$a = \cos\chi_a$, $b = \cos\chi_b$, and $0 \le \chi_b < \chi_a \le \pi$,

$$E_{u,v}\big((a,b)\big) = \frac{1}{2\pi}\int_{\chi_b}^{\chi_a} \big(\mathcal{F}u\big)(\cos\chi)\overline{\big(\mathcal{F}v\big)(\cos\chi)}\frac{d\chi}{|c(e^{i\chi})|^2},$$

$$\big(\mathcal{F}u\big)(x) = \langle u, \phi_x\rangle = \sum_{l=-\infty}^{\infty} w_l f_l(\cos\chi)u_l.$$

This shows that $[-1,1]$ is contained in the continuous spectrum of L.

(4.5.7) For $|x| > 1$ we can calculate as in (4.5.6) the integrand in the Stieltjes-Perron inversion formula, but now we use that $x = \mu(y)$ with $|y| < 1$, see (4.5.5). This gives

$$\lim_{\varepsilon\downarrow 0}\langle G(x+i\varepsilon)u, v\rangle = 2\sum_{k\le l}\frac{w_kF_k(y)w_lf_l(y)}{c(y^{-1})(y-y^{-1})}\big(u_l\bar v_k + u_k\bar v_l\big)(1-\frac{1}{2}\delta_{k,l}),$$

and since the limit $\lim_{\varepsilon\downarrow 0}\langle G(x+i\varepsilon)u,v\rangle$ gives the same result, we see, as in the case of the Meixner functions, that we can only have discrete mass points for $|x| > 1$ in the spectral measure at the zeroes of the Wronskian, i.e. at the zeroes of $y \mapsto c(y^{-1})$ with $|y| < 1$ or at $y = \pm 1$. Let us assume that all zeroes of the c-function are simple, so that the spectral measure at these points can be easily calculated.

The zeroes of the c-function can be read off from the expressions in (4.5), and they are $\{cq^k/d \mid k \in \mathbb{Z}_{\ge 0}\}$, $\{dq^k \mid k \in \mathbb{Z}_{\ge 0}\}$ and $\{q^k/dr \mid k \in \mathbb{Z}\}$. Assuming that $|c/d| < 1$ and $|d| < 1$, we see that the first two sets do not contribute. In the more general case we have that the product is less than 1, since the product equals $c < 1$. We leave this extra case to the reader. The last set, labeled by Z always contributes to the spectral measure. Now for $u, v \in \mathcal{D}(\mathbb{Z})$ we let $x_p = \mu(y_p)$, $y_p = q^p/dr$, $p \in \mathbb{Z}$, with $|q^p/dr| > 1$, so that, cf. (4.4.9),

$$E_{u,v}(\{x_p\}) = \mathrm{Res}_{y=y_p^{-1}}\Big(\frac{-1}{c(y^{-1})y}\Big)w_kF_k(y_p^{-1})w_lf_l(x_p)\big(u_l\bar v_k + u_k\bar v_l\big)(1-\frac{1}{2}\delta_{k,l})$$

after substituting $x = \mu(y)$. Now from (4.5) we find $f_k(x_p) = c(y_p)F_k(y_p^{-1})$, since $c(y_p^{-1}) = 0$ and we assume here that $c(y_p) \ne 0$. Hence, we can symmetrise the sum again and find

$$E_{u,v}(\{x_p\}) = \Big(\mathrm{Res}_{y=y_p}\frac{1}{c(y^{-1})c(y)y}\Big)\big(\mathcal{F}u\big)(x_p)\overline{\big(\mathcal{F}v\big)(x_p)}$$

switching to the residue at y_p.

(4.5.8) We can combine the calculations in the following theorem. Note that most of the regularity conditions can be removed by continuity after calculating explicitly all the residues. The case of an extra set of finite mass points is left to the reader, cf. (4.5.7), as well as the case of other choices of the parameters c, d and r for which the expression under the square root sign in a_k in (4.5.1) is positive. See [13, App. A] for details.

