Orthogonal Polynomials

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Contents

Chapter 1

Herglotz functions

1.1 Defintions and topological properties

We will work with three classes of functions. All of them will have certain advantages and are in an (almost) bijective correspondence.

1.1.1 Definition. Let $\Omega \subset \mathbb{C}$ be open. We denote by $\mathrm{Hol}(\Omega)$, the set of holomorphic functions on Ω.

- Let $f \in \mathrm{Hol}(\mathbb{D})$. f is called a *Schur function*, if $f(\mathbb{D}) \subset \overline{\mathbb{D}}$. The set of all Schur functions is denoted by $\mathcal{S}$.
- Let $f \in \mathrm{Hol}(\mathbb{D})$. f is called a *Caratheordory function*, if $\mathrm{Re}\, f(z) \geq 0$, for all $z \in \mathbb{D}$,
- Let $f \in \mathrm{Hol}(\mathbb{C}_+)$. f is called a *Herglotz function*, if $\mathrm{Im}\, f(z) \geq 0$, for all $z \in \mathbb{C}_+$. The set of all Herglotz functions is denoted by $\mathcal{N}_0$.

The following example of a Herglotz functions is the main reason for the importance of Herglotz functions in the spectral theory of self-adjoint operators:

1.1.2 Example. Let $\mathcal{H}$ be a Hilbert space, A a bounded linear, self-adjoint operator on $\mathcal{H}$ and $v \in \mathcal{H}$. Define for $z \in \mathbb{C}_+$

$$m_v(z) = \langle (A - z)^{-1} v, v \rangle.$$

Then $m_v \in \mathcal{N}_0$. Since $R_A(z) := (A-z)^{-1}$ is analytic (with values in $L_b(\mathcal{H})$), m_v is analytic in $\mathbb{C}_+$. Moreover,

$$\frac{m_v(z) - \overline{m_v(z)}}{z - \overline{z}} = \frac{\langle ((A - z)^{-1} - (A - \overline{z})^{-1}) v, v \rangle}{z - \overline{z}} = \langle (A - \overline{z})^{-1} (A - z)^{-1} v, v \rangle = \|(A - z)^{-1} v\|^2 \geq 0.$$

Let us note that if f is a Schur class function and $|f(z_0)| = 1$ for some $z \in \mathbb{D}$, then by the maximum modulus principle, $f(z) \equiv= c$, with $|c| = 1$. That is, by considering Schur class functions taking values in $\overline{\mathbb{D}}$ rather than $\mathbb{D}$, we "only" add unimodular constants. Let us recall the following fact from comoplex analysis. Let Ω be a domain and K_n a compact exhaustion. That is, $K_n \subset \Omega$ are compact, $K_n \subset \mathrm{int}(K_{n+1})$ and $\cup K_n = \Omega$. Then we define a metric on $\mathrm{Hol}(\Omega)$ by,

$$d(f, g) = \sum_{k=1}^{\infty} 2^{-n} \min(\sup_{z \in K_n} |f(z) - g(z)|, 1). \tag{1.1}$$

With this metric $(Hol(\Omega), d)$ is a complete metric space and this metric induces uniform convergence on compact subsets of Ω.

1.1.3 Lemma. *$(\mathcal{S}, d|_{\mathcal{S}\times\mathcal{S}})$ is a compact metric space.*

Proof. Since $\sup\{|f(z)| \mid z \in \mathbb{D}, f \in \mathcal{S}\} \leq 1$, $\mathcal{S}$ is precompact by Montel's theorem. Thus, we only need to show that it is closed in $(Hol(\Omega), d)$. We need to show that if $f_n \in \mathbb{D}$ and $d(f_n, f) \to 0$, then $|f| \leq 1$ on $\mathbb{D}$. This is an immediate consequence of the fact that convergence with respect to d implies pointwise convergence. ❑

1.1.4 Corollary. *Let $g_n \in \mathcal{S}$ and assume that there exists $D \subset \mathbb{D}$ wich accumulates in $\mathbb{D}$ such that for all $z \in D$ $\lim_n g_n(z)$ exists. Then there exists $g \in \mathbb{D}$ such that $d(g_n, g) \to 0$.*

Proof. It suffices to show that every subsequence of g_n has a subsequence which converges to g in d. Let g_{n_1} be an arbitrary subsequence, then by compactness we find a subsequence g_{n_2} and $h \in \mathcal{S}$, so that $d(g_{n_2}, h) \to 0$. Fix $z \in D$. Then we have

$$|g(z) - h(z)| \leq |g(z) - g_{n_2}(z)| + |g_{n_2}(z) - h(z)| \to 0.$$

Thus, by the identity theorem we conclude that $h \equiv g$. ❑

We see that we there are three domains that play an important role in the definitions of these classes of functions. Namely, $\mathbb{D}$, $\mathbb{C}_+$, and $\mathbb{H}_+ = \{z \in \mathbb{C} \mid \operatorname{Re} z \geq 0\}$. Let us note that these domains can be mapped into each other by means of Möbius transformations. We have that the following mappings are conformal mappings of the corresponding domains

$$\tau = \begin{cases} \mathbb{H}_+ & \to & \mathbb{C}_+ \\ z & \mapsto & iz \end{cases} \qquad \varphi = \begin{cases} \mathbb{C}_+ & \to & \mathbb{D} \\ z & \mapsto & \frac{z-i}{z+i} \end{cases}$$

Clearly if f is a Caratheodory function, then

$$g(z) = \tau(f(\varphi(z)))$$

is a Herglotz function and this sets a bijection between these class of functions. This is not precisely true for the class $\mathcal{S}$. Note that $\varphi^{-1}(u) = i\frac{1+u}{1-u}$. Thus, $\varphi^{-1}(1) = \infty$. For this reason, it is sometimes convenient to consider the set $\overline{\mathcal{N}_0} = \mathcal{N}_0 \cup \{\infty\}$. Then again, we have that if $f \in \mathcal{S}$, then

$$f \in \mathcal{S} \implies g(z) = \varphi^{-1}(f(\varphi(z))) \in \overline{\mathcal{N}_0}.$$

In particular, the function $f \equiv 1$ is mapped onto the function $g \equiv \infty$. This mapping sets up a bijection. In fact, if we define for $f, g \in \overline{\mathcal{N}_0}$ the metric

$$d_{\mathcal{N}_0}(f, g) = \sum_{k=1}^{\infty} 2^{-n} \min(sup_{z\in K_n} d_\chi(f(z), g(z)), 1),$$

where d_χ denotes the chordal metric on the Riemann sphere, then this mapping even becomes a homeomorphism.

1.1.5 Corollary. *$(\overline{\mathcal{N}_0}, d_{\mathcal{N}_0})$ is a compact metric space.*

1.1.6 Corollary. *Let f_n. Assume that there exists $D \subset \mathbb{C}_+$ which accumulates in $\mathbb{C}_+$ such that for all $z \in D$ $\lim_n f_n(z)$ exists. Then there exists $f \in \overline{\mathcal{N}_0}$ such that $d(f_n, f)_{\mathcal{N}_0} \to 0$.*

1.2 J-expanding matrix functions

Let us consider points $z \in \overline{\mathbb{C}}$ (the Riemann spere) in their projective coordinates. That is, we consider vectors in $\mathbb{C}^2 \setminus \{(0,\ 0)^\intercal\}$, with the equivalence relation

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \sim \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \iff \exists c \in \mathbb{C} : \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = c \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}$$

The projective line is defined by $\mathbb{CP}^1 = (\mathbb{C} \setminus \{(0,0)^\intercal\}/\sim)$. The quotient space can be identified with the Riemann sphere $\overline{\mathbb{C}}$, bu using the quotient map $\pi : \mathbb{C}^2 \setminus \{(0,\ 0)^\intercal\}$ defined by

$$\pi\left(\begin{pmatrix} w_1 \\ w_2 \end{pmatrix}\right) = \begin{cases} \frac{w_1}{w_2} & w_2 \neq 0 \\ \infty & w_2 = 0 \end{cases}$$

$\overline{\mathbb{C}}$ is embedded into $\mathbb{CP}^1$ is embedded into the $\mathbb{CP}^1$ by $z \mapsto (z,\ 1)^\intercal$, if $z \neq \infty$ and $\infty \mapsto (1,0)^\intercal$. Projective coordinates are particularly convenient if working with Möbius transformations. Let $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ be so that $\det A = 1$. To this we can associate the Möbius transformation

$$z \mapsto f_A(z) := \frac{az+b}{cz+d}.$$

Note that this can be rephrased to

$$f_A \circ \pi = \pi \circ A.$$

It will be convenient to introduce an abbreviation for this

$$A \star z := f_A(z).$$

1.2.1 Lemma. *Let $A, B \in \mathbb{C}^{2\times 2}$, be invertible. Then the following hold*

(i) $f_A = \mathrm{id}$ *if and only if* $A = zI$ *for some* $z \in \mathbb{C} \setminus \{0\}$*;*

(ii) $f_{AB} = f_A \circ f_B$*;*

(iii) The map f_A *is a bijection of* $\overline{\mathbb{C}}$ *onto itself;*

Proof. (i): Assume that $f_A = \mathrm{id}$ and let $x \in \mathbb{C}^2 \setminus \{(0,\ 0)^\intercal\}$. Then

$$\pi(Ax) = f_A(\pi(x)) = \pi(x).$$

This means that x is an eigenvector for A. Since x was arbitrary, we have shown that any x is an eigenvector of A, implying that $A = zI$ for some $z \in \mathbb{C} \setminus \{0\}$;
(ii) We have

$$f_{AB} \circ \pi = \pi \circ A \circ B = f_A \circ \pi \circ B = f_A \circ f_B \circ \pi.$$

Since π is surjective, this implies that $f_{AB} = f_A \circ f_B$.
(iii) Follows from (i) and (ii) since

$$f_A \circ f_{A^{-1}} = f_{A^{-1}} \circ f_A = \mathrm{id}.$$

❑

Note that in particular this implies that for any $\lambda \neq 0$, $f_{\lambda A} = f_A$ since

$$f_{\lambda A} = f_{\lambda I A} = f_{\lambda I} \circ f_A = f_A.$$

Thus, it suffices to consider matrices with $\det A = 1$. Recall that

$$\mathbb{SL}(\mathbb{C}, 2) = \{A \in \mathbb{C}^{2\times 2} \mid \det A = 1\}.$$

The following lemma will be crucial in the course of the lecture. We will call a set a generalized circle on $\overline{\mathbb{C}}$ if it is either a standard circle or a straight line. Interpreting a straight line as a circle containing ∞. Note that generalized circles are exactly given by equations of the form

$$\alpha z\overline{z} + \beta z + \overline{\beta}\overline{z} + \gamma = 0, \tag{1.2}$$

where $\alpha, \beta \in \mathbb{R}, \beta \in \mathbb{C}$ and $|\beta|^2 > \alpha\gamma$. In particular, $\alpha = 0$ corresponds to straight lines.

1.2.2 Lemma. *Let $A \in \mathbb{SL}(2, \mathbb{C})$, $A = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$. Then f_A maps the set of generalized circles onto itself. In particular, $\overline{\mathbb{R}}$ is mapped onto a circle with radius and center given by*

$$m = \frac{b\overline{c} - a\overline{d}}{\overline{c}d - c\overline{d}}, \quad r = \frac{1}{|d\overline{c} - c\overline{d}|}.$$

If $\operatorname{Im} d\overline{c} = 0$, then the circle degenerates to a line.

Proof. Assume first that $c \neq 0$. Then we can write

$$M = \begin{pmatrix} 1 & a/c \\ 0 & 1 \end{pmatrix}\begin{pmatrix} 1/c & 0 \\ 0 & c \end{pmatrix}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & d/c \\ 0 & 1 \end{pmatrix} \tag{1.3}$$

Note that this shows that M is a composition of translations, a dilation, a rotation and the inversion $z \mapsto -1/z$. It is clear that transations, dilations and rotations leave the set of generalized circles invariant. That this also holds for inversions follows from (1.2). Thus, the first claim is proved in the case $c \neq 0$. If $c = 0$, $\det A = 1$ implies $d \neq 0$ and $a = 1/d$. From this we see that

$$M = \begin{pmatrix} 1 & ab \\ 0 & 1 \end{pmatrix}\begin{pmatrix} a & 0 \\ 0 & 1/a \end{pmatrix}$$

and the claim also follows.
It remains to compute the image of $\overline{\mathbb{R}}$. Let us assume that $\operatorname{Im}(c\overline{d} \neq 0)$. Then using (1.3) we can trace to image of all the above transformations. We get

$$\begin{aligned} \mathbb{R} \cup \{\infty\} \mapsto \{x + iy_0 \mid x \in \mathbb{R} \cup \{\infty\}\} &\mapsto \left\{ z \mid \left| z - \frac{i}{2y_0} \right|^2 = \frac{1}{4y_0^2} \right\} \mapsto \left\{ w \mid \left| w - \frac{i}{2y_0 c^2} \right|^2 = \frac{1}{4y_0^2 |c|^4} \right\} \\ &\mapsto \left\{ u \mid \left| u - \left(\frac{a}{c} + \frac{i}{2y_0 c^2} \right) \right|^2 = \frac{1}{4y_0^2 |c|^4} \right\}. \end{aligned}$$

One can now directly check that

$$\frac{1}{4y_0^2|c|^4} = r \quad \text{and} \quad \frac{a}{c} + \frac{i}{2y_0 c^2} = m.$$

If $\operatorname{Im} c\overline{d} = 0$, then $y_0 \in \mathbb{R}$ and hence $\{x + iy_0 \mid x \in \mathbb{R} \cup \infty\} = \mathbb{R} \cup \{\infty\}$. Since $z \mapsto -1/z$ preserves $\mathbb{R} \cup \{\infty\}$ and all other transformations map lines onto lines, we see that in this case the image is a line.

❑

Let J denote the signature matrix

$$J := \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Let $w = \binom{u_1}{u_2} \in \mathbb{C}^2 \setminus \left\{\binom{0}{0}\right\}$. Then a direct computations shows that

$$-iw^*Jw \begin{cases} > 0 & \iff & \pi(w) \in \mathbb{C}_+ \\ < 0 & \iff & \pi(w) \in \mathbb{C}_- \\ = 0 & \iff & \pi(w) \in \overline{\mathbb{R}} \end{cases} \tag{1.4}$$

Let $v = (z, 1)^\intercal$. Then, we see that $v^*Jv = z - \overline{z}$. Thus, $\operatorname{Im} z \geq 0$, if and only if $v^*Jv/i \geq 0$. This motivates the following definition.

1.2.3 Definition. Let $M : \mathbb{C} \to \mathbb{C}^{2\times 2}$ so that each entry of M belongs to $\operatorname{Hol}(\mathbb{C})$. We call

- M J-expanding if $-i(M(z)^*JM(z) - J) \geq 0$ for every $z \in \mathbb{C}_+$
- M J-inner, if M is J-expanding and $M(z)^*JM(z) - J = 0$ for $z \in \mathbb{R}$.

A constant function M is called J unitary, if it is J inner, i.e, $M^*JM = J$.

The special linear group is given by

$$\mathbb{SL}(2, \mathbb{R}) := \{A \in \mathbb{R}^{2\times 2} \mid \det A = 1\} \tag{1.5}$$

One can show that

$$\mathbb{SL}(2, \mathbb{R}) = \{A \mid A \text{ is J unitary, } \det A = 1\}.$$

Note that $\mathbb{SL}(2, \mathbb{R})$ correspond exactly to those Möbius transformations which are conformal automorphisms of $\mathbb{C}_+$. It is now easy to see that $A \in \mathbb{SL}(2, \mathbb{R})$ preserves $\mathbb{C}_+$. This follows, since A being j-unitary implies that $\operatorname{Im} f_A(z) > 0$ if and only if $\operatorname{Im} z > 0$.

1.2.4 Lemma. *The following statements hold.*

(i) If $M \in \mathbb{SL}(2, \mathbb{C})$ satisfies $-i(M^*JM - J) \geq 0$, then $z \mapsto M \star z$ defines a Herglotz function.

(ii) If $M(z)$ is J-expanding matrix function and $f \in \mathcal{N}_0$, then $M \star f \in \overline{\mathcal{N}_0}$. If there exists $z \in \mathbb{C}_+$ such that $\operatorname{Im} f(z) > 0$ or $-i(M(z)^*jM(z) - j) > 0$, then $M \star f \in \mathcal{N}_0$.

(iii) Let $(M_n(z))_{n\in\mathbb{N}}$ be a sequence of J-expanding matrix function and $(f_n)_{n\in\mathbb{N}_0}$ a sequence of Herglotz functions. Assume that for every $z \in \mathbb{C}_+$, $M_n(z) \star f_n(z)$ has a limit $m(z)$. Then $m \in \overline{\mathcal{N}_0}$.

Proof. (i): Let us first show that for $z \in \mathbb{C}_+$, $M \star z \neq \overline{\mathbb{R}}$. Let $v = \binom{z}{1}$, $w = Mv$ and recall that $M \star z = \pi(w)$. Then from (1.4) it follows that

$$-iw^*Jw \geq -iv^*Jv > 0$$

and hence $\pi(w) \in \mathbb{C}_+$. In particular $\pi(w) \neq \infty$. This implies that $M \star z \in \operatorname{Hol}(\mathbb{C}_+)$ and $\operatorname{Im} M \star z > 0$.
(ii): Clearly $M(z) \star f(z)$ is meromorphic. Let as before $v = \binom{f(z)}{1}$, $w = Mv$ Now we conclude

$$-iw^*Jw \geq -iv^*Jv \geq 0 \tag{1.6}$$

and hence $M(z) \star f(z) = \pi(w) \in \overline{\mathcal{N}_0}$. Note that this means that either $\operatorname{Im} M(z) \star f(z) > 0$ for all $z \in \mathbb{C}_+$ or $\operatorname{Im} M(z) \star f(z) = c$ for $c \in \overline{\mathbb{R}}$. Hence, we conclude that $\operatorname{Im} M(z) \star f(z) > 0$ for all $z \in \mathbb{C}_+$ if there exists $z \in \mathbb{C}_+$ such that one of the inequalities is strict in (1.6).
(iii) $g_n(z) =: M_n(z) \star f_n(z)$ is a sequence of Herglotz functions that converges pointwise. Thus, by Corollary 1.1.5 it converges in $d_{\mathcal{N}_0}$ and the limit is again a Herglotz function.
❑

1.3 Integral representation

The goal of this section is to show that $f \in \mathcal{N}_0$ if and only if there exists $\alpha \in \mathbb{R}, \beta > 0$ and a positive Borel measure μ with $\int \frac{d\mu(x)}{1+x^2} < \infty$ such that

$$m(z) = \alpha + \beta z + \int \left(\frac{1}{x-z} - \frac{x}{1+x^2} \right) d\mu(x). \tag{1.7}$$

We will establish first an integral representation for Caratheordory functions and then use their bijective correspondence with Herglotz functions to obtain (1.7).
In the following let $\mathbb{T} = \partial\mathbb{D} + \{z \in \mathbb{C} \mid |z| = 1\}$. By $dm(\zeta)$, we denote the normalized Lebesgue measure on $\mathbb{T}$.

1.3.1 Definition. On $\mathbb{D} \times \mathbb{T}$, we define the Poisson kernel:

$$P(z, \zeta) := \operatorname{Re} \frac{\zeta + z}{\zeta - z} = \frac{1 - |z|^2}{|\zeta - z|^2}.$$

Let μ be a complex (i.e., in particular finite) Borel measure on $\mathbb{T}$, then we define the Poisson integral of μ by

$$\mathcal{P}[d\mu](z) = \int_{\mathbb{T}} P(z, \zeta) d\mu(\zeta).$$

Note that for $(z, \zeta) \in \mathbb{D} \times \mathbb{T}$

$$\frac{\zeta + z}{\zeta - z} = 1 + 2 \sum_{k=1}^{\infty} \left(\frac{z}{\zeta} \right)^k$$

and the series converges uniformly for $\zeta \in \mathbb{T}$. This implies that for a complex (thus finite) measure μ we have

$$\int_{\mathbb{T}} \frac{\zeta + z}{\zeta - z} d\mu(\zeta) = \mu(\mathbb{T}) + 2 \sum_{k=1}^{\infty} \int_{\mathbb{T}} \zeta^{-k} d\mu(\zeta).$$

Hence $\int_{\mathbb{T}} \frac{\zeta+z}{\zeta-z} d\mu(\zeta) \in \operatorname{Hol}(\mathbb{D})$ and $P(z, \zeta) = \operatorname{Re} \int_{\mathbb{T}} \frac{\zeta+z}{\zeta-z} d\mu(\zeta)$ is harmonic. The Poisson kernel is an approximate identity:

1.3.2 Lemma. *The Poisson kernel has the properties:*

(i) For $z \in \mathbb{D}$ and $\zeta \in \mathbb{T}$, it holds that $P(z, \zeta) > 0$;

(ii) For $z \in \mathbb{D}$ it holds that $\int_{\mathbb{T}} P(z, \zeta) dm(\zeta) = 1$;

(iii) For every $\delta > 0$ and $\zeta_0 \in \mathbb{T}$ it holds that

$$\lim_{z \to \zeta_0} \sup_{|\zeta - \zeta_0| > \delta} P(z, \zeta) = 0.$$

Proof. (i): This follows directly from the definition.
(ii): By Cauchy's integral formula, we obtain

$$\begin{aligned}\int_{\mathbb{T}} P(z,\zeta)dm(\zeta) &= \mathrm{Re}\left(\frac{1}{2\pi i}\int_{|\zeta|=1}\frac{\zeta+z}{\zeta-z}\frac{d\zeta}{\zeta}\right)\\ &= \mathrm{Re}\left(\frac{1}{2\pi i}\int_{-\pi}^{\pi}\left(\frac{2}{\zeta-z}-\frac{1}{\zeta}\right)d\zeta\right)\\ &= \mathrm{Re}\,(2-1) = 1.\end{aligned}$$

(iii): If $|z-\zeta_0| < \delta$ and $|\zeta-\zeta_0| \geq \delta$, then

$$|\zeta - z|^2 = |\zeta-\zeta_0+\zeta_0-z|^2 \geq (\delta - |z-\zeta_0|)^2$$

and thus,

$$\sup_{|\zeta-\zeta_0|\geq\delta} P(z,\zeta) \leq \frac{1-|z|^2}{(\delta-|z-\zeta_0|)^2} \to 0$$

as $z \to \zeta_0$. ❑

1.3.3 Lemma. *Let $h \in C(\overline{\mathbb{D}})$ and harmonic in $\mathbb{D}$. Then*

$$h(z) = \int_{-\pi}^{\pi} P(z,\zeta)h(\zeta)dm(\zeta).$$

Proof. Define

$$g(z) = \int_{-\pi}^{\pi}\frac{1-|z|^2}{|\zeta-z|^2}h(\zeta)dm(\zeta).$$

We have already seen that g is harmonic in $\mathbb{D}$. Fix $\zeta_0 \in \mathbb{T}$ and $\epsilon > 0$. Choose $\delta > 0$, such that for $|\zeta-\zeta_0| \leq \delta$

$$|h(\zeta) - h(\zeta_0)| \leq \frac{\epsilon}{2}$$

Moreover, choose ϵ_1 such that for $|z-\zeta_0| < \delta_1$ we have that

$$\sup_{|\zeta-\zeta_0|>\delta} P(z,\zeta) < \frac{\epsilon}{4\|h\|_{\mathbb{T}}}.$$

With this we have

$$\begin{aligned}&\left|\int_{\mathbb{T}} P(z,\zeta)h(\zeta)dm(\zeta) - h(\zeta_0)\right|\\ &\leq \int_{\mathbb{T}} |P(z,\zeta)h(\zeta) - P(z,\zeta)h(\zeta_0)|\,dm(\zeta)\\ &= \int_{\mathbb{T}\cap|\zeta-\zeta_0|\leq\delta} P(z,\zeta)\,|h(\zeta)-h(\zeta_0)|\,dm(\zeta) + \int_{\mathbb{T}\cap|\zeta-\zeta_0|>\delta} P(z,\zeta)\,|h(\zeta)-h(\zeta_0)|\,dm(\zeta)\\ &< \frac{\epsilon}{2} + 2\|h\|_{[-\pi,\pi]}\frac{\epsilon}{4\|h|_{\mathbb{T}}} = \epsilon.\end{aligned}$$

Hence $g(z)$ is harmonic in $\mathbb{D}$ and for any $\zeta_0 \in \mathbb{T}$,

$$\lim_{\substack{z\to\zeta\\ z\in\mathbb{D}}} g(z) = h(\zeta_0).$$

That is, $g(z)$ is a solution of the Dirichlet problem with boundary function $h|_{\mathbb{T}}$. The claim follows by uniqueness of the Dirichlet problem. ❑

1.3.4 Theorem. *Let f be a Caratheodory function. Then there exists unique $a \in \mathbb{R}$ and a finite measure ν on $\partial\mathbb{D}$ such that*

$$f(z) = ia + \int \frac{\zeta + z}{\zeta - z} d\nu(\zeta). \tag{1.8}$$

Proof. For $r \in (0, 1)$ define $f_r(z) = f(rz)$ and $h_r = \operatorname{Re} f_r$. Then h_r satisfies the assumptions of Lemma 1.3.3 and hence, with $d\nu_r(\zeta) = \operatorname{Re} h_r(\zeta) dm(\zeta)$, where m denotes the normalized Lebesgue measure on $\partial\mathbb{D}$. Since $h_r \geq 0$ these are positive measure. Moreover,

$$\|\nu_r\| = \int_{\partial\mathbb{D}} h_r(\zeta) dm(\zeta) = h_r(0) = \operatorname{Re} f(0).$$

Hence, the Banach-Alaoglu theorem provides us with a measure ν and $r_n \to 1$ such that

$$\lim_{n\to\infty} \nu_{r_n} \to \nu$$

in the weak* topology of $(C(\partial\mathbb{D}), \|\cdot\|_\infty)^*$. Thus

$$\begin{aligned} \operatorname{Re} f(z) &= \lim_{n\to\infty} h_{r_n}(z) \\ &= \lim_{n\to\infty} \int \frac{1 - |z|^2}{|\zeta - z|^2} d\nu_{r_n}(\zeta) \\ &= \int \frac{1 - |z|^2}{|\zeta - z|^2} d\nu(\zeta). \end{aligned}$$

Adding the complex conjugate, we get (1.8).
Uniqueness: It remains to show uniqueness: Let μ be a complex measure and set $\nu = \mathcal{P}[\mu]$. We need to show that $\nu = 0$ implies $\mu = 0$. Choose $f \in C(\mathbb{T})$ and set $u = \mathcal{P}[f]$. Since for $\zeta, z \in \mathbb{T}$, $P(r\zeta, z) = P(rz, \zeta)$ it follows from Fubini that

$$\int_{\mathbb{T}} u_r(\zeta) d\mu(\zeta) = \int_{\mathbb{T}} \nu_r(z) f(z) dm(z).$$

Since $\nu = 0$ also $\nu_r = 0$. Note that in the proof of Lemma 1.3.3 we have shown that for a continuous f:

$$u(z) = \begin{cases} \mathcal{P}[f](z) & z \in \mathbb{D} \\ f(z) & z \in \mathbb{T} \end{cases}$$

defines a continuous function on $\overline{\mathbb{D}}$. Thus it is uniformly continuous and we conclude that $\lim_{r\nearrow} \|u_r - f\|_\infty = 0$. Therefore,

$$\int_{\mathbb{T}} f d\mu = 0, \tag{1.9}$$

for every $f \in C(\mathbb{T})$. Recall that by the Riesz-Representation theorem $C(\mathbb{T})^*$ is the set of all complex Borel measures on $\mathbb{T}$. If we denote the functional defined by (1.9) with Λ_μ, then since Riesz Representation gives an isometry, we know that $\|\Lambda_\mu\| = |\mu|(\Omega)$. Thus, we conlude from (1.9) that $\mu = 0$. ❑

1.3.5 Theorem. *Let $f \in \mathcal{N}_0$. Then there exists unique $\alpha \in \mathbb{R}$, $\beta \geq 0$ and a finite measure σ on $\mathbb{R}$ such that*

$$f(z) = \alpha + \beta z + \int_{\mathbb{R}} \frac{1 + zx}{x - z} d\sigma(x). \tag{1.10}$$

Proof. Let $\varphi : \mathbb{C}_+ \to \mathbb{D}$ be defined by

$$\varphi(z) = \frac{z-i}{z+i}.$$

Then

$$F(u) = -if(\varphi^{-1}(u))$$

is analytic in $\mathbb{D}$ and $\operatorname{Re} F \geq 0$. Hence by Theorem 1.3.4 we find a finite measure ν and $a \in \mathbb{R}$ such that

$$F(u) = ia + \int \frac{\zeta + u}{\zeta - u} d\nu(\zeta).$$

Hence

$$f(z) = iF(\varphi(z)) = -a + i\nu(\{1\})\frac{1+\varphi(z)}{1-\varphi(z)} + i\int_{\partial\mathbb{D}\setminus\{1\}} \frac{\zeta + \varphi(z)}{\zeta - \varphi(z)} d\nu(\zeta).$$

Now we note that

$$i\frac{1+\varphi(z)}{1-\varphi(z)} = i(-i)\varphi^{-1}(\varphi(z)) = z.$$

Moreover, a direct computation shows that

$$\frac{\varphi(x)+\varphi(z)}{\varphi(x)-\varphi(z)} = -i\frac{1+xz}{x-z}.$$

Hence, with $\sigma = \varphi_*^{-1}(\nu|_{\partial\mathbb{D}\setminus\{1\}})$ we get

$$\int_{\partial\mathbb{D}\setminus\{1\}} \frac{\zeta + \varphi(z)}{\zeta - \varphi(z)} d\nu(\zeta) = -i\int_{\mathbb{R}} \frac{1+xz}{x-z} d\sigma(x).$$

The proof has shown that $\alpha = -a$ and $\beta = \nu(\{1\})$.
The steps can be reveresed. Starting with a representation (1.10). We get an integral representation of a Caratheordory function of the form (1.8) with $a = -\alpha$ and $\nu = \beta\delta_{\{1\}} + \varphi_\star\sigma$. Hence, uniqueness, follows from the uniqueness claim in Theorem 1.3.4. ❑

1.3.6 Remark. Instead of splitting up the point mass at ∞ it will also be convenient to consider $\varphi : \overline{\mathbb{R}} \to \mathbb{T}$ and to consider $\sigma^\infty = \varphi_\star^{-1}\nu = \sigma + \beta\delta_{\{\infty\}}$. In this case the integral representation reads as

$$f(z) = \alpha + \int_{\overline{\mathbb{R}}} \frac{1+zx}{x-z} d\sigma^\infty(x). \tag{1.11}$$

1.3.7 Corollary. *Let $f \in \mathcal{N}_0$. Then there exists unique $\alpha \in \mathbb{R}$, $\beta > 0$ and a positive measure μ on $\mathbb{R}$ with $\int \frac{d\mu(x)}{1+x^2} < \infty$ such that*

$$f(z) = \alpha + \beta z + \int \frac{1}{x-z} - \frac{x}{1+x^2} d\mu(x). \tag{1.12}$$

Proof. For $f \in \mathcal{N}_0$, let α, β, σ be the data from the integral representation (1.10). Define μ by $d\mu(x) := (1+x^2)d\sigma(x)$ and note that

$$\frac{1}{x-z} - \frac{x}{1+x^2} = \frac{1+xz}{x-z}\frac{1}{1+x^2}.$$

The claim follows. ❑

1.3.8 Proposition. *Let $f_n, f \in \mathcal{N}_0$ and $\alpha_n, \beta_n, \sigma_n^\infty, \sigma_n$ the data from the integral representations* (1.10), (1.11). *Then the following are equivalent:*

(i) There exists a $D \subset \mathbb{C}_+$ which accumulates in $\mathbb{C}_+$, such that for all $z \in D$ $f_n(z) \to f(z)$;

(ii) Uniformly on compact subsets of $\mathbb{C}_+$, we have $f_n \to f$;

(iii) $\alpha_n \to \alpha$, and $\sigma_n^\infty \to \sigma^\infty$ in the weak topology of $C(\overline{\mathbb{R}})'$;*

(iv) $\alpha_n \to \alpha$, and $\sigma_n(\mathbb{R}) + \beta_n \to \sigma(\mathbb{R}) + \beta$ and $\sigma_n \to \sigma$ in the weak topology of $C_0(\overline{\mathbb{R}})'$;*

Proof. $(i) \iff (ii)$: This is already shown in Corollary 1.1.6.
That $(iii) \iff (iv)$: This follows, since every $f \in C(\overline{\mathbb{R}})$ can be written as a sum of a constant and a function which vanishes at ∞.
$(iii) \implies (i)$: This is clear, since for every $z \in \mathbb{C}_+$, $(x \mapsto \frac{1+xz}{x-z}) \in C(\overline{\mathbb{R}})$.
$(ii) \implies (iii)$: This will follow from uniqueness of the data and compactness of $\overline{\mathcal{N}_0}$. Write

$$f_n(z) = \alpha_n + \int_{\mathbb{R}} \frac{1 + zx}{x - z} d\sigma_n^\infty(x)$$

and similarly f. Note that $f_n(i) = \alpha_n + i\sigma_n^\infty(\overline{\mathbb{R}})$.Thus, we conclude that $\alpha_n \to \alpha$ and σ_n^∞ is a bounded sequence of measures. Thus, the Banach-Alaoglu theorem provides us with a subsequence $\sigma_{n_j}^\infty$ which converges to some finite measure ρ on $\overline{\mathbb{R}}$. It remains to show that $\rho = \sigma^\infty$. Assume the contrary. Then, we define

$$g(z) = \alpha + \int_{\overline{\mathbb{R}}} \frac{1 + xz}{x - z} d\rho(x)$$

and uniqueness of the integral representation implies $g \neq f$. On the other hand, since $\alpha_n \to \alpha$ and $\sigma_{n_j}^\infty \to \rho$, we conlude from $(iii) \implies (ii)$ that $f_{n_j} \to g$. A contradiction. ❑

We have already seen in the proof above that

$$f(i) = \alpha + i\sigma^\infty(\overline{\mathbb{R}}) = \alpha + i(\beta + \sigma(\mathbb{R})).$$

Thus, by taking real and imaginary part, we can extract α and $\beta + \sigma(\mathbb{R})$. However, extracting β, requires to take a limit.