Theorem. *Assume $r < 0$, $0 < c \le q^2$, $d \in \mathbb{R}$ with $|d| < 1$ and $|c/d| < 1$ such that the zeroes of $y \mapsto c(y)$ are simple and $c(y) = 0$ implies $c(y^{-1}) \ne 0$. Then the spectral measure for the Jacobi operator on $\ell^2(\mathbb{Z})$ defined by (4.5.1) is given by, $A \subset \mathbb{R}$ a Borel set,*

$$\langle E(A)u,v\rangle = \int_{\cos\chi\in[-1,1]\cap A}\big(\mathcal{F}u\big)(\cos\chi)\overline{\big(\mathcal{F}v\big)(\cos\chi)}\frac{d\chi}{|c(e^{i\chi})|^2}$$
$$+ \sum_{p\in\mathbb{Z},|q^p/dr|>1,\mu(q^p/dr)\in A}\Big(Res_{y=q^p/dr}\frac{1}{c(y^{-1})c(y)y}\Big)\big(\mathcal{F}u\big)(\mu(q^p/dr))\overline{\big(\mathcal{F}v\big)(\mu(q^p/dr))}.$$

Proof. It only remains to prove that ± 1 is not contained in the point spectrum. These are precisely the points for which $F(y)$ and $F(y^{-1})$ are not linearly independent solutions. We have to show that $\phi_{\pm 1} \notin \ell^2(\mathbb{Z})$, and this can be done by determining its asymptotic behaviour as $k \to -\infty$, see [10], [12] for more information. □

Take $A = \mathbb{R}$ and $u = e_k$ and $v = e_l$, then we find the following orthogonality relations for the ${}_2\varphi_1$-series as in Lemma (4.5.2);

$$\int_0^\pi f_k(\cos\chi) f_l(\cos\chi) \frac{d\chi}{|c(e^{i\chi})|^2} + \sum_{p\in\mathbb{Z}, |q^p/dr|>1} \Big(\mathrm{Res}_{y=q^p/dr} \frac{1}{c(y^{-1})c(y)y}\Big) f_k(\mu(\frac{q^p}{dr})) f_l(\mu(\frac{q^p}{dr})) = \frac{\delta_{k,l}}{w_k^2}.$$

(4.5.9) In Theorem (4.5.8) we have made the assumption $0 < c \le q^2$ in order to have L as an essentially self-adjoint operator. From the general considerations in (4.3.1)-(4.3.4) it follows that the previous calculations, and in particular Theorem (4.5.8), remain valid for $q^2 < c < 1$ if we can show that there exists a self-adjoint extension of L satisfying the assumptions of (4.3.2). It suffices to check (2) of (4.3.2), or, by Lemma (4.2.3), the existence of a $\theta \in [0, 2\pi)$ such that

$$\lim_{k\to\infty} [wf(z), e^{i\theta} wF(i(1-\sqrt{2})) + e^{-i\theta} wF(-i(1-\sqrt{2}))]_k = 0. \tag{4.6}$$

Indeed, $wF(\pm i(1-\sqrt{2}))$ is the element $\Phi_{\pm i}$ up to the normalisation of the length. This is not important for showing the existence of θ satisfying (4.6).