1.3.9 Proposition. *Let $f \in \mathcal{N}_0$ with representation* (1.10). *Then*

$$\beta = \lim_{y\to\infty} \frac{f(iy)}{iy}. \tag{1.13}$$

Proof. In order to show (1.13), we need to show that

$$\lim_{y\to\infty} \int_{\mathbb{R}} \frac{1}{iy} \frac{1 + xiy}{x - iy} d\sigma(x) = 0. \tag{1.14}$$

The integrand converges to 0 pointwise as $y \to \infty$, so (1.14) follows from dominated convergence (having in mind that $\sigma(\mathbb{R})$ is finite) with the bound

$$\left| \frac{1}{iy} \frac{1 + xiy}{x - iy} \right| = \frac{1}{y} \frac{\sqrt{1 + x^2y^2}}{\sqrt{x^2 + y^2}} = \frac{\sqrt{1 + x^2y^2}}{\sqrt{y^2x^2 + y^4}} \leq 1,$$

which is valid for $y \geq 1$. ❑

1.3.10 Proposition. *Let $f \in \mathcal{N}_0$. Then there exists a finite measure μ on $\mathbb{R}$ such that*

$$f(z) = \int \frac{1}{x - z} d\mu(x), \tag{1.15}$$

if and only if there exists $C > 0$ such that for all $z \in \mathbb{C}_+$

$$|f(z)| \leq \frac{C}{\operatorname{Im} z}. \tag{1.16}$$

Proof. If f is of the form (1.15) and μ is finite then

$$|f(z)| \leq \int \frac{1}{|x - z|} d\mu(x) \leq \frac{\mu(\mathbb{R})}{\operatorname{Im} z},$$

and the claim follows with $C = \mu(\mathbb{R})$.
Conversely, assume that $|f(z)| \leq \frac{C}{\operatorname{Im} z}$. By Proposition 1.3.9, $\beta = 0$. Write f as in (1.12). Then we have

$$\operatorname{Im} f(iy) = \int \frac{y}{x^2 + y^2} d\mu(x).$$

Monotone convergence implies that

$$\lim_{y \to \infty} y \operatorname{Im} f(iy) = \lim_{y \to \infty} \int \frac{y^2}{x^2 + y^2} d\mu(x) = \mu(\mathbb{R}).$$

Thus, by (1.16) we conclude that $\mu(\mathbb{R}) \leq C < \infty$ and therefore, $\frac{1}{x-z}, \frac{x}{1+x^2} \in L^1(\mathbb{R}, \mu)$ and we get

$$f(z) = \alpha - \int \frac{x}{1 + x^2} d\mu(x) + \int \frac{1}{x - z} d\mu(x) = \gamma + \int \frac{1}{x - z} d\mu(x).$$

Dominated convergence and (1.16) imply that $\gamma = \lim_{y \to \infty} f(iy) = 0$. ❑

1.4 Stieltjes inversion

We have already seen in that the data in the integral representation of a Herglotz function f is uniquely determined by f. However, in many cases it is useful to know, how to recover this data from f. We have already seen, that if f is written as

$$f(z) = \alpha + \beta z + \int \left(\frac{1}{x - z} - \frac{x}{1 + x^2} \right) d\mu(x), \tag{1.17}$$

then we have

$$a = \operatorname{Re} f(i), \quad \beta = \lim_{y \to \infty} \frac{f(iy)}{iy}.$$

In fact, also the measure can be recovered from f. The formula is known as Stieltjes inversion formula. We start with a Lemma:

1.4.1 Lemma. *Let f be a Herglotz function, with α, β, μ as in* (1.17). *Then f defines an analytic function on $\mathbb{C} \setminus \operatorname{supp} \mu$, which obeys $f(\overline{z}) = \overline{f(z)}$.*

Proof. For any $1 \le R < \infty$ and z such that $\operatorname{dist}(z, \operatorname{supp}\mu) \ge R^{-1}$, $|z| \le R$, it holds that

$$\left|\frac{1+xz}{x-z}\right| \le 4R^3. \tag{1.18}$$

Indeed, if $|x| > 2R$, we have

$$\left|\frac{1+xz}{x-z}\right| \le \frac{1+R|x|}{|x|-|z|} \le \frac{2R|x|}{|x|/2} = 4R$$

and for $x \in \operatorname{supp}\mu \cap [-2R, 2R]$, we have

$$\left|\frac{1+xz}{x-z}\right| \le R(1+|x|R) \le 4R^3.$$

Since $\int \frac{d\mu(x)}{1+x^2} < \infty$ and $\frac{1}{x-z} - \frac{x}{1+x^2} = \frac{1+xz}{x-z}\frac{1}{1+x^2}$, the integral in (1.17) is convergent for such z and defines a continuous function on $\mathbb{C} \setminus \operatorname{supp}\mu$. By Morera's theorem, it suffices to show that the integral over every null-homotopic curve γ in $\mathbb{C} \setminus \operatorname{supp}\mu$ vanishes. Fix such γ. Since $\operatorname{ran}\gamma$ is compact, we find R such that for any $z \in \operatorname{ran}\gamma$ we have $\operatorname{dist}(z, \operatorname{supp}\mu) \ge R^{-1}$ and $|z| \le R$. Thus, by (1.18) we can apply Fubini's theorem to conclude

$$\int_\gamma \int_{\mathbb{R}} \left(\frac{1}{x-z} - \frac{x}{1+x^2}\right) d\mu(x) dz = \int_{\mathbb{R}} \int_\gamma \left(\frac{1}{x-z} - \frac{x}{1+x^2}\right) dz d\mu(x) = 0.$$

❑

1.4.2 Theorem. *Let $f \in \mathcal{N}_0$. Then the measure μ in its integral representation can be reconstructed via the Stieltjes inversion formula*

$$\frac{1}{2}\left(\mu((a,b)) + \mu([a,b])\right) = \lim_{\epsilon \to 0} \frac{1}{\pi} \int_a^b \operatorname{Im} f(x+i\epsilon) dx. \tag{1.19}$$

Proof. By Lemma 1.4.1 we can assume that

$$f(z) = \int \frac{d\mu(x)}{x-z}, \quad \mu(\mathbb{R}) < \infty. \tag{1.20}$$

Indeed, for general f and fixed $R > 0$, we can write $f(z) = \int \frac{d\tilde{\mu}(x)}{x-z} + g(z)$, where $\tilde{\mu}$ coincides with μ on subsets of $(-2R, 2R)$ and g is a Herglotz function whose measure is supported on $\mathbb{R} \setminus [-2R, 2R]$. Hence, by Lemma 1.4.1, for $(a,b) \subset [-R, R]$, the limit in (1.19) for $\int \frac{d\tilde{\mu}(x)}{x-z}$ and for f are the same. Since also the measures coincide there, it suffices to consider f as in (1.20).
Tonelli's theorem shows that

$$\begin{aligned}\frac{1}{\pi}\int_a^b \operatorname{Im} f(x+i\epsilon)dx &= \frac{1}{\pi}\int_{\mathbb{R}} \frac{\epsilon}{(x-t)^2+\epsilon^2} d\mu(t) dx \\ &= \int_{\mathbb{R}} \frac{1}{\pi}\int_a^b \frac{\epsilon}{(x-t)^2+\epsilon^2} dx d\mu(t).\end{aligned}$$

Pointwise, we have

$$\frac{1}{\pi}\int_a^b \frac{\epsilon}{(x-t)^2+\epsilon^2}dx = \frac{1}{\pi}\left(\arctan\frac{b-t}{\epsilon} - \arctan\frac{a-t}{\epsilon}\right) \to \frac{1}{2}\left(\chi_{[a,b]}(t) - \chi_{(a,b)}(t)\right)$$

as $\epsilon \to 0$. Since $0 \le \arctan\frac{b-t}{\epsilon} - \arctan\frac{a-t}{\epsilon} \le \pi$, the result follows from dominated convergence. ❑

As a corollary, we get

1.4.3 Corollary. *If* $\mathrm{Im}\, f$ *can be continuously extended to* $\mathbb{C}_+ \cup (a, b)$*, for some interval* $(a, b) \subset \mathbb{R}$*, then* $\chi_{(a,b)} d\mu$ *is absolutely continuous with density* $\frac{1}{\pi}\chi_{(a,b)}(x)\,\mathrm{Im}\, f(x)$.

It is also interesting to compute point masses of μ.

1.4.4 Lemma. *For any* $x_0 \in \mathbb{R}$ *we have*

$$\mu(\{x_0\}) = \lim_{\epsilon\to 0}(-i\epsilon) f(x_0 + i\epsilon) = \lim_{\epsilon\to 0} \epsilon\, \mathrm{Im}\, f(i\epsilon). \tag{1.21}$$

Proof. As in the proof of Theorem 1.4.2 it suffices to consider f of the form (1.20). Thus, in order to prove the first equality in (1.21) it remains to show

$$\mu(\{x_0\}) = \lim_{\epsilon\to 0} \int \frac{-i\epsilon}{x - (x_0 + i\epsilon)} d\mu(x).$$

Pointwise, we have

$$\lim_{\epsilon\to 0} \frac{-i\epsilon}{x - (x_0 + i\epsilon)} = \chi_{x_0}.$$

Since $|\frac{-i\epsilon}{x-(x_0+i\epsilon)}| \le 1$, the claim follows by dominated convergence. Now the second equality in (1.21) follows by taking the real part of the first one. ❑

Chapter 2

Orthogonal polynomials and Jacobi matrices

Assume that we are given a probability measure, μ, supported on $\mathbb{R}$ such that for all $n \in \mathbb{N}_0$ we have

$$\int_{\mathbb{R}} |x|^n d\mu(x) < \infty.$$

To such a measure, we can associate a sequence

$$s_n = s_n(\mu) = \int_{\mathbb{R}} x^n d\mu(x).$$

Such a sequence will be called the *moment sequence* associated to μ. Assume for a second, that μ is not a pure point measure supported on finitely many atoms, that is, $\# \operatorname{supp} \mu = \infty$. Let

$$H_n := \begin{pmatrix} s_0 & s_1 & s_2 & \cdots & s_{n-1} \\ s_1 & s_2 & s_3 & \cdots & s_n \\ \vdots & \vdots & \vdots & \ldots & \vdots \\ s_{n-1} & s_n & s_{n+1} & \cdots & s_{2n-2} \end{pmatrix}$$

be the *Hankel matrix* associated to s_n. Then a simple computation shows that for $\xi = (c_0,\ c_1, \ldots,\ c_{n-1}) \neq 0$ we have

$$\xi^* H_n \xi = \sum_{j=0}^{n-1} \sum_{i=0}^{n-1} \overline{c_j} s_{i+j} c_i = \int_{\mathbb{R}} \sum_{j=0}^{n-1} \sum_{i=0}^{n-1} \overline{c_j} x^{i+j} c_i d\mu(x) = \int_{\mathbb{R}} \sum_{j=0}^{n-1} \overline{c_j} x^j \sum_{i=0}^{n-1} x^i c_i d\mu(x) = \langle P, P \rangle_{L^2(\mu)} > 0, \tag{2.1}$$

where $P(x) = \sum_{i=0}^{n-1} c_i x^i$. That is, H_n is positive definite. We will encounter, that this is a characteristic property of moment sequences. This means, given $(s_n)_{n \in \mathbb{N}_0} \in \mathbb{R}^{\mathbb{N}_0}$ such that $H_n > 0$ for all n (and $s_0 = 1$ in case we assume μ to be a probability measure), there exists a measure with this given moment sequence. In the first sections we will discuss existence and uniqueness for this problem. Along with this, we will encounter many properties of associated orthogonal polynomials. We start with proving existence of a measure for a given moment sequence. Given a moment sequence, it will be helpful to always have in mind that it should be given by $s_n = \int_{\mathbb{R}} x^n d\mu(x)$. All the definitions below are motivated by this identity.

2.1 Moment sequences

We start with the definition of a (non trivial) moment sequence. The name will be justified later in this chapter.

2.1.1 Definition. Let $s = (s_n)_{n\in\mathbb{N}_0} \in \mathbb{R}^{\mathbb{N}_0}$ with $s_0 = 1$. To s we associate the *Hankel matrix*

$$H_n := \begin{pmatrix} s_0 & s_1 & s_2 & \cdots & s_{n-1} \\ s_1 & s_2 & s_3 & \cdots & s_n \\ \vdots & \vdots & \vdots & \cdots & \vdots \\ s_{n-1} & s_n & s_{n+1} & \cdots & s_{2n-2} \end{pmatrix}$$

and the *Hankel determinant*

$$D_n := \det H_n.$$

The sequence s is called a (non-trivial) moment sequence, if for all $n \in \mathbb{N}_0$

$$D_n > 0.$$

2.1.2 Remark. The addition "non trivial" comes from assuming that all D_n is strictly positive. Note that if $\dim\ker H_n \geq 1$ for some $n \in \mathbb{N}$, then this holds for all $m \geq n$. In fact, if

$$m_0 = \inf\{n \in \mathbb{N}_0 \mid \dim\ker H_n \geq 1\}$$

then we can associated a measure μ with the given moments and μ will be supported on $m_0 - 1$ atoms. For now we want to exclude this trivial case. The reason for this is, that if μ is supported on n atoms, then by taking P the polynomial of degree n with zeros at these atoms, we see that $\|P\|^2_{L^2(\mu)} = \int |P(x)|^2 d\mu(x) = 0$; see (2.1).

Let $\mathcal{P}$ denote the set of polynomials with complex coefficients. With $\mathcal{P}_n$, we denote the subspace of polynomials of degree at most n.

2.1.3 Definition. Let $t = (t_i)_{i\in\mathbb{N}_0} \in \mathbb{R}^{\mathbb{N}_0}$, $t_0 = 1$. To t we associate the linear functional in $\mathcal{P}^*$ by

$$\Phi(P) = \Phi[t](P) = \sum_{i=0}^{n} c_i t_i,$$

where $P(z) = \sum_{i=0}^{n} c_i z^i$. We say that $\Phi[t]$ is *positive*, if $P \geq 0$ on $\mathbb{R}$ and $P \not\equiv 0$ implies that $\Phi[t](P) > 0$.

We say that $\Phi[t]$ is positive, if $P \geq 0$ on $\mathbb{R}$ and $P \not\equiv 0$ implies that $\Phi[t](P) > 0$. For $P \in \mathcal{P}$, $P = \sum_{i=0}^{n} c_i z^i$ we introduce the notation

$$P^{\#}(z) = \sum_{i=0}^{n} \overline{c_i} z^i = \overline{P(\overline{z})}.$$

Note that $P = P^{\#}$ if and only if P is real. This can either be stated by saying that $P(x) \in \mathbb{R}$ for $x \in \mathbb{R}$ or by saying that P has real coefficients. Let $R \in \mathcal{P}$, $R(z) = \sum_{i=0}^{n} c_i z^i$. Let us compute

$$\Phi[t](RR^{\#}) = \Phi[t]\left(\sum_{i=0}^{n} c_i z^i \sum_{j=0}^{n} \overline{c_j} z^j\right) = \sum_{i=0}^{n}\sum_{j=0}^{n} c_i \overline{c_j} t_{i+j} = \xi^* H_{n+1}\xi, \tag{2.2}$$

with $\xi = (c_0, \ldots, c_n)$ and H_n is the Hankel matrix for the sequence $(t_j)_{j=0}^{2n}$. This motivates the following factorization:

2.1.4 Lemma. *Let $n \in \mathbb{N}_0$, $P \in \mathcal{P}_{2n}$ has the property that $P(x) \geq 0$ for $x \in \mathbb{R}$ and $P \not\equiv 0$, if and only if there exists $R \in \mathcal{P}_n$, $R \not\equiv 0$, so that $P = RR^{\#}$.*

Proof. That $RR^{\#}$ has the desired property is clear. Let us thus start with $P \in \mathcal{P}_{2n}$ as above. Note that the assumption in particular implies that $P^{\#} = P$. From this it follows that complex zeros can only occur in conjugate pairs. Positivity on $\mathbb{R}$ implies that real zeros must be of even degree. We conclude that there exist $z_1, \dots, z_n$ and $r > 0$ so that

$$P(z) = r \prod_{k=1}^{m} (z - z_k)(z - \overline{z_k}).$$

Then $R(z) = \sqrt{r} \prod_{k=1}^{m} (z - z_k)$ gives the desired factorization. ❑

Note that the assumption on P, that it is of even degree follows also from non-negativity on $\mathbb{R}$.
Together with (2.2), we can now make the connection between moment sequences and sequences inducing positive functionals.

2.1.5 Corollary. *$s \in \mathbb{R}^{\mathbb{N}_0}$ with $s_0 = 1$ is a moment sequence, if and only if $\Phi[s]$ is a positive functional.*

We can use Φ to define an inner product on $\mathcal{P}$. Let s be a moment sequence. For $P, Q \in \mathcal{P}$ define

$$\langle P, Q \rangle_s := \Phi[s](PQ^{\#}). \tag{2.3}$$

2.1.6 Proposition. *$\langle \cdot, \cdot \rangle_s$ defines an inner product on the vector space $\mathcal{P}$.*

Proof. Let's write $P(z) = \sum_{i=0}^{n} a_i z^i$, $Q(z) = \sum_{j=0}^{m} b_i z^i$. Then a direct computation shows that

$$\langle P, Q \rangle_s = \sum_{i=0}^{n} \sum_{j=0}^{m} a_i \overline{b_j} s_{i+j}.$$

From this, linearity and $\overline{\langle P, Q \rangle_s} = \langle Q, P \rangle_s$ is clear. That $\langle P, P \rangle_s \geq 0$ and $\langle P, P \rangle_s = 0$ if and only if P is zero, follows from the fact that s is a moment sequence. ❑

We can thus apply the Gram-Schmidt orthogonalization procedure to the sequence $(z^n)_{n=0}^{\infty} \in \mathcal{P}^{\mathbb{N}_0}$ with respect to the scalar product $\langle \cdot, \cdot \rangle_s$.

2.1.7 Definition. Let s be a moment sequence. Then we denote by $p_n(z) = p_n(z, s)$ the nth *orthonormal polynomial* with respect to the inner product $\langle \cdot, \cdot \rangle_s$. Likewise, we denote by P_n the nth *monic, orthogonal polynomial*. Let γ_n denote the leading coefficient of p_n, i.e.,

$$\gamma_n = \frac{1}{\langle P_n, P_n \rangle_s} > 0.$$

2.1.8 Remark. It is important to mention, that D_n being strictly positive, guarantees that $\dim((\mathcal{P}_n, \langle \cdot, \cdot \rangle_s)) = n + 1$ for all n.

There is an explicit formula for p_n in terms of Hankel determinants.

2.1.9 Lemma. *The orthonormal polynomials are given explicitly by*

$$p_n(z) = \frac{1}{\sqrt{D_n D_{n+1}}} \det \begin{pmatrix} s_0 & s_1 & s_2 & \cdots & s_n \\ s_1 & s_2 & s_3 & \cdots & s_{n+1} \\ \vdots & \vdots & \vdots & \ldots & \vdots \\ s_{n-1} & s_n & s_{n+1} & \cdots & s_{2n-1} \\ 1 & z & z^2 & \cdots & z^n \end{pmatrix}$$

Proof. It follows from the definition that

$$p_n(z) = \sqrt{\frac{D_n}{D_{n+1}}} z^n + Q, \quad Q \in \mathcal{P}_{n-1}.$$

Thus, using that $(z^j)^\# = z^j$, we need to show that

$$\Phi(p_n(z)z^j) = \begin{cases} 0, & j < n \\ \sqrt{\frac{D_{n+1}}{D_n}}, & j = n. \end{cases}$$

From the definition of p_n and Φ it follows that

$$\Phi(p_n(z)z^j) = \frac{1}{\sqrt{D_n D_{n+1}}} \det \begin{pmatrix} s_0 & s_1 & s_2 & \cdots & s_n \\ s_1 & s_2 & s_3 & \cdots & s_{n+1} \\ \vdots & \vdots & \vdots & \dots & \vdots \\ s_{n-1} & s_n & s_{n+1} & \cdots & s_{2n-1} \\ s_j & s_{j+1} & s_{j+2} & \cdots & s_{j+n} \end{pmatrix}.$$

From this, the claim is clear. ❑

2.1.10 Definition. Let $a_{n+1} > 0, b_n \in \mathbb{R}$, for $n \geq 0$. The formal "difference operator" acting on sequences $(y_n)_{n\in\mathbb{N}_0}$ by

$$\begin{aligned} (\mathcal{J}y)_n &= a_{n+1}y_{n+1} + b_n y_n + a_n y_{n-1}, \quad n \geq 1 \\ (\mathcal{J}y)_1 &= a_1 y_1 + b_0 y_0. \end{aligned} \tag{2.4}$$

is called *Jacobi operator*.

It is sometimes convenient to visualize $\mathcal{J}$ as as an infinite dimensional three-diagonal matrix of the the form

$$\mathcal{J} = \begin{pmatrix} b_0 & a_1 & 0 & 0 & 0 \\ a_1 & b_1 & a_2 & 0 & 0 \\ 0 & a_2 & b_2 & a_3 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots \end{pmatrix}$$

2.1.11 Remark. At this stage it is not justified to call this an operator. We will see that $\mathcal{J}$ will act after specifying the correct domains (possibly unbounded) as an operator on $\ell^2(\mathbb{N}_0)$.

The connection to orthogonal polynomials is the following:

2.1.12 Proposition. *Let s be a moment sequence. Define for* $n \geq 0$

$$a_{n+1} = \frac{\|P_{n+1}\|_s}{\|P_n\|_s} > 0, \quad b_n = \frac{\langle zP_n, P_n\rangle_s}{\|P_n\|_s^2} \in \mathbb{R}.$$

Then for the monic orthogonal polynomials it holds that

$$\begin{aligned} zP_n(z) &= P_{n+1}(z) + b_n P_n(z) + a_n^2 P_{n-1}(z), \quad n \geq 1 \\ zP_0(z) &= P_1(z) + b_0 P_0(z). \end{aligned}$$

For the orthonormal polynomials we have

$$\begin{aligned} zp_n(z) &= a_{n+1}p_{n+1}(z) + b_n p_n(z) + a_n p_{n-1}(z), \quad n \geq 1 \\ zp_0(z) &= a_1 p_1(z) + b_0 p_0(z). \end{aligned} \tag{2.5}$$

In particular

$$\|P_n\|_s = \prod_{j=1}^{n} a_j.$$

Proof. We consider only $n \geq 1$. Let $j < n-1$ (if $n > 1$) then $\deg(zP_j(z)) < n$. Using orthogonality and the fact that $(zP_n(z))P_m^{\#}(z) = (zP_n(z))P_m(z) = P_n(z)(zP_m(z))^{\#}$, it follows that

$$\langle zP_n(z), P_j(z)\rangle_s = \langle P_n(z), zP_j(z)\rangle_s = 0.$$

Hence we get that

$$zP_n(z) = P_{n+1}(z) + \tilde{b}_n P_n(z) + c_n P_{n-1}(z)$$

for $\tilde{b}_n, c_n \in \mathbb{R}$. Let us check that $\tilde{b}_n = b_n$ and $c_n = a_n^2$. We have

$$\tilde{b}_n \|P_n\|_s^2 = \langle zP_n(z), P_n(z)\rangle_s.$$

For c_n note that $zP_n(z) - P_{n+1}(z)$ is a polynomial of degree at most n. Thus, taking the inner product with respect to P_{n+1} yields

$$\langle zP_n(z), P_{n+1}(z)\rangle_s = \|P_{n+1}\|_s^2.$$

Therefore

$$c_n = \frac{\langle zP_n(z), P_{n-1}(z)\rangle_s}{\|P_{n-1}\|_s^2} = \frac{\langle P_n(z), zP_{n-1}(z)\rangle_s}{\|P_{n-1}\|_s^2} = \left(\frac{\|P_n\|_s}{\|P_{n-1}\|_s}\right)^2 = a_n^2.$$

Passing to the recursion for the orthonormal polynomials is now an exercise. ❑

We have thus, defined a map from the set of positive sequences into the set of Jacobi operators. Our next goal is to show that this map is in fact a bijection.
Let us start with a Jacobi operator J. We can define the sequence of polynomials p_n by $p_0(z) = 1$, $p_1(z) = \frac{z-b_0}{a_1}$ and for $n \geq 1$

$$p_{n+1}(z) = \frac{1}{a_{n+1}}\left((z-b_0)p_n(z) - a_n p_{n-1}(z)\right).$$

Note that this in particular implies that $\deg p_n = n$.

2.1.13 Lemma. *We have $\mathcal{P}_n = \operatorname{span}\{p_k \mid 0 \leq k \leq n\}$. Moreover, if $P = \sum_{k=0}^{n} c_k p_k(z)$ with $c_n \neq 0$, then this representation is unique.*

Proof. We prove by induction that this is true for $(z^n)_{n\in\mathbb{N}_0}$. The induction start follows from $p_0(z) = 1$. Now assume that $z^n = \sum_{j=0}^{m} c_j p_j(z)$. Then we have

$$z^{n+1} = zz^n = \sum_{j=0}^{m} c_j z p_j(z) = \sum_{j=0}^{m} c_j(a_{j+1}p_{j+1}(z) + b_j p_j(z) + a_j p_{j-1}(z)).$$

We also show the second claim using induction. We need to show that if for $n \in \mathbb{N}$ $\sum_{k=0}^{n} c_k p_k(z) = 0$, then $c_k = 0$ for all $0 \le k \le n$. Clearly, this holds for $n = 0$. Now assume that

$$0 = \sum_{k=0}^{n+1} c_k p_k(z) = a_{n+1} p_{n+1}(z) + \sum_{k=0}^{n} c_k p_k(z).$$

Since $\deg p_{n+1} = n + 1$ and $\deg \sum_{k=0}^{n} c_k p_k(z) \le n$, we conclude that $c_{n+1} = 0$ and the induction hypothesis implies that $c_k = 0$ for $0 \le k \le n$. ❑

Our goal is to define a functional Φ on $\mathcal{P}$ with

$$\Phi(p_n p_m^{\#}) = \delta_{nm}.$$

It is a priori not clear that this is well defined. Let us therefore, for $R = \sum_{k=0}^{n} c_k p_k$ and $Q = \sum_{j=0}^{m} d_j p_j$ define

$$\tilde{\Phi}(R, Q) = \sum_{k=0}^{\min\{n,m\}} c_k \overline{d_k}.$$

It is easy to see that

$$\tilde{\Phi}(R, Q) = \overline{\tilde{\Phi}(Q, R)}$$

and that for $\lambda \in \mathbb{C}$ and $R_1, R_2, Q \in \mathcal{P}$

$$\tilde{\Phi}(\lambda R_1 + R_2, Q) = \lambda \tilde{\Phi}(R_1, Q) + \tilde{\Phi}(R_2, Q).$$

2.1.14 Lemma. *Let* $R_i = \sum_{k=0}^{n_i} c_k^i p_k$, $Q_i = \sum_{j=0}^{m_i} d_j^i p_j$, *for* $i = 1, 2$ *and assume that* $R_1 Q_1^{\#} = R_2 Q_2^{\#}$. *Then it holds that*

$$\tilde{\Phi}(R_1, Q_1) = \tilde{\Phi}(R_2, Q_2).$$

Proof. We first show the claim for $R_1(z) = z p_k(z), Q_1(z) = p_j(z)$ and $R_2(z) = p_k(z), Q_1(z) = z p_j(z)$. We show the claim for $j, k > 0$. The case $j = 0$ or $k = 0$ can be included by setting below $a_{-1} = 0$. Recall that

$$z p_i(z) = a_{i+1} p_{i+1}(z) + b_i p_i(z) + a_i p_{i-1}(z).$$

Hence,

$$\tilde{\Phi}(z p_k(z), p_j(z)) = a_{k+1} \delta_{k+1,j} + b_k \delta_{k,j} + a_k \delta_{k-1,j},$$
$$\tilde{\Phi}(p_k(z), z p_j(z)) = a_{j+1} \delta_{k,j+1} + b_j \delta_{k,j} + a_j \delta_{k,j-1},$$

which shows that $\tilde{\Phi}(z p_k(z), p_j(z)) = \tilde{\Phi}(p_k(z), z p_j(z))$. Using linearity, we conclude that for $R, Q \in \mathcal{P}$ it holds that $\tilde{\Phi}(zR, Q) = \tilde{\Phi}(R, zQ)$. Note also that for $\lambda \in \mathbb{C}$ it holds that $\tilde{\Phi}(\lambda R, Q) = \tilde{\Phi}(R, \overline{\lambda} Q)$ and $\lambda R Q\# = R(\overline{\lambda} Q)^{\#}$. Now writing $R_1 Q_1$ as a product of its zeros, this and linearity allows us to move factors between R and Q and the claim follows. ❑

Let $P = RQ^{\#}$, then due to Lemma 2.1.14 we can define

$$\Phi(P) := \tilde{\Phi}(R, Q).$$

Note that we always have the trivial factorization $P(z) = P(z) \cdot 1$.
We can now define s_k associated to J by

$$s_k := \Phi(z^k). \tag{2.6}$$

2.1.15 Lemma. *Let J be a Jacobi matrix, Φ the associated functional and $s_k = \Phi(z^k)$. Then $(s_k)_{k\in\mathbb{N}_0}$ is a moment sequence.*

Proof. Let $P(z) = \sum_{i=0}^n c_i z^i$. Then we have

$$\Phi(PP^\#) = \sum_{i=0}^n \sum_{j=0}^n c_i\overline{c_j}\Phi(z^{i+j}) = \sum_{i=0}^n \sum_{j=0}^n c_i\overline{c_j}s_{i+j}.$$

On the other hand, let

$$P = \sum_{i=0}^n \xi_i p_i.$$

Then by definition of Φ, we have

$$\Phi(PP^\#) = \sum_{i=0}^n |\xi_i|^2.$$

Thus, if $P \not\equiv 0$ we have $\sum_{i=0}^n \sum_{j=0}^n c_i\overline{c_j}s_{i+j} > 0$ and we conclude that $(s_k)_{k\in\mathbb{N}_0}$ is a moment sequence. ❑

2.1.16 Theorem. *There is a bijective correspondence between the set of Jacobi matrices and the set of moment sequences.*

Let us consider J as an operator acting on $\ell^2(\mathbb{N}_0)$. In general J can be unbounded. However, there is a clear criterion, when it is bounded.

2.1.17 Lemma. *Let J be a Jacobi matrix with coefficients a_{k+1}, b_k. Then J is bounded if and only if*

$$\sup_{k\in\mathbb{N}_0}(|a_k| + |b_k|) < \infty. \tag{2.7}$$

In this case J defines a self-adjoint operator on $\ell^2(\mathbb{N}_0)$.

Proof. We first show that boundedness of J implies (2.7). Let $e_n \in \ell^2(\mathbb{N}_0)$ denote the standard basis in $\ell^2(\mathbb{N}_0)$, i.e., $(e_n)_k = \delta_{n,k}$. Then we have

$$\langle Je_n, e_{n-1}\rangle = a_n, \quad \langle Je_n, e_n\rangle = b_n.$$

Thus, it follows that

$$a_n \le \|J\|, \quad b_n \le \|J\|.$$

Conversely, let $y = (y_k) \in \ell^2(\mathbb{N}_0)$ and $\alpha = \sup|a_n|, \beta = \sup|b_n|$. Then we have

$$\begin{aligned}|(Jy)_n|^2 = |a_{n+1}y_{n+1} + b_n y_n + a_n y_{n-1}|^2 &= \left|\left\langle \begin{pmatrix}\sqrt{a_{n+1}}\\ \sqrt{b_n}\\ \sqrt{a_n}\end{pmatrix}, \begin{pmatrix}\sqrt{a_{n+1}}y_{n+1}\\ \sqrt{b_n}y_n\\ \sqrt{a_n}y_{n-1}\end{pmatrix}\right\rangle\right|^2 \\ &\le (2\alpha+\beta)(\alpha|y_{n+1}|^2 + \beta|y_n|^2 + \alpha|y_{n-1}|^2).\end{aligned}$$

Taking the sum of all n shows that $\|Jy\|^2 \le (2\alpha+\beta)^2\|y\|^2$ and thus

$$\|J\| \le 2\sup_n |a_{n+1}| + \sup_n |b_n|.$$

It remains to show that J is self adjoint. We need to show that $\langle Ju, v\rangle$, for all $u, v \in \ell^2(\mathbb{N}_0)$. We first check that this holds for the basis vectors e_n:

$$\langle Je_n, e_m\rangle = \langle e_n, Je_m\rangle = \begin{cases} b_n & \text{if } n = m, \\ a_m & \text{if } m = n+1, \\ a_n & \text{if } n = m+1, \\ 0 & |n-m| > 1. \end{cases}$$

By linearity it thus holds for all vectors which are compactly supported and then by continuity for all $u, v \in \ell^2(\mathbb{N}_0)$. ❑

Recall that (p_n) satisfies the recursion

$$zp_n(z) = a_{n+1}p_{n+1}(z) + b_n p_n(z) + a_n p_{n-1}(z).$$

It is convenient to bring this into matrix form. For $(z, a, b) \in \mathbb{C} \times \mathbb{R}_{>0} \times \mathbb{R}$, let us define the one step transfer matrix by

$$A(z, a, b) := \begin{pmatrix} \frac{z-b}{a} & \frac{1}{a} \\ -a & 0 \end{pmatrix} \tag{2.8}$$

Then it holds that

$$\begin{pmatrix} p_{n+1}(z) \\ -a_{n+1}p_n(z) \end{pmatrix} = A(z, a_{n+1}, b_n) \begin{pmatrix} p_n(z) \\ -a_n p_{n-1}(z) \end{pmatrix}^1.$$

This holds also for $n = 0$, if we set $p_{-1}(z) = 0$. That is, if we start with the initial condition

$$\begin{pmatrix} p_1(z) \\ -a_1 p_0(z) \end{pmatrix} = A(z, a_1, b_0) \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

If we define

$$T_n(z) = A(z, a_n, b_{n-1})A(z, a_{n-1}, b_{n-2}) \dots A(z, a_1, b_0). \tag{2.9}$$

then we clearly have that

$$\begin{pmatrix} p_n(z) \\ -a_n p_{n-1}(z) \end{pmatrix} = T_n(z) \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

It will be convenient to also introduce the second solution of the system.

2.1.18 Definition. Let J be a Jacobi matrix. Then we define the *orthonormal polynomials of the second kind* by

$$\begin{pmatrix} q_n(z) \\ -a_n q_{n-1}(z) \end{pmatrix} = T_n(z) \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Setting $n = 1$, we get

$$q_1(z) = \frac{1}{a_1}, \quad q_0(z) = 0$$

and all others are given by

$$zq_n(z) = a_{n+1}q_{n+1}(z) + b_n q_n(z) + a_n q_{n-1}(z). \tag{2.10}$$

In particular, we see that $\deg q_n = n - 1$.

---

[1] Although it is standard to define the transfer matrix so that there is no minus sign in the second entry, there are good reasons for this choice. We will encounter some in the course of the lecture.

2.1.19 Lemma. *Let J be a Jacobi matrix and Φ the associated functional. Then we have for $n \geq 0$*

$$q_n(z) = \Phi_t\left(\frac{p_n(z) - p_n(t)}{z - t}\right).$$

Proof. Note first that $\frac{p_n(z)-p_n(t)}{z-t}$ is a polynomial of degree $n-1$ in z and t. Thus, we can apply Φ with respect to the variable t. The identity is easy to check for $n = 0, 1$. For $n > 1$ it thus suffices to check that $\tilde{q}_n(z) = \Phi_t\left(\frac{p_n(z)-p_n(t)}{z-t}\right)$ satisfies (2.10). We have

$$\begin{aligned} z\tilde{q}_n(z) &= \Phi_t\left(\frac{zp_n(z) - zp_n(t) + tp_n(t) - tp_n(t)}{z - t}\right) \\ &= \Phi_t\left(\frac{zp_n(z) - tp_n(t)}{z - t}\right) \\ &= a_{n+1}\tilde{q}_n(z) + b_n\tilde{q}_n(z) + a_n\tilde{q}_{n-1}(z), \end{aligned}$$

where for the last step we used the recursion for $zp_n(z)$ and $tp_n(t)$. ❑

Let us note that

$$T_n(z) = \begin{pmatrix} p_n(z) & q_n(z) \\ -a_n p_{n-1}(z) & -a_n q_{n-1}(z) \end{pmatrix} \tag{2.11}$$

2.1.20 Corollary. *The following Wronskian identity holds for all $n \geq 1$ and $z \in \mathbb{C}$:*

$$1 = a_n(p_{n-1}(z)q_n(z) - q_{n-1}(z)p_n(z)) \tag{2.12}$$

Proof. Due to (2.8),(2.9), $\det T_n(z) = 1$. Thus, the claim follows from (2.11). ❑

2.1.21 Definition. The Christoffel-Darboux kernel is given by

$$K_n(z, w) = \sum_{j=0}^{n-1} p_j(z)\overline{p_j(w)}, \quad z, w \in \mathbb{C}.$$

Due to Theorem 2.1.16 it is the same whether to start with a moment sequence of a Jacobi matrix. In any case we can associate a functional, which then defines an inner product $\langle \cdot, \cdot \rangle_s$ on $\mathcal{P}$ by (2.3). Although $(\mathcal{P}, \langle \cdot, \cdot \rangle_s)$ will not be complete, this is obviously true for $(\mathcal{P}_n, \langle \cdot, \cdot \rangle_s)$. Thus, $(\mathcal{P}_n, \langle \cdot, \cdot \rangle_s)$ is a Hilbert space of functions on $\mathbb{C}$. As $\mathcal{P}_n$ is finite dimensional, point evaluation is a continuous functional and hence, $(\mathcal{P}_n, \langle \cdot, \cdot \rangle_s)$ is a reproducing kernel Hilbert space. Let us recall the definition

2.1.22 Definition. Let Ω be a set and $\mathcal{H} \subseteq \mathbb{C}^\Omega$ be a Hilbert space with inner product $\langle \cdot, \cdot \rangle$. If for every $w \in \Omega$, the point evaluation functional at w is continuous, then $(\mathcal{H}, \langle \cdot, \cdot \rangle)$ is called a reproducing kernel Hilbert space. In this case, there exists $K_\mathcal{H}(z, w) : \Omega \times \Omega \to \mathbb{C}$ such that

- $\forall w \in \Omega\ K_\mathcal{H}(\cdot, w) \in \mathcal{H}$,
- $\forall f \in \mathcal{H}, w \in \Omega, f(w) = \langle f, K_\mathcal{H}(\cdot, w) \rangle$.

The function $K_\mathcal{H}$ is called the reproducing kernel of $\mathcal{H}$.

Since p_j forms an orthonormal basis for $(\mathcal{P}_n, \langle \cdot, \cdot \rangle_s)$, it is easy to check that $K_{n+1}(z, w)$ is the reproducing kernel for $(\mathcal{P}_n, \langle \cdot, \cdot \rangle_s)$. We will prove a convenient formula for K_n.