For (4.6) we need to know the asymptotic behaviour of $F_k(y)$ as $k \to \infty$. The same result in basic hypergeometric series that results in (4.5) can be used to prove that

$$F_k(y) = a(y)\, f_k(y) + b(y)\, g_k(y),$$
$$a(y) = \frac{(qdy/c, qy/d, qcy/dr, dr/cy; q)_\infty}{(qy^2, q/c, qc/d^2r, d^2r/c; q)_\infty}, \quad b(y) = \frac{(dy, cy/d, q^2y/dr, dr/yq; q)_\infty}{(qy^2, c/q, qc/d^2r, d^2r/c; q)_\infty},$$

for $y^2, c \notin q^{\mathbb{Z}}$, so that $F_k(y) = a(y)\mathcal{O}(1) + b(y)\mathcal{O}((q/c)^k)$. It follows that

$$\lim_{k\to\infty} [wf(z), wF(y)]_k = \frac{1}{2}\Big|\frac{c}{dr}\Big|(1 - \frac{c}{q})\, b(y),$$

so that the limit in (4.6) equals

$$\frac{\big|\frac{c}{dr}\big|(1-\frac{c}{q})}{2\|F(i(1-\sqrt{2}))\|}\big(e^{i\theta} b(i(1-\sqrt{2})) + e^{-i\theta} b(-i(1-\sqrt{2}))\big).$$

The term in parentheses is $2\Re(e^{i\theta} b(i(1-\sqrt{2})))$, which is zero for $\theta = -\frac{\pi}{2} + \arg b(i(1-\sqrt{2}))$.

(4.5.10) The Meixner functions can formally be obtained as a limit case as $q \uparrow 1$ from the spectral analysis of the second order q-difference operator as considered here. For this we make the following specialisation; $c \mapsto qs^{-2}$, $d \mapsto q^{1+\lambda}s^{-1}$, $r \mapsto q^{-\varepsilon-\lambda}$, where ε and λ have the same meaning as in (4.4.1). Note that $r < 0$ is no longer valid but the operator is well-defined under suitable conditions on λ, cf. (4.4.1). The operator L with (4.5.1) has the same type of spectral measure (exercise). Now consider the operator

$$L_q = \frac{2L - s - s^{-1}}{1-q}, \qquad L_q f_k = a_k^q\, f_{k+1} + b_k^q\, f_k + a_{k-1}^q\, f_{k-1}$$

for $f_k = e_{-k}$, then a calculation shows that $a_k^q \to a_k$, $b_k^q \to b_k$ with a_k and b_k as in (4.4.1) with $2a = s + s^{-1}$ as $q \uparrow 1$. We now assume $a \ge 1$ as in the previous subsection on Meixner functions.

Now the operator L_q has continuous spectrum supported on $[(-2-s-s^{-1})/(1-q), (2-s-s^{-1})/(1-q)]$. For $s + s^{-1} > 2$ the continuous spectrum will disappear to $-\infty$ as $q \uparrow 1$; it will tend to $(-\infty, 0]$ for $s+s^{-1}=2$, and it will tend to $\mathbb{R}$ if $0 \leq s+s^{-1} < 2$. The discrete spectrum (or at least the infinite number of discrete mass points) is of the form

$$s\frac{q^{p-1+\varepsilon}-1}{1-q}+s^{-1}\frac{q^{1-\varepsilon-p}-1}{1-q}, \qquad p\in\mathbb{Z},\ |sq^{p+1-\varepsilon}|>1.$$

As $q \uparrow 1$ this tends to $(p+\varepsilon-1)(s^{-1}-s)$ with $p \in \mathbb{Z}$ for $|s|>1$ and it will disappear for $|s| \leq 1$. So for $a>1$ only the discrete spectrum survives and this corresponds precisely to Theorem (4.4.9). For $0 \leq a \leq 1$ the discrete spectrum disappears in the limit.

It is also possible to show that the solutions for the q-hypergeometric difference operator tend to to solutions of the operator for the Meixner functions. This requires the transformation as in (4.4.6), and one of Heine's transformations.

So we have motivated, at least formally, that the orthogonality relations for the Meixner functions can be obtained as a limit case of the ${}_2\varphi_1$-series that arise as solutions of the second order q-difference hypergeometric equation, and that the limit transition remains valid on the level of (the support of) the spectral measure. For the Laguerre and Meixner-Pollaczek functions the limit remains valid on the level of the support of the spectral measure.

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