2.1.23 Lemma. *The following identity holds for $z, w \in \mathbb{C}$ and $n \geq 1$:*

$$J - T_n(w)^* J T_n(z) = (z - \overline{w}) \sum_{k=0}^{n-1} \begin{pmatrix} p_k(z)\overline{p_k(w)} & q_k(z)\overline{p_k(w)} \\ p_k(z)\overline{q_k(w)} & q_k(z)\overline{q_k(w)} \end{pmatrix}. \tag{2.13}$$

Proof. Since $T_n(z) = A(z, a_n, b_{n-1}) T_{n-1}(z)$ we have

$$\begin{aligned} J - T_n(w)^* J T_n(z) &= J - T_{n-1}(w)^* J T_{n-1}(z) + T_{n-1}(w)^* J T_{n-1}(z) - T_n(w)^* J T_n(z) \\ &= J - T_{n-1}(w)^* J T_{n-1}(z) + T_{n-1}(w)^* (J - A(w, a_n, b_{n-1})^* J A(z, a_n, b_{n-1})) T_{n-1}(z). \end{aligned}$$

A direct computation shows that

$$\begin{aligned} T_{n-1}(w)^* (J - A(w, a_n, b_{n-1})^* J A(z, a_n, b_{n-1})) T_{n-1}(z) &= T_{n-1}(w)^* \begin{pmatrix} z - \overline{w} & 0 \\ 0 & 0 \end{pmatrix} T_{n-1}(z) \\ &= (z - \overline{w}) \begin{pmatrix} p_{n-1}(z)\overline{p_{n-1}(w)} & q_{n-1}(z)\overline{p_{n-1}(w)} \\ p_{n-1}(z)\overline{q_{n-1}(w)} & q_{n-1}(z)\overline{q_{n-1}(w)} \end{pmatrix} \end{aligned}$$

Thus, the claim follows by iterating this identity. ❑

2.1.24 Corollary. *For $n \geq 1$, $T_n(z)$ is a J contractive matrix function.*

Proof. We need to show that for $z \in \mathbb{C}_+$, $-i(J - T_n(z)^* J T_n(z)) \geq 0$. This follows since $(J - T_n(z)^* J T_n(z))/(z - \overline{z}) = -i(T_n(z)^* J T_n(z) - J)/(2 \operatorname{Im} z)$ and

$$\begin{pmatrix} p_k(z)\overline{p_k(z)} & q_k(z)\overline{p_k(z)} \\ p_k(z)\overline{q_k(z)} & q_k(z)\overline{q_k(z)} \end{pmatrix} = \begin{pmatrix} p_k(z) \\ q_k(z) \end{pmatrix} \begin{pmatrix} p_k(z) \\ q_k(z) \end{pmatrix}^* \geq 0.$$

❑

Conjugating (2.13) with $(w,\ 1)^{\intercal}$ yields:

2.1.25 Corollary. *For $w \in \mathbb{C}$, $z \in \mathbb{C} \setminus \mathbb{R}$ and $n \geq 1$ we have*

$$\operatorname{Im} z \sum_{k=0}^{n-1} |w p_k(z) + q_k(z)|^2 = \operatorname{Im} w + a_n \operatorname{Im} \Big((w p_n(z) + q_n(z))(\overline{w}\overline{p_{n-1}(z)} + \overline{q_{n-1}(z)}) \Big). \tag{2.14}$$

Looking at the 1-1 entry of (2.13), we get the Christoffel-Darboux formula:

2.1.26 Proposition (Christoffel-Darboux formula)**.** *It holds that*

$$K_n(z, w) = a_n \frac{p_n(z)\overline{p_{n-1}(w)} - p_{n-1}(z)\overline{p_n(w)}}{z - \overline{w}} \tag{2.15}$$

We can now make the first connection to Herglotz functions

2.1.27 Corollary. *$p_n(z) \neq 0$ for $z \in \mathbb{C} \setminus \mathbb{R}$. Moreover, if we define*

$$g_n(z) = -\frac{p_n(z)}{a_{n+1} p_{n+1}(z)}.$$

Then $g_n \in \mathcal{N}_0$. As a consequence the zeros of p_n are real and simple and zeros of p_n and p_{n+1} interlace.

Proof. Let $z \in \mathbb{C} \setminus \mathbb{R}$. Then $z - \overline{z} = 2i \operatorname{Im} z \neq 0$. Hence, if $p_n(z) = 0$, we get

$$K_{n+1}(z, z) = a_{n+1} \frac{p_{n+1}(z)\overline{p_n(z)} - p_n(z)\overline{p_{n+1}(z)}}{z - \overline{z}} = 0$$

which is a contradiction. The same argument shows that p_n and p_{n+1} cannot vanish simultaneously.
Hence $g_n(z)$ is analytic in $\mathbb{C}_+$. Moreover, for $z \in \mathbb{C}_+$

$$0 < K_{n+1}(z, z) = a_{n+1} \frac{p_{n+1}(z)\overline{p_n(z)} - p_n(z)\overline{p_{n+1}(z)}}{z - \overline{z}} = |a_{n+1} p_{n+1}(z)|^2 \frac{\operatorname{Im} g_n(z)}{\operatorname{Im} z}.$$

Thus, $g_n \in \mathcal{N}_0$. Write $p_n(z) = \prod_{j=1}^{n} \gamma_n (z - \xi_j)$. Due to the integral representation for g_n, there exists $\sigma_j > 0$ such that

$$g_n(z) = \sum_{j=1}^{n} \frac{\sigma_j}{\xi_j - z}.$$

Hence, g_n is increasing between λ_j and λ_{j+1}, giving exactly one zero of p_n between consecutive zeros of p_{n+1}. Thus there is exactly one zero of p_{n+1} in each (ξ_j, ξ_{j+1}), which shows the interlacing property. ❑

Note that m_n is normalized so that

$$g_n(z) \sim -\frac{1}{z}, \quad z \to \infty$$

which is the same as

$$\sum_{j=1}^{n+1} \sigma_j = 1.$$

Another family of Herglotz functions will play an important role. Note that from (2.13) it follows that $T_n(z)^{-1}$ is J-expanding. Thus, from Lemma 1.2.4 it follows that for $\tau \in \overline{\mathbb{R}}$,

$$m_n(z, \tau) := T_n(z)^{-1} \star \tau = -\frac{q_n(z) + a_n \tau q_{n-1}(z)}{p_n(z) + a_n \tau p_{n-1}(z)} \tag{2.16}$$

is a Herglotz function. The functions

$$p_n(z, \tau) := p_n(z) + a_n \tau p_{n-1}(z), \quad q_n(z, \tau) = q_n(z) + a_n \tau q_{n-1}(z)$$

are called *quasi-orthogonal polynomials*. For $\tau = \infty$, we set $p_n(z, \infty) = -a_n p_{n-1}(z)$, $q_n(z, \infty) = -a_n q_{n-1}(z)$. We collect their most important properties below.

2.1.28 Proposition. *Let s be a moment sequence, $\tau \in \overline{\mathbb{R}}$. Then the quasi-orthogonal polynomials have the following properties*

(i) All the zeros of a quasi-orthogonal polynomial are real and simple;

(ii) The zeros of $p_n(z, \tau)$ and $q_n(z, \tau)$ interlace;

(iii) For $\tau \in \overline{\mathbb{R}} \setminus \{0\}$, and $j < n - 1$, we have

$$\Phi_t(p_n(t, \tau) t^j) = 0;$$

(iv) We have

$$\Phi_t(p_n(t, 0) t^{n-1}) = 0;$$

Proof. (i): By definition we have

$$T_n(z)^{-1}\begin{pmatrix}\tau\\1\end{pmatrix}\begin{pmatrix}-q_n(z,\tau)\\p_n(z,\tau)\end{pmatrix}.$$

Therefore, p_n and q_n cannot vanish identically. Since m_n is a Herglotz function, which is not constant 0 or ∞, it cannot vanish or have a pole at $\mathbb{C}_+$.
(ii) follow as in Corollary 2.1.27.
(iii) and (iv) follow from the definition and the fact that $p_n(z)$ are orthogonal polynomials for Φ. ❑

2.2 Quadrature formulae

Remember the rectangle rule with the left endpoint

$$Q_0^{[a,b]}(f) := (b-a)f(a)$$

which is exact for constant polynomials and the trapezoid rule

$$Q_1^{[a,b]}(f) := (b-a)\frac{f(a)+f(b)}{2}$$

which is exact for linear polynomials. Note that if we consider the midpoint rule,

$$Q^{[a,b]}(f) := (b-a)f\left(\frac{a+b}{2}\right)$$

we can integrate also linear polynomials exact with only one evaluation point. Gauss suggested that an integration scheme is optimal, if it is exact for a certain degree of polynomials and we will see that the above can be obtained for arbitrary number of sampling points and degree of polynomials. That is for n interior sampling points we are able to integrate exactly polynomials up to degree $2n-1$.

2.2.1 Lemma (Lagrange interpolation)**.** *Let $z_1,\cdots,z_n$ and $\alpha_1,\cdots,\alpha_n$ be complex numbers. Assume that all the z_j are distinct. There exists a unique polynomial $P\in\mathcal{P}_{n-1}$ such that*

$$P(z_j)=\alpha_j. \tag{2.17}$$

It is explicitly given by

$$P(z)=\sum_{j=1}^{n}\alpha_j\prod_{k\neq j}\frac{z-z_k}{z_j-z_k}=\sum_{j=1}^{n}\alpha_j\frac{Q(z)}{Q'(z_j)(z-z_j)},$$

where $Q(z)=A\prod_{j=1}^{n}(z-z_j)$ (here $A\in\mathbb{C}$ is arbitrary).

Proof. We will omit the proof. ❑

2.2.2 Proposition. *Let $\Phi:\mathcal{P}\to\mathbb{C}$ be a positive functional and $\tau\in\overline{\mathbb{R}}$. Let $p_n(z,\tau)$ be the quasi-orthonormal polynomial constructed from Φ and let $(\xi_j)_{j=1}^{n}$ be the zeros of $p_n(z,\tau)$. Then*

$$\Phi(R)=\sum_{j=1}^{n}\Phi_t\left(\frac{p_n(t,\tau)}{p_n'(\xi_j,\tau)(t-\xi_j)}\right)R(\xi_j) \tag{2.18}$$

for any $R\in\mathcal{P}_{2n-2}$. If $\tau=0$, (2.18) *also holds for $R\in\mathcal{P}_{2n-1}$*

Proof. Let $p_{n,\tau}(z) = p_n(z,\tau)$ and let $R \in \mathcal{P}_{2n-2}$. By polynomial division we can write $R = p_{n,\tau}S + T$, where $S \in \mathcal{P}_{n-2}, T \in \mathcal{P}_{n-1}$. Using orthogonality of $p_{n,\tau}$ and $p^{\#}_{n,\tau} = p_{n,\tau}$, we get

$$\Phi(R) = \Phi(p_{n,\tau}S) + \Phi(T) = \Phi(T) \tag{2.19}$$

$$= \sum_{j=1}^{n} T(\xi_j)\Phi_t\left(\frac{p_{n,\tau}(t)}{(t-\xi_j)p'_{n,\tau}(\xi_j)}\right) \tag{2.20}$$

$$= \sum_{j=1}^{n} R(\xi_j)\Phi_t\left(\frac{p_{n,\tau}(t)}{(t-\xi_j)p'_{n,\tau}(\xi_j)}\right), \tag{2.21}$$

where we used Lagrange interpolation in the second line and the fact that $R(\xi_j) = T(\xi_j)$ for the last line. If $\tau = 0$, then we can choose $R \in \mathcal{P}_{2n-1}$, i.e., $S \in \mathcal{P}_{n-1}$ and still $\Phi(p_{n,\infty}S) = 0$. ❑

There is an alternative expression for the coefficient in the interpolation forumla in terms of the Christoffel-Darboux kernel

2.2.3 Lemma. *In the setting of Proposition 2.2.2 we have*

$$\Phi_t\left(\frac{p_n(t)}{p'_n(\xi_j)(t-\xi_j)}\right) = \frac{q_n(\xi_j,\tau)}{p'_n(\xi_j,\tau)} = \frac{1}{K_{n-1}(\xi_j,\xi_j)}.$$

In particular, these coefficients are positive.

Proof. Since $p_n(\xi_j,\tau) = 0$ we have

$$\Phi_t\left(\frac{p_n(t,\tau)}{(t-\xi_j)}\right) = \Phi_t\left(\frac{p_n(t,\tau) - p_n(\xi_j,\tau)}{(t-\xi_j)}\right) = q_n(\xi_j,\tau).$$

Hence

$$\Phi_t\left(\frac{p_n(t)}{p'_n(\xi_j)(t-\xi_j)}\right) = \frac{q_n(\xi_j,\tau)}{p'_n(\xi_j,\tau)}.$$

On the other hand, using that $p_n(\xi_j,\tau) = p_n(\xi_j) - a_n\tau p_{n-1}(\xi_j) = 0$, and hence, $a_n\tau = \frac{p_n(x_j)}{p_{n-1}(x_j)}$, we see that

$$\frac{q_n(\xi_j,\tau)}{p'_n(\xi_j,\tau)} = \frac{p_{n-1}(\xi_j)q_n(\xi_j) - p_n(\xi_j)q_{n-1}(\xi_j)}{p_{n-1}(\xi_j)p'_n(\xi_j) - p_n(\xi_j)p'_{n-1}(\xi_j)}.$$

Recall that by (2.12) we have $1 = a_n(p_{n-1}(\xi_j)q_n(\xi_j) - q_{n-1}(\xi_j)p_n(\xi_j))$ On the other hand, by the CD-formula (2.15)

$$K_{n-1}(\xi_j,\xi_j) = a_n(p'_n(\xi_j)p_{n-1}(\xi_j) - p'_{n-1}(\xi_j)p_n(\xi_j)).$$

Hence,

$$\frac{a_n(p_{n-1}(\xi_j)q_n(\xi_j) - p_n(\xi_j)q_{n-1}(\xi_j))}{a_n(p_{n-1}(\xi_j)p'_n(\xi_j) - p_n(\xi_j)p'_{n-1}(\xi_j))} = \frac{1}{K_{n-1}(\xi_j,\xi_j)}.$$

❑

2.3 Existence of a solution for the Hamburger moment problem

At this place we are already able to show that $(s_n)_{n\in\mathbb{N}_0}$ being a positive sequence is necessary and sufficient to have a non-trivial solution to the Hamburger moment problem.

2.3.1 Theorem. *Let $(s_n)_{n\in\mathbb{N}_0} \in \mathbb{R}^{\mathbb{N}_0}$. Then there exists a real measure μ, which is not supported on finitely many points such that for all $n \in \mathbb{N}_0$*

$$s_n = \int_{\mathbb{R}} x^n d\mu(x),$$

if and only if $(s_n)_{n\in\mathbb{N}_0}$ is a moment sequence.

From the introduction we already see that the only thing to prove is the "if" direction.

2.3.2 Lemma. *Let $(s_n)_{n\in\mathbb{N}_0} \in \mathbb{R}^{\mathbb{N}_0}$ be a moment sequence. Fix $n \in \mathbb{N}$ and define*

$$m_n(z,\tau) = -\frac{q_n(z,\tau)}{p_n(z,\tau)}.$$

Then $m_n(z,\tau)$ is a Herglotz function and if

$$\mu_{n,\tau} = \sum_{\xi_j | p_n(\xi_j,\tau)=0} c_j \delta_{\xi_j}$$

is the measure in its integral representation, then it holds that

$$s_j = \int x^j d\mu_{n,\tau}(x), \quad 0 \le j \le 2n-2.$$

If $\tau = 0$, this also holds for $j = 2n-1$. In particular, $\mu_{n,\tau}(\mathbb{R}) = s_0 = 1$.

Proof. We have already seen that $m_n(z,\tau)$ is a Herglotz function. Thus, the integral representation is given by

$$-\frac{q_n(z,\tau)}{p_n(z,\tau)} = \sum_{\xi_j | p_n(\xi_j,\tau)=0} \frac{c_j}{\xi_j - z} = \int \frac{1}{x-z} d\mu_n(x),$$

where

$$c_j = \lim_{y\to 0} m_n(\xi_j + iy)(\xi_j - (\xi_j + iy)) = \frac{q_n(\xi_j,\tau)}{p_n'(\xi_j,\tau)} = \frac{1}{K_{n-1}(\xi_j,\xi_j)},$$

where we used Lemma 2.2.3 in the last step. By definition of the function (2.6) we have $\Phi_t(t^k) = s_k$. On the other hand, for every polynomial $R \in \mathcal{P}_{2n-2}$

$$\Phi[R] = \sum_{\xi_j | p_n(\xi_j)=0} \Phi_t\left(\frac{p_n(t,\tau)}{p_n'(\xi_j,\tau)(t-\xi_j)}\right) R(\xi_j) = \sum_{\xi_j | p_n(\xi_j,\tau)=0} c_j R(\xi_j) = \int R(x) d\mu_n(x).$$

Thus, this holds in particular for the monomials $(x^j)_{j=0}^{2n-2}$. The changes for $\tau = 0$ are obvious. ❑

Our general strategy is to take a weak-* limit of the sequence μ_n and show that this limit has all the right moments. Some caution is required at this place, since x^j are not bounded functions on $\mathbb{R}$, so convergence of μ_n does not imply directly convergence of the moments. We therefore prove the following lemma. Let us first clarify what convergence of measures we have in mind. All μ_n are measures on $\mathbb{R}$. We can extend them to measures on $\overline{\mathbb{R}}$ by setting $\mu_n(\{\infty\}) = 0$. Then we can identify them as elements of $(C(\overline{\mathbb{R}}), \|\cdot\|_\infty)^*$. We will understand convergence of measures in the corresponding weak-* topology.

2.3.3 Lemma. *Let μ_n be measures supported on $\mathbb{R}$ and $(s_n)_{n\in\mathbb{N}_0}$ a moment sequence. Assume that*

$$\int x^j d\mu_n(x) = s_j \quad 0 \le j \le 2n-1.$$

Then, there exists a subsequence μ_{n_k} convergent to a measure μ with

$$\int x^j d\mu(x) = s_j, \quad j \in \mathbb{N}_0.$$

Proof. Let m_n be as in (2.3.2) for some fixed choice of τ. Consider μ_n as elements of $(C(\overline{\mathbb{R}}), \|\cdot\|_\infty)^*$, extended to $\overline{\mathbb{R}}$ by $\mu_n(\{\infty\}) = 0$. Since $s_0 = 1$, we have $\mu_n(\mathbb{R}) = \mu_n(\overline{\mathbb{R}}) = 1$, and thus are precompact by Banach-Alaoglu. Thus, we find a subsequence and a measure μ such that

$$\lim_{k\to\infty} \mu_{n_k} = \mu,$$

where the limit is taken in the weak-* topology of $(C(\overline{\mathbb{R}}), \|\cdot\|_\infty)^*$. That is integrated agains continuous functions on $\overline{\mathbb{R}}$. Note that in principle mass could be lost to ∞. We first show that this is not the case. Since for all $n \ge 2$

$$\int x^2 d\mu_n = s_2,$$

we get for any $R > 0$,

$$\int_{|x|\ge R} d\mu_n \le \int \frac{x^2}{R^2} d\mu_n(x) = \frac{s_2}{R^2}$$

Let f_R be a function on $\overline{\mathbb{R}}$, which is constant 1 on $\overline{\mathbb{R}} \setminus [-2R, 2R]$, constant 0 on $[-R, R]$ and linearly interpolated in between. Then we clearly have

$$\int_{\overline{\mathbb{R}}} f_R(x) d\mu_n(x) \le \int_{|x|\ge R} d\mu_n(x) \le \frac{s_2}{R^2}.$$

On the other hand

$$\lim_{k\to\infty} \int_{\overline{\mathbb{R}}} f_R(x) d\mu_{n_k}(x) = \int_{\overline{\mathbb{R}}} f_R(x) d\mu(x)$$

and thus

$$\int_{\overline{\mathbb{R}}} f_R(x) d\mu(x) \le \frac{s_2}{R^2}.$$

Sending $R \to \infty$ shows that $\mu(\{\infty\}) = 0$.
We define a function

$$f_{j,R}(x) = \begin{cases} x^j, & x \in [-R, R] \\ R^j(1 - \frac{x-R}{R}), & x \in [R, 2R] \\ (-R)^j(1 - \frac{-x-R}{R}), & x \in [-2R, -R] \\ 0 & x \in \overline{\mathbb{R}} \setminus [-2R, 2R] \end{cases}$$

For any m and k so that $m \leq n_k - 1$ we have

$$\int f_{2m,R}(x) d\mu_{n_k} \leq s_{2m}. \tag{2.22}$$

Since $f_{j,R}$ is continuous on $\overline{\mathbb{R}}$ we get

$$\lim_{k\to\infty} \int f_{j,R}(x) d\mu_{n_k}(x) = \int f_{j,R}(x) d\mu(x).$$

and thus

$$\int f_{2m,R}(x) d\mu \leq s_{2m}$$

and the monotone convergence theorem implies that

$$\int_{\mathbb{R}} x^{2m} d\mu(x) \leq s_{2m}.$$

That is μ has finite moments. Dominated convergence, implies that

$$\lim_{R\to\infty} \int f_{j,R}(x) d\mu(x) = \int x^j d\mu(x). \tag{2.23}$$

Fix j and choose $2m > j$ and k sufficiently large so that $n_k - 1 > m$. Then we have

$$\begin{aligned}\int \left| f_{j,R}(x) - x^j \right| d\mu_{n_k}(x) &\leq 2 \int_{|x|\geq R} |x|^j \, d\mu_{n_k}(x) \\ &\leq 2 \int_{|x|\geq R} \left| \frac{x}{R} \right|^{2m-j} |x|^j d\mu_{n_k}(x) \\ &\leq 2R^{j-2m} s_{2m}.\end{aligned}$$

Hence

$$\lim_{R\to\infty} \int f_{j,R}(x) d\mu_{n_k}(x) = \int x^j d\mu_{n_k}(x) \tag{2.24}$$

uniformly in k. Fix $\epsilon > 0$. Using that the limit in (2.23) is finite, we write

$$\begin{aligned}\left| \int x^j d\mu(x) - \int x^j d\mu_{n_k}(x) \right| \leq \left| \int x^j d\mu(x) - \int f_{j,R}(x) d\mu(x) \right| + \left| \int f_{j,R}(x) d\mu(x) - \int f_{j,R}(x) d\mu_{n_k}(x) \right| \\ + \left| \int f_{j,R}(x) d\mu_{n_k}(x) - \int x^j d\mu_{n_k} \right|.\end{aligned}$$

Using uniformity in (2.24) we can first choose R big enough so that the first and the third expression are smaller than ϵ for all sufficiently large k. Then we find k_0 so that for $k \geq k_0$ the second term becomes smaller than ϵ. ❑

Combining these statements we have proven Theorem 2.3.1.

2.4 Weyl discs and Weyl m-function

From Corollary 2.1.24 it follows that $T_n(z)^{-1}$ is J-expanding in $\mathbb{C}_+$. Thus, considered as a Möbius transform $T_n(z)^{-1}$, by Lemma 1.2.4 maps $\overline{\mathbb{C}_+} = \mathbb{C}_+ \cup \mathbb{R} \cup \{\infty\}$ into itself. Let us also introduce $\overline{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$. This motivates the definition of the Weyl disc

2.4.1 Definition. For every $n \geq 1$ and $z \in \mathbb{C}_+$ the Weyl disc $\mathcal{D}_n(z)$ and the Weyl circle $C_n(z)$ are defined by

$$\mathcal{D}_n(z) = \left\{ T_n(z)^{-1} \star \tau \mid \tau \in \overline{\mathbb{C}_+} \right\}, \quad \Gamma_n(z) = \left\{ T_n(z)^{-1} \star \tau \mid \tau \in \overline{\mathbb{R}} \right\}.$$

2.4.2 Lemma. *For every $n \geq 1$ and $z \in \mathbb{C}_+$ the Weyl circle $\Gamma_n(z)$ is a circle in $\mathbb{C}_+ \cup \mathbb{R}$ with center $c_n(z)$ and radius $r_n(z)$ given by*

$$c_n(z) = \frac{q_{n-1}(z)\overline{p_n(z)} - q_n(z)\overline{p_{n-1}(z)}}{p_n(z)\overline{p_{n-1}(z)} - p_{n-1}(z)\overline{p_n(z)}}, \quad r_n(z) = \frac{1}{|z - \overline{z}| K_n(z, z)}.$$

Proof. Note that since $\det T_n(z) = 1$

$$T_n(z)^{-1} = \begin{pmatrix} -a_n q_{n-1}(z) & -q_n(z) \\ a_n p_{n-1}(z) & p_n(z) \end{pmatrix}.$$

The forumla for $c_n(z)$ follows readily from Lemma 1.2.2. The forumla for r_n follows from Lemma 1.2.2 together with the CD-formula (2.15). That $C_n(z)$ must be contained in $\overline{\mathbb{C}_+}$ follows from the fact that $T_n(z)$ is J-expanding. Since $r_n(z) < \infty$, we conclude that it is indeed a circle and not a half space. ❑

2.4.3 Lemma. *For every $n \geq 1$ and $z \in \mathbb{C}_+$ the Weyl disc $\mathcal{D}_n(z)$ is a disc in the upper half plane. Moreover, the discs are nested, i.e.,*

$$\mathcal{D}_{n+1}(z) \subset \mathcal{D}_n(z).$$

Proof. We have $T_{n+1}(z) = A(z, a_{n+1}, b_n) T_n(z)$. If M is a *Mbius* transform and $S \subset \overline{\mathbb{C}}$, let us denote $M(S) = \{M \star \tau \mid \tau \in S\}$. Since $A(z, a_n, b_{n-1})$ is J-expanding, we have $A(z, a_n, b_{n-1})^{-1}(\overline{\mathbb{C}_+}) \subset \overline{\mathbb{C}}_+$. It follows that

$$\mathcal{D}_{n+1}(z) = T_{n+1}(z)^{-1}\left(\overline{\mathbb{C}_+}\right) = T_n(z)^{-1}\left(A(z, a_{n+1}, b_n)^{-1}\left(\overline{\mathbb{C}_+}\right)\right) \subset T_n(z)^{-1}\left(\overline{\mathbb{C}_+}\right) = \mathcal{D}_n(z).$$

❑

We will give an alternative description for the Weyl disc and the Weyl circle:

2.4.4 Lemma. *For any $z \in \mathbb{C}_+$, $n \geq 1$ we have*

$$\Gamma_n(z) = \left\{ w \mid \frac{\operatorname{Im} w}{\operatorname{Im} z} = \sum_{k=0}^{n-1} |w p_k(z) + q_k(z)|^2 \right\}, \mathcal{D}_n(z) \quad = \left\{ w \mid \frac{\operatorname{Im} w}{\operatorname{Im} z} \geq \sum_{k=0}^{n-1} |w p_k(z) + q_k(z)|^2 \right\}.$$

In particular $\mathcal{D}_n(z) \subset \mathbb{C}_+$.

Proof. Recall that $w \in \Gamma_n(z)$ if $w = T_n(z)^{-1} \star \tau$, for $\tau \in \overline{\mathbb{R}}$. If f_A denotes the Möbius transformation generated by A as in Lemma 1.2.1 this is by definition

$$w = f_{T_n(z)^{-1}}(\tau)$$

and hence,

$$T_n(z) \star w = f_{T_n(z)}(w) = f_{T_n(z)}(f_{T_n(z)^{-1}}(\tau)) = f_{T_n(z) \circ T_n(z)^{-1}}(\tau) = \tau.$$

Therefore

$$T_n(z) \star w = \tau \in \overline{\mathbb{R}}.$$

This is,

$$\frac{p_n(z)w + q_n(z)}{p_{n-1}(z)w + q_{n-1}(z)} \in \overline{\mathbb{R}},$$

which is equivalent to

$$(p_n(z)w + q_n(z))(\overline{p_{n-1}(z)}\overline{w} + \overline{q_{n-1}(z)}) \in \mathbb{R}.$$

Inserting this into (2.14) yields that $w \in \Gamma_n(z)$ if and only if

$$\frac{\operatorname{Im} w}{\operatorname{Im} z} = \sum_{k=0}^{n-1} |wp_k(z) + q_k(z)|^2.$$

For the description of $\mathcal{D}_n$ we note that the same arguments show that $w \in \mathcal{D}_n(z)$ if and only if

$$\operatorname{Im}(p_n(z)w + q_n(z))(\overline{p_{n-1}(z)}\overline{w} + \overline{q_{n-1}(z)}) \geq 0.$$

Hence, the claim follows again by (2.14).
It remains to show that $\mathcal{D}_n(z) \subset \mathbb{C}_+$. Note that $\operatorname{Im} w = 0$, implies that for $0 \leq k < n$, $wp_k(z) + q_k(z) = 0$. This implies that $-q_k(z)/p_k(z) \in \mathbb{R}$. Since $T_k(z)^{-1}$ is J-expanding, we see that

$$m_k(z) = T_k(z)^{-1} \star 0 = -\frac{q_k(z)}{p_k(z)}$$

is a Herglotz function. Thus if for $z \in \mathbb{C}_+$, $m_k(z) \in \mathbb{R}$, it follows that m_k is constant. This gives a contradiction. ❑

Recall that

$$m_n(z, \tau) = T_n(z)^{-1} \star \tau, \tau \in \overline{\mathbb{R}}$$

and that by Lemma 2.3.2, the measure in its integral representation $\mu_{n,\tau}$ is a solution of the moment problem for $0 \leq j \leq 2n - 2$. On the other hand, by construction

$$\Gamma_n(z) = \{m_n(z, \tau) \mid \tau \in \overline{\mathbb{R}}\}.$$

Allowing $\tau \in \overline{\mathbb{C}_+}$ and all solutions of the moment problem gives a corresponding relation of $\mathcal{D}_n(z)$. Let us introduce for a general finite measure μ,

$$w_\mu(z) = \int_{\mathbb{R}} \frac{d\mu(x)}{x - z}.$$

Recall also that for measure with k finite moments, we denote

$$s_k[\mu] = \int x^n d\mu(x).$$

2.4.5 Proposition. *For $n \geq 0$ and $z \in \mathbb{C}_+$ it holds that*

$$\mathcal{D}_n(z) = \{w_\mu(z) \mid s_k[\mu] = s_k, 0 \leq k \leq 2n - 2\}.$$

Proof. Let us start with the inclusion $\subset$: As seen above, we know the statement already for $w \in \Gamma_n(z)$. It thus suffices to take $w \in \operatorname{int}(\mathcal{D}_n(z))$. Since $\mathcal{D}_n(z)$ is a circle, we find $w_1, w_2 \in \Gamma_n(z)$ and $\theta \in (0, 1)$ so that

$$w = \theta w_1 + (1 - \theta)w_2.$$

Moreover, there are $\tau_1, \tau_2 \in \overline{\mathbb{R}}$ with

$$w_i = m_{n,\tau_i}(z), \quad i = 1, 2.$$

Now set

$$\mu = \theta\mu_{n,\tau_1} + (1-\theta)\mu_{n,\tau_2},$$

then clearly

$$s_j[\mu] = s_j, \quad 0 \le j \le 2n-2,$$

and

$$w_\mu(z) = \theta m_{n,\tau_1}(z) + (1-\theta)m_{n,\tau_2}(z) = \theta w_1 + (1-\theta)w_2 = w.$$

We prove $\supset$: Let μ be a solution of the moment problem for $0 \le k \le 2n-2$. Let $(p_k)_{k=0}^{n-1}$ be the orthonormal polynomials associated to $(s_k)_{k=0}^{2n-2}$. Note that by assumption and Lemma 2.1.9, they also form an orthonormal system in $L^2(\mu)$. Since μ is a finite measure $f(x) = \frac{1}{x-z}$ belongs to $L^2(\mu)$ and thus by Bessel's inequality we get

$$\int |f(x)|^2 d\mu(x) \ge \sum_{k=0}^{n-1} \left| \int f(x)p_k(x)d\mu(x) \right|^2.$$

Since

$$|f(x)|^2 = \frac{1}{x-z}\frac{1}{x-\overline{z}} = \frac{1}{z-\overline{z}}\left(\frac{1}{x-z} - \frac{1}{x-\overline{z}}\right),$$

we see that

$$\int |f(x)|^2 d\mu(x) = \frac{\operatorname{Im} w_\mu(z)}{\operatorname{Im} z}.$$

On the other hand, for $0 \le k \le n-1$

$$\int f(x)p_k(x)d\mu(x) = \int \frac{p_n(x)-p_k(z)}{x-z}d\mu(x) + p_k(z)\int \frac{1}{x-z}d\mu(x) = q_k(z) + p_k(z)w_\mu(z).$$

Appealing to Lemma 2.4.4 shows that $w_\mu(z) \in \mathcal{D}_n(z)$. ❑

2.4.1 Invariablity

Due to Lemma 2.4.2, $\mathcal{D}_n(z)$ is a non-degenerated disc (i.e., not a straight line) and due to 2.4.3 for fixed z, the discs $\mathcal{D}$ are nested. Hence, we can define

$$\mathcal{D}_\infty(z) = \bigcap_n \mathcal{D}_n(z)$$

and this will be either a disc or a point. It turns out that this is a property of the moment sequence in the sense that $\mathcal{D}_\infty(z)$ is a disc for one $z \in \mathbb{C}_+$ then this holds for all $z \in \mathbb{C}_+$. By Lemma 2.4.2, $\mathcal{D}_\infty(z)$ is a disc if and only if

$$\lim_{n\to\infty} K_n(z,z) = \sum_{k=0}^{\infty} |p_k(z)|^2 < \infty.$$

In fact, this also implies summablity if q_k.

2.4.6 Lemma. *Let $z \in \mathbb{C}_+$. Then $\mathcal{D}_\infty(z)$ is a disc, if and only if*

$$\sum_{k=0}^{\infty}(|p_k(z)|^2 + |q_k(z)|^2) < \infty. \tag{2.25}$$

Proof. From the discussion preceding the Lemma, we obtain that (2.25) implies that $\mathcal{D}_\infty(z)$ is a disc.
On the other hand, choose $w \in \mathcal{D}_\infty(z)$. Then Lemma 2.4.4 implies that

$$\sum_{k=0}^{\infty} |wp_k(z) + q_k(z)|^2 \leq \frac{\operatorname{Im} w}{\operatorname{Im} z}.$$

That is, $(p_k(z))_k, (wp_k(z) + q_k(z))_k \in \ell^2(\mathbb{N}_0)$ and thus also $(q_k(z))_k \in \ell^2(\mathbb{N}_0)$. ❑

2.4.7 Lemma. *Let* $A = (\alpha_{k,j})_{k,j=0}^{\infty}$ *such that*

$$a_{k,j} = 0 \quad \textit{for} \quad j \geq k \quad \textit{and} \quad \sum_{k,j\in\mathbb{N}_0^2} |a_{k,j}|^2 < \infty.$$

Then, there exists a constant C *(depending on* A*) such that for any* $(y_j)_{j\in\mathbb{N}_0}, \in \ell^2(\mathbb{N}_0)$*, there exists a unique solution* $(x_j)_{j\in\mathbb{N}_0}$ *so that*

$$y_k = x_k - \sum_{j=0}^{k-1} \alpha_{k,j} x_j. \tag{2.26}$$

Moreover, we have

$$\sum_{k=0}^{\infty} |x_k|^2 \leq C \sum_{k=0}^{\infty} |y_k|^2,$$

i.e., $(I - A)^{-1} \in L_b(\ell^2(\mathbb{N}_0))$.

Proof. Let $A_n = (\alpha_{k,j})_{k,j=0}^{n-1}$. Note that $I - A$ is lower triangular. Therefore, for all $n \in \mathbb{N}$, $I - A$ maps $(\mathbb{C}^n)^\perp = \{(x_j) \in \ell^2 \mid x_j = 0, \quad 0 \leq j \leq n-1\}$ into itself. Thus, uniqueness of the solution follows from invertibility of $I_n - A_n$, where I_n is the identiy on $\mathbb{C}^n$. Let us first consider vectors in $x^n, y^n \in \mathbb{C}^n$. Since $(I_n - A_n)$ is invertible and as linear map between finite dimensional Hilbert spaces bounded, we find C_n so that

$$\|x^n\| \leq C_n \|y^n\|.$$

Let $(y_j)_{j\in\mathbb{N}_0} \in \ell^2(\mathbb{N}_0)$ and $(x_j)_{j\in\mathbb{N}_0}$ be the unique solution of (2.26). Moreover, for $N \in \mathbb{N}$ let $x^N = (x_j)_{j=0}^N$. Set

$$n = \min\left\{ m \mid \sum_{k\geq m} \sum_{j=0}^{k-1} |a_{k,j}|^2 < \frac{1}{8} \right\}.$$

In the following assume that $N \geq n$. By the above it holds that

$$\sum_{j=0}^{n-1} |x_j|^2 \leq C_n^2 \|y\|^2. \tag{2.27}$$

Set

$$J(x) = \left\{ n \leq k \leq N \mid |x_k| \leq 2\sqrt{\sum_{j=0}^{k-1} |a_{k,j}|^2}\, \left\|x^N\right\| \right\}.$$

Then

$$\sum_{k\in J(x)} |x_k|^2 \leq 4 \sum_{k\in J(x)} \sum_{j=0}^{k-1} |a_{k,j}|^2 \left\|x^N\right\|^2 \leq 4 \sum_{n\leq k} \sum_{j=0}^{k-1} |a_{k,j}|^2 \left\|x^N\right\|^2 \leq \frac{1}{2} \left\|x^N\right\|^2.$$

That is,

$$\sum_{\substack{n\le k\le N\\ k\in J(x)}} |x_k|^2 \le \sum_{k=0}^{n-1} |x_k|^2 + \sum_{\substack{n\le k\le N\\ k\notin J(x)}} |x_k|^2. \tag{2.28}$$

On the other hand, for $n \le k \le N$, $k \notin J(x)$ we have

$$|y_k| \ge |x_k| - \sum_{j=0}^{k-1} |a_{k,j}||x_j| \ge |x_k| - \sqrt{\sum_{j=0}^{k-1} |a_{k,j}|^2}\,\left\|x^N\right\| > \frac{1}{2}|x_k|.$$

Hence,

$$\frac{1}{4} \sum_{\substack{n\le k\le N\\ k\notin J(x)}} |x_k|^2 \le \|y\|^2. \tag{2.29}$$

Combining (2.27), (2.28) and (2.29), we get

$$\begin{aligned}\sum_{k=0}^{N} |x_k|^2 &= \sum_{k=0}^{n-1} |x_k|^2 + \sum_{\substack{n\le k\le N\\ k\notin J(x)}} |x_k|^2 + \sum_{\substack{n\le k\le N\\ k\in J(x)}} |x_k|^2\\ &\le 2\left(\sum_{k=0}^{n-1} |x_k|^2 + \sum_{\substack{n\le k\le N\\ k\notin J(x)}} |x_k|^2\right)\\ &\le 2(C_n^2+4)\|y\|^2.\end{aligned}$$

Since this estimate holds for all $N \ge n$, we conclude that

$$\sum_{k=0}^{\infty} |x_k|^2 \le 2(C_n^2+4)\|y\|^2,$$

which finishes the proof. ❑

2.4.8 Theorem. *The following are equivalent:*

(i) There exists $z_0 \in \mathbb{C}_+$ so that $\sum_{k=0}^{\infty}(|p_k(z)|^2 + |q_k(z)|^2) < \infty$;

(ii) For all $z_0 \in \mathbb{C}_+$ so that $\sum_{k=0}^{\infty}(|p_k(z)|^2 + |q_k(z)|^2) < \infty$;

(iii) There exists $z_0 \in \mathbb{C}_+$ so that $\mathcal{D}_\infty(z_0)$ is a disc;

(iv) For all $z_0 \in \mathbb{C}_+$ so that $\mathcal{D}_\infty(z_0)$ is a disc;

Proof. $(i) \iff (iii)$ and $(ii) \iff (iv)$ follows from Lemma 2.4.6. We show $(i) \iff (ii)$. $(ii) \implies (i)$ is trivial.
Assume that (i) holds. Then we have

$$\sum_{k=0}^{\infty} |p_k(z_0)|^2 < \infty \quad \text{and} \quad \sum_{k=0}^{\infty} |q_k(z_0)|^2 < \infty.$$

Since

$$\frac{p_n(z) - p_n(z_0)}{z - z_0} \in \mathcal{P}_{n-1},$$

we find $\alpha_{n,k}$ so that

$$\frac{p_n(z) - p_n(z_0)}{z - z_0} = \sum_{k=0}^{n-1} \alpha_{n,k}(z_0) p_k(z). \tag{2.30}$$

Applying Φ yields

$$\begin{aligned}
\alpha_{n,k}(z_0) &= \Phi\left(\frac{p_n(t) - p_n(z_0)}{t - z_0} p_k(t)\right) \\
&= p_k(z_0)\Phi\left(\frac{p_n(t) - p_n(z_0)}{t - z_0}\right) + \Phi\left(\frac{p_n(t) - p_n(z_0)}{t - z_0}(p_k(t) - p_k(z_0))\right) \\
&= p_k(z_0)q_n(z_0) + \Phi\left(\frac{p_k(t) - p_k(z_0)}{t - z_0} p_n(t)\right) - p_k(z_0)\Phi\left(\frac{p_k(t) - p_k(z_0)}{t - z_0}\right) \\
&= p_k(z_0)q_n(z_0) - p_n(z_0)q_k(z_0).
\end{aligned}$$

Hence,

$$\sum_{n=0}^{\infty} |\alpha_{n,k}(z_0)|^2 \leq 4 \sum_{k=0}^{\infty} |p_k(z_0)|^2 \sum_{k=0}^{\infty} |q_k(z_0)|^2 < \infty.$$

Invoking Lemma 2.4.7 shows that $(p_k(z))_{k\in\mathbb{N}_0} \in \ell^2(\mathbb{N}_0)$, which concludes the proof. ❑

2.4.9 Definition. We say that a moment sequence s corresponds to an indeterminate moment problem, if one (and hence all) of the properties of Theorem 2.4.8 hold. Otherwise, we call the moment problem determinate.

2.4.10 Proposition. *If s corresponds to an indeterminate moment problem, then there is only one measure μ, such that for every $n \in \mathbb{N}_0$*

$$s_n = \int x^n d\mu(x).$$

Proof. Assume that there are μ_1, μ_2, such that for every n, $s_n = s_n[\mu_1] = s_n[\mu_2]$. Fix $z \in \mathbb{C}_+$. Then Proposition 2.4.5 implies that $w_{\mu_1}(z)$ and $w_{\mu_2(z)}$ belong to $\mathcal{D}_n(z)$ for every n. Thus, they belong to $\mathcal{D}_\infty(z)$, which implies that $w_{\mu_1}(z) = w_{\mu_2(z)}$. Since this holds for every $z \in \mathbb{C}_+$, we conclude that $w_{\mu_1} \equiv w_{\mu_2}$. Uniqueness of the measure in the integral representation, cf. Theorem 1.3.5 shows that $\mu_1 = \mu_2$. ❑

We will now focus on the case of an indeterminate moment problem. In this case, there exists a whole family of solutions, which can be explicitly parametrized. We will end this section by studying the functions, which will ultimately lead to the parametrization of all solutions.
Recall the identity

$$\frac{T_n(w)^* J T_n(z) - J}{\overline{w} - z} = \sum_{k=0}^{n-1} \begin{pmatrix} p_k(z)\overline{p_k(w)} & q_k(z)\overline{p_k(w)} \\ p_k(z)\overline{q_k(w)} & q_k(z)\overline{q_k(w)}, \end{pmatrix}$$

which needs to be interpreted appropriately if $z = \overline{w}$. Define

$$\mathcal{K}_n(z, w) = \frac{T_n(w)^* J T_n(z) - z}{\overline{w} - z}.$$

Since $T_n(0) \in \mathrm{SL}(2,\mathbb{R})$, we have $T_n(0)^* J T_n(0) = J$ and hence

$$\mathcal{K}_n(z,0) = \frac{J - JT_n(0)^{-1}T_n(z)}{z}$$

and thus

$$T_n(0)^{-1}T_n(z) = I + zJ\mathcal{K}_n(z,0).$$

Note also, that $T_n(0)$ as a Möbius transform acts as a bijection from $\overline{\mathbb{C}}_+$ to $\overline{\mathbb{C}}_+$. We define polynomials A_n, B_n, C_n, D_n by

$$\begin{pmatrix} A_n(z) & B_n(z) \\ C_n(z) & D_n(z) \end{pmatrix} = T_n(z)^{-1}T_n(0).$$

Note that by (2.12) we have

$$\det T_n(z)^{-1}T_n(0) = A_n(z)D_n(z) - B_n(z)C_n(z) = 1.$$

Explicitly, we get

$$A_n(z) = 1 + z\sum_{k=0}^{n-1} q_k(z)p_k(0), \qquad B_n(z) = z\sum_{k=0}^{n-1} q_k(z)q_k(0),$$
$$C_n(z) = -z\sum_{k=0}^{n-1} p_k(z)p_k(0), \qquad D_n(z) = 1 - z\sum_{k=0}^{n-1} p_k(z)q_k(0).$$

Our goal is to show that, provided to s corresponds to an indeterminate moment problem, A_n, B_n, C_n, D_n converge to entire functions as $n \to \infty$.

2.4.11 Proposition. *Assume that s corresponds to an indeterminate moment problem. Then, for z in a compact subset of $\mathbb{C}$,*

$$\sum_{k=0}^{\infty} |p_k(z)|^2, \quad \textit{and} \quad \sum_{k=0}^{\infty} |q_k(z)|^2$$

are uniformly bounded.

Proof. We start with proving the claim for p_k. Fix $z_0 \in \mathbb{C}_+$. In Theorem 2.4.8 it is shown, that there exists a Hilbert-Schmidt operator $A = (a_{k,j})$ (depending on z_0) with $a_{k,j} = 0$ for $j \geq k$, so that

$$p_k(z_0) = p_k(z) - (z - z_0)\sum_{j=0}^{k-1} a_{k,j}p_j(z).$$

If $v(z) = (p_k(z))_{k=0}^{\infty}$, then we can write this as

$$v(z_0) = (I - (z - z_0)A)v(z).$$

That is,

$$v(z) = (I - (z - z_0)A)^{-1}v(z_0).$$

We claim that

$$z \mapsto (I - (z - z_0)A)^{-1} \tag{2.31}$$

is analytic and hence in particular continuous. To see this, fix $z_1 \in \mathbb{C}$ and write

$$(I-(z-z_0)A) = (I-(z-z_1+z_1-z_0)A) = (I-(z_1-z_0)A)(I-(z-z_1)(I-(z_1-z_0)A)^{-1}A).$$

Now if z is so that

$$|z-z_1|\|I-(z_1-z_0)A)^{-1}A\| < 1$$

we can form the Neumann series for $(I-(z-z_1)(I-(z_1-z_0)A)^{-1}A)^{-1}$ to prove analyticity of (2.31). Hence, for $K \subset \mathbb{C}$ there exists $C > 0$ so that

$$\|(I-(z-z_0)A)^{-1}\| < C.$$

In particular, this shows that

$$\|v(z)\| \leq C\|v(z_0)\|,$$

showing uniform boundedness of

$$\sum_{k=0}^{\infty} |p_k(z)|^2.$$

The same proof works for $\sum_{k=0}^{\infty} |q_k(z)|^2$, once we know that

$$q_n(z) = q_n(z_0) + (z-z_0)\sum_{k=0}^{n-1} \alpha_{n,k}(z_0) q_k(z). \tag{2.32}$$

Using (2.31) we find that

$$\begin{aligned} \frac{p_n(z)-p_n(t)}{z-t} &= \sum_{k=0}^{n-1} \alpha_{n,k}(z_0)\left(\frac{p_k(z)(z-z_0)-p_k(t)(t-z_0)}{z-t}\right), \\ \frac{p_n(z_0)-p_n(t)}{z_0-t} &= \sum_{k=0}^{n-1} \alpha_{n,k}(z_0) p_k(t). \end{aligned}$$

Subtracting these equations and applying Φ proves (2.32). ❑

2.4.12 Theorem. *The functions A_n, B_n, C_n, D_n converge uniformly on compact subsets of $\mathbb{C}$ and thus*

$$\begin{aligned} A(z) &= 1 + z\sum_{k=0}^{\infty} q_k(z)p_k(0), & B(z) &= z\sum_{k=0}^{\infty} q_k(z)q_k(0), \\ C(z) &= -z\sum_{k=0}^{\infty} p_k(z)p_k(0), & D(z) &= 1 - z\sum_{k=0}^{\infty} p_k(z)q_k(0). \end{aligned}$$

define entire functions. Moreover, we have

$$A(z)D(z) - B(z)C(z) = 1. \tag{2.33}$$

Define

$$W(z) := \begin{pmatrix} A(z) & B(z) \\ C(z) & D(z) \end{pmatrix}$$

Then, W is J-expanding on $\mathbb{C}_+$ and

$$\mathcal{D}_\infty(z) = \left\{ W(z) \star \tau \mid \tau \in \overline{\mathbb{C}_+} \right\}.$$

Proof. We show the claim for A, A_n. All other cases follow analogously. Fix $K \subset \mathbb{C}$ compact and $\epsilon > 0$. Let $C = \sup_{z\in K} \sum_{k=0}^{\infty} |q_k(z)|^2$. Let n_0, so that for $n, m \geq n_0$

$$\sum_{k=m+1}^{n} |p_k(0)|^2 < \frac{\epsilon}{C}.$$

Then, we get

$$|A_n(z) - A_m(z)|^2 \leq \left(\sum_{k=m+1}^{n} |q_k(z) p_k(0)| \right)^2 \leq \sum_{k=m+1}^{n} |q_k(z)|^2 \sum_{k=m+1}^{n} |p_k(0)|^2 < \epsilon.$$

Recall, that by definition of A_n, B_n, C_n, D_n, we have

$$A_n(z) D_n(z) - B_n(z) C_n(z).$$

Thus, sending $n \to \infty$ proves (2.33). To show that $W(z)$ is J-expansive is equivalent to showing that $W^{-1}(z)$ is J-contractive. Define $W_n(z) = T_n(z)^{-1} T_n(0)$. Then $W_n(z)^{-1} = T_n(0)^{-1} T_n(z)$. Using that $(T_n(0)^{-1})^* J T_n(0)^{-1} = J$, we get

$$\frac{(W_n(z)^{-1})^* J W_n(z)^{-1} - J}{\overline{z} - z} = \frac{T_n(z)^* (T_n(0)^{-1})^* J T_n(0)^{-1} T_n(z) - J}{\overline{z} - z} = \frac{T_n(z)^* J T_n(z) - J}{\overline{z} - z} \geq 0.$$

Sending $n \to \infty$ preserved the inequality showing that W is J-expanding in $\mathbb{C}_+$. For the remaining claim note that $T_n(0)$ maps $\mathbb{C}_+$ onto itself and thus that $W_n(z)(\overline{\mathbb{C}_+}) = \mathcal{D}_n(z)$. Using that $\mathcal{D}_n(z) \searrow \mathcal{D}_\infty(z)$ and $W_n \to W_\infty$ the last claim follows. ❑

2.5 Function theoretic approach to the moment problem

In 1922 Nevanlinna proposed to not work with the moments directly, but instead consider asymptotic expansions of w_μ at ∞. We start with a definition:

2.5.1 Definition. Let $\Omega \subset \mathbb{C}$ be an undbounded set and $0 \notin \Omega$. A function $f : \Omega \to \mathbb{C}$ has an asymptotic expansion in Ω at ∞, if there exists $a_k \in \mathbb{C}$, $k \in \mathbb{N}_0$, so that for all $n \in \mathbb{N}_0$,

$$\lim_{\substack{z\to\infty \\ z\in\Omega}} z^n \left(f(z) - \sum_{k=0}^{n-1} \frac{a_k}{z^k} \right) = a_n.$$

In this case we write

$$f(z) \sim \sum_{k=0}^{\infty} \frac{a_k}{z^k}.$$

We will be mainly concerned with Ω of the form

$$\Omega_\delta = \{z \in \mathbb{C} \setminus \{0\} \mid \delta < \arg z < \pi - \delta\}, \quad 0 < \delta < \frac{\pi}{2}.$$

Induction shows that the a_ns are uniquely determined by f, if they exist. However, a_n do not determine f uniquely. E.g. $f(x) = e^{-x}$ and $g(x) = 0$ have the same asymptotic expansion in $\Omega = (0, \infty)$. We will if s corresponds to an indeterminate moment problem, then every representing measure will have the same asymptotic expansion. Note also that the series $\sum_{k=0}^{\infty} \frac{a_k}{z^k}$ in an asymptotic expansion can be divergent. It merely says that the partial sums are good approximations of f in the sense that

$$f(z) - \sum_{k=0}^{n-1} \frac{a_k}{z^k} = O\left(\frac{1}{z^n}\right), \quad z \to \infty, z \in \Omega.$$

The following argument will be used later. Assume that for some n and $a_n \in \mathbb{C}$.

$$\lim_{z\to\infty} z^n \left(f(z) - \sum_{k=0}^{n-1} \frac{a_k}{z^k} \right) = -a_n$$

This implies that

$$0 = \lim_{z\to\infty} z^{n-1} \left(f(z) - \sum_{k=0}^{n-1} \frac{a_k}{z^k} \right) = \lim_{z\to\infty} z^{n-1} \left(f(z) - \sum_{k=0}^{n-2} \frac{a_k}{z^k} \right) - a_{n-1},$$

showing that

$$\lim_{z\to\infty} z^{n-1} \left(f(z) - \sum_{k=0}^{n-2} \frac{a_k}{z^k} \right) = a_{n-1}.$$

The following theorem is in this spirit and shows that the moments of a measure can be seen from the asymptotic expansion of the corresponding Herglotz function. Recall that

$$w_\mu(z) = \int \frac{1}{x-z} d\mu(x).$$

2.5.2 Proposition. *Assume that μ has $n+1$ finite moments,*

$$s_k = s_k[\mu] = \int_{\mathbb{R}} x^k d\mu(x), \quad 0 \le k \le n.$$

Then for any $0 < \delta < \frac{\pi}{2}$, it holds that

$$\lim_{\substack{z\to\infty \\ z\in\Omega_\delta}} z^{n+1} \Big(w_\mu(z) + \frac{s_0}{z} + \frac{s_1}{z^2} + \ldots \frac{s_{n-1}}{z^n} \Big) = -s_n. \tag{2.34}$$

If μ has $n+2$ finite moments and n is odd, then this limit is uniform among all measures with the same $n+2$ moments.

Proof. Assume that μ has $n+1$ finite moments. It can be directly verified that

$$\frac{1}{x-z} + \frac{1}{z} + \ldots \frac{x^{n-1}}{z^n} = \frac{x^n}{z^n} \frac{1}{x-z}. \tag{2.35}$$

Integrating this with respect to μ yields

$$z^{n+1} \Big(f(z) + \frac{s_0}{z} + \ldots \frac{s_{n-1}}{z^n} \Big) = \int \frac{x^n z}{x-z} d\mu(x) = -s_n + \int \frac{x^{n+1}}{x-z} d\mu(x).$$

Thus, it is required to estimate the last integral. Note that for $\delta \le \arg z \le \pi - \delta$ and $x \in \mathbb{R}$ it holds that

$$|x-z| \ge |z| \sin\delta, \quad |x-z| \ge |x| \sin\delta.$$

In the first case, this can be seen by considering the ray, $\arg z = \delta$ and realizing that for fixed z the extremal configuration corresponds to $\operatorname{Re} z = x$, i.e. $|\operatorname{Re} z - z| = \operatorname{dist}(\mathbb{R}, z)$, where one has equality. Any other x increases $|x - z|$. The second inequaliy can be obtained in the same way by fixing x and varying z.
Assume first that also the s_{n+1} is finite and $n+1$ is even. Then

$$\int \frac{|x|^{n+1}}{|x-z|} d\mu(x) \leq \frac{1}{|z| \sin \delta} \int x^{n+1} d\mu(x) = \frac{s_{n+1}}{|z| \sin \delta}. \tag{2.36}$$

Thus, we proved the uniformity statement. Without this extra assumption, we have for arbitrary $A > 0$,

$$\int \frac{|x|^{n+1}}{|x-z|} d\mu(x) \leq \frac{1}{|z| \sin \delta} \int_{(-A,A)} |x|^{n+1} d\mu(x) + \frac{1}{\sin \delta} \int_{|x| \geq A} |x|^{n} d\mu(x).$$

Thus, for given $\epsilon > 0$, we can first choose A big enough to make the second integral smaller than $\epsilon/2$ and then for fixed A choose $|z|$ big enough. ❑

Note that (2.34) is equivalent to

$$w_\mu(z) + \frac{s_0}{z} + \frac{s_1}{z} + \cdots + \frac{s_n}{z^{n+1}} = o\left(\frac{1}{z^{n+1}}\right) \quad z \to \infty, z \in \Omega.$$

The following proposition is a converse to this statement.

2.5.3 Proposition. *Let $f \in \mathcal{N}_0$, $n \in \mathbb{N}$ and $s_k \in \mathbb{R}$, $0 \leq k \leq 2n$ so that*

$$\lim_{y \to \infty} (iy)^{2n+1} \left(f(iy) + \frac{s_0}{iy} + \frac{s_1}{(iy)^2} + \ldots \frac{s_{2n-1}}{(iy)^{2n}} \right) = -s_{2n}. \tag{2.37}$$

Then $f = w_\mu$ for some μ with

$$s_k = \int_{\mathbb{R}} x^k d\mu(x), \quad 0 \leq k \leq 2n.$$

Proof. From (2.37) it follows that

$$\lim_{y \to \infty} iy f(iy) = -s_0$$

and hence by Proposition 1.3.10 there exists a finite measure μ such that

$$f(z) = \int \frac{d\mu(x)}{x - z} = w_\mu(z).$$

Since,

$$\operatorname{Re} iy f(iy) = -y \operatorname{Im} f(iy),$$

we conclude from the proof of Proposition 1.3.10 that $\lim_{y \to \infty} iy f(iy) = -\mu(\mathbb{R})$ and hence $s_0 = \mu(\mathbb{R})$. From (2.37) it follows that for all $m \leq n$

$$\lim_{y \to \infty} (iy)^{2m+1} \left(f(iy) + \frac{s_0}{iy} + \frac{s_1}{(iy)^2} + \cdots + \frac{s_{2m-1}}{(iy)^{2m}} \right) = -s_{2m}. \tag{2.38}$$

We proceed by induction over m. Assume that for $m \leq n$ it holds that

$$\int x^k d\mu(x) = s_k, \quad 0 \leq k \leq 2m - 2.$$

Inserting this into (2.38) and using (2.35) yields

$$\lim_{y\to\infty}\left(\int \frac{(iy)^2 x^{2m-1}}{x-iy} + iy s_{2m-1}\right) = -s_{2m}. \tag{2.39}$$

In particular,

$$\lim_{y\to\infty}\int \frac{iy x^{2m-1}}{x-iy} = -s_{2m-1}. \tag{2.40}$$

Splitting off the real part in (2.39) and (2.40) we get

$$\lim_{y\to\infty}\int \frac{y^2 x^{2m}}{x^2+y^2} d\mu(x) = s_{2m},$$
$$\lim_{y\to\infty}\int \frac{y^2 x^{2m-1}}{x^2+y^2} d\mu(x) = s_{2m-1}.$$

By monotone convergence, we conclude from the first equation that

$$\int x^{2m} d\mu(x) = s_{2m}.$$

In particular, $\int |x|^{2m-1} d\mu(x) < \infty$. And hence, by dominated convergence, we get from the second equation that

$$\int x^{2m-1} d\mu(x) = s_{2m-1}.$$

This finishes the proof. ❑

We get an alternative proof of Lemma 2.3.3.

2.5.4 Corollary. *Let $(s_k)_{k=0}^{2n}$ be given and assume that $(\mu_\ell)_{\ell\in\mathbb{N}_0}$ are measures such*

$$\int x^k d\mu_n(x) = s_k \quad 0 \le k \le 2n.$$

Then, there exists a convergent subsequence $(\mu_{\ell_j})_{j\in\mathbb{N}}$ (in $C(\overline{\mathbb{R}})'$). Moreover, for any convergent subsequence and limit $\mu = \lim \mu_{\ell_j}$ we have

$$\int x^k d\mu_n(x) = s_k \quad 0 \le k \le 2n-1.$$

Proof. That there exists a convergent subsequence follows again by Banach-Alaoglu. Now take a convergent subsequence (μ_{n_j}) with limit μ and define

$$w_{\mu_{\ell_j}}(z) = \int \frac{1}{x-z} d\mu_{\ell_j}(x), \quad w_\mu(z) = \int \frac{1}{x-z} d\mu(x).$$

Then, by (1.3.8) we conclude that

$$\lim_j w_{\mu_{\ell_j}} = w_\mu$$

uniformly on compact subsets of $\mathbb{C}_+$. In the proof of Theorem 2.5.2, specifically (2.36) we have shown that

$$\left|(iy)^{2n}\left(w_{\mu_{\ell_j}}(iy) + \frac{s_0}{iy} + \cdots + \frac{s_{2n-2}}{(iy)^{2n-1}} + \frac{s_{2n-1}}{(iy)^{2n}}\right)\right| \le \frac{s_{2n}}{y},$$

which holds pointwise for all y. Sending $j \to \infty$ shows that

$$\left|(iy)^{2n}\left(w_\mu(iy) + \frac{s_0}{iy} + \cdots + \frac{s_{2n-2}}{(iy)^{2n-1}} + \frac{s_{2n-1}}{(iy)^{2n}}\right)\right| \le \frac{s_{2n}}{y},$$

which implies by Theorem 2.5.2 that

$$\int x^k \mu(x) = s_k, \quad 0 \le k \le 2n-1.$$

❑

We are now ready to prove the main theorem of this section. Recall that

$$W(z) = \begin{pmatrix} A(z) & B(z) \\ C(z) & D(z), \end{pmatrix}$$

as given in Theorem 2.4.12.

2.5.5 Theorem. *Assume that s corresponds an indeterminate moment problem. Define the map*

$$\Xi[s] := \begin{cases} \overline{\mathcal{N}_0} & \to & \overline{\mathcal{N}_0} \\ \phi & \mapsto & (z \mapsto W(z) \star \phi(z)) \end{cases}$$

Then Ξ is injective and $\mu \in \Xi[s](\overline{\mathcal{N}_0})$ if and only if

$$s_k[\mu] = s_k, \quad k \in \mathbb{N}_0. \tag{2.41}$$

Proof. That Ξ maps into $\overline{\mathcal{N}_0}$ follows from the fact that W is J-expanding. Injectivity follows from the fact that W is invertivible and the uniqueness claim in Theorem 1.3.5. Thus, it remains to determine the range of $\Xi[s]$. Assume that μ is so that w_μ satisfies (2.41). Then, for fixed $z \in \mathbb{C}_+$, $w_\mu(z)$ belongs to $\mathcal{D}_n(z)$ for all $n \in \mathcal{N}_0$ and thus to $\mathcal{D}_\infty(z)$. Hence, Theorem 2.4.12 implies that

$$\phi(z) := W(z)^{-1} \star w_\mu(z) \in \overline{\mathbb{C}_+}.$$

We conclude that $\phi \in \overline{\mathcal{N}_0}$.
It remains to show that for any $\phi \in \overline{\mathcal{N}_0}$, $\Xi[s](\phi)$ is of the form

$$\int \frac{d\mu(x)}{x-z},$$

for some measure μ satisfying (2.41).
Recall that

$$W_n(z) := \begin{pmatrix} A_n(z) & B_n(z) \\ C_n(z) & D_n(z) \end{pmatrix} = T_n(z)^{-1} T_n(0).$$

$J \star \phi = -\frac{1}{\phi}$, which maps $\overline{\mathcal{N}_0}$ onto itself, we can also consider

$$W_n(z)J = \begin{pmatrix} B_n(z) & -A_n(z) \\ D_n(z) & -C_n(z) \end{pmatrix}.$$

Let $\phi \in \mathcal{N}_0$ and assume that $\lim \frac{\operatorname{Im}\phi(iy)}{y} > 0$. Define

$$w_n(z) = W_n(z)J \star \phi = \frac{B_n(z)\phi(z) - A_n(z)}{D_n(z)\phi - C_n(z)}.$$

Using that $A_n(z)D_n(z) - B_n(z)C_n(z) = 1$ we get

$$w_n(z) = \frac{B_n(z)}{D_n(z)} - \frac{1}{D_n(z)(D_n(z)\phi(z) - C_n(z))}.$$

We have

$$C_n(z) = -z\sum_{k=0}^{n-1} p_k(z)p_k(0), \qquad D_n(z) = 1 - z\sum_{k=0}^{n-1} p_k(z)q_k(0).$$

Assume that $q_{n-1}(0) \neq 0$, then using $\lim \frac{\operatorname{Im}\phi(iy)}{y} > 0$, we have

$$\frac{1}{D_n(iy)(D_n(iy)\phi(iy) - C_n(iy))} = o\left(\frac{1}{z^{2n}}\right),$$

Since

$$\frac{B_n(iy)}{D_n(iy)} + \frac{s_0}{iy} + \cdots + \frac{s_{2n-2}}{(iy)^{2n-1}} = o\left(\frac{1}{(iy)^{2n-1}}\right),$$

we have

$$w_n(z) + \frac{s_0}{iy} + \cdots + \frac{s_{2n-2}}{(iy)^{2n-1}} = o\left(\frac{1}{(iy)^{2n-1}}\right). \tag{2.42}$$

Let μ_n be the measure in the integral representation of w_n. Then it follows from Propostion 2.5.3 that

$$s_k[\mu_n] = s_k, \quad 0 \leq k \leq 2n-2.$$

If $q_{n-1}(0) = 0$, then $q_n(0) \neq 0$, since $-\frac{q_{n-1}}{q_n}$ is a Herglotz function and thus has interlacing zeros. In any case, we find a subsequence such that (2.42) holds. Sending $n \to \infty$ and appealing to Corollary 2.5.4 we conclude that

$$\lim_{n\to\infty} w_n(z) = \frac{B(z)\phi(z) - A(z)}{D(z)\phi - C(z)},$$

is a Herglotz function whose measure in the integral representation is a solution of the moment problem.

It remains to discuss the assumption $\lim \frac{\operatorname{Im}\phi(iy)}{y} > 0$, if this limit is zero consider $\phi_n(z) = \frac{1}{n}z + \phi(z)$. Then by the above, the statement holds for

$$w_{\phi_n}(z) = \frac{B(z)\phi_n(z) - A(z)}{D(z)\phi_n(z) - C(z)}.$$

Since $w_{\phi_n} \to w_\phi$ the claim follows again by Corllary 2.5.4.

❑

2.6 Are polynomial dense?

Recall that

$$\mathcal{D}_n(z) = \left\{ w \mid \frac{\operatorname{Im} w}{\operatorname{Im} z} \geq \sum_{k=0}^{n-1} |w p_k(z) + q_k(z)|^2 \right\}.$$

and

$$\mathcal{D}_\infty(z) = \bigcap_n \mathcal{D}_n(z).$$

Sending $n \to \infty$ shows that

$$\mathcal{D}_\infty(z) = \left\{ w \mid \frac{\operatorname{Im} w}{\operatorname{Im} z} \geq \sum_{k=0}^{\infty} |w p_k(z) + q_k(z)|^2 \right\}.$$

If we are in the indeterminate case, this shows that for the unique solution of the moment probplem μ, it holds that

$$\frac{\operatorname{Im} w_\mu(z)}{\operatorname{Im} z} \geq \sum_{k=0}^{\infty} |w_\mu(z) p_k(z) + q_k(z)|^2$$

Let us briefly argue that in the indeterminate case we have

$$\Gamma_\infty(z) = \partial \mathcal{D}_\infty(z) = \left\{ w \mid \frac{\operatorname{Im} w}{\operatorname{Im} z} = \sum_{k=0}^{\infty} |w p_k(z) + q_k(z)|^2 \right\} \tag{2.43}$$

In this case $(q_k), (p_k) \in \ell^2$ and we can rewrite

$$\frac{\operatorname{Im} w}{\operatorname{Im} z} = \sum_{k=0}^{\infty} |w p_k(z) + q_k(z)|^2$$

as

$$0 = f(w, \overline{w})$$

where

$$f(w, \overline{w}) = w\overline{w} \sum_{k=0}^{\infty} |p_k(z)|^2 (z - \overline{z})^2 + w \left(\sum_{k=0}^{\infty} p_k(z) \overline{q_k(z)} (z - \overline{z}) - 1 \right) + \overline{w} \left(\sum_{k=0}^{\infty} q_k(z) \overline{p_k(z)} (z - \overline{z}) + 1 \right) + (z - \overline{z}) \sum_{k=0}^{\infty} |q_k(z)|^2$$

By continuity of f we get that $w \in \Gamma_\infty(z)$ implies $f(w, \overline{w}) = 0$. Moreover, we see that $\{w \in \mathbb{C} \mid f(w, \overline{w}) = 0\}$ is a circle, since it is exactly of the form (1.2). Hence we have

$$\Gamma_\infty(z) \subset \{w \in \mathbb{C} \mid f(w, \overline{w}) = 0\}$$

and both are circles, which implies equality. In the determinate case we have $\mathcal{D}_\infty = \{w_\mu(z)\} = \Gamma_\infty(z)$, where μ is the unique solution of the moment problem.
Let s be a moments sequence and μ be a solution of the associated moment problem. We will investigate, when

$$\mathcal{P} = \operatorname{span}\{z^n \mid n \in \mathbb{N}_0\}$$

is dense in $L^2(\mu)$. Let (p_n) denote the orthonormal polynomials associated to s. Note that they are determined solely by s and that (p_n) form an orthonormal set in $L^2(\mu)$. For $f \in L^2(\mu)$, let c_k denote its Fourier coefficients,

$$c_k = \int f(x)p_k(x)d\mu(x), \quad k \in \mathbb{N}_0.$$

Moreover, let $S_n(f)$ denote the partial sum

$$S_n(f)(x) = \sum_{k=0}^{n} c_k p_k(x),$$

which is the orthogonal projection onto $\mathcal{P}_n$ in $L^2(\mu)$.
For a finite measure μ (not necessarily positive), define the Stieltjes transform by

$$s_\mu(z) = \int \frac{1}{x-z} d\mu(x)$$

For positive measures, this is a Herglotz function and we have seen that in this case the measure is uniquely determined by s_μ. The uniqueness proof in Theorem 1.3.4, however also worksfor complex finite measures. In fact, there is an explicit formula for reconstructing the measure, which we provide without proof. It is called Stieltjes inversion formula:

$$\lim_{\epsilon \searrow 0} \int_a^b s_\mu(x+i\epsilon)dx = \frac{1}{2}\mu(\{a\}) + \mu((a+b)) + \frac{1}{2}\mu(\{b\}).$$

2.6.1 Theorem. *Let s be a moment sequence and μ be a solution of the moment problem. Then the following are equivalent:*

(i) There exists $z_0 \in \mathbb{C}_+$ so that $w_\mu(z_0) \in \Gamma_\infty(z_0)$;

(ii) For all $z_0 \in \mathbb{C}_+$ so that $w_\mu(z_0) \in \Gamma_\infty(z_0)$;

(iii) $\mathcal{P}$ is dense in $L^2(\mu)$;

(iv) $(p_n)_{n\in\mathbb{N}_0}$ form an orthonormal basis of $L^2(\mu)$;

Proof. Clearly $(ii) \implies (i)$ and $(iii) \iff (iv)$.
We show $(iv) \implies (ii)$. Fix $z_0 \in \mathbb{C}_+$. Then $f_{z_0}(x) = \frac{1}{x-z_0} \in L^2(\mu)$. As in the proof of Proposition 2.4.5 we see that

$$c_k = \int f_{z_0}(x)p_k(x)d\mu(x) = w_\mu(z_0)p_k(z_0) + q_k(z_0)$$

and

$$\|f_{z_0}\|^2_{L^2(\mu)} = \frac{\operatorname{Im} w_\mu(z_0)}{\operatorname{Im} z_0}.$$

Since the (p_k) for an ONB, we get

$$\sum_{k=0}^{\infty} |w_\mu(z_0)p_k(z_0) + q_k(z_0)|^2 = \sum_{k=0}^{\infty} |c_k|^2 = \|f_{z_0}\|^2_{L^2(\mu)} = \frac{\operatorname{Im} w_\mu(z_0)}{\operatorname{Im} z_0},$$

and hence by (2.43), $w_\mu(z_0) \in \Gamma_\infty(z_0)$.

It remains to show $(i) \implies (iii)$: Let $H = \operatorname{clos}\mathcal{P}$, where the closure is taken in $L^2(\mu)$. By the above computation, the assumption implies that $f_{z_0} \in H$. We want to show that $f_{z_0}^n \in H$, for $n \geq 0$. Assume that it holds for n. Then we find $P \in \mathcal{P}$ so that $\|f_{z_0}^n - P\|_{L^2(\mu)} < \epsilon \operatorname{Im}(z_0)$. Writing $P(z) = (z - z_0)Q(z) + a$, where $a = P(z_0)$, we get

$$\begin{aligned}\|f_{z_0}^{n+1} - af_{z_0} - Q\|_{L^2(\mu)}^2 &= \int \frac{1}{|x-z_0|^2}\left|f_{z_0}^n(x) - a - (x-z_0)Q(x)\right|^2 d\mu(x)\\ &\leq \frac{1}{\operatorname{Im} z_0}\|f_{z_0} - P\|_{L^2(\mu)}^2 < \epsilon^2.\end{aligned}$$

since $af_{z_0} + Q \in H$, we conclude that $f_{z_0}^{n+1} \in H$. Suppose now that $g \in L^2(\mu)$ is orthogonal to H. Then consider

$$s(z) = \int \frac{g(x)}{x-z} d\mu(x).$$

It follows that $s^{(n)}(z_0) = 0$ for all $n \in \mathbb{N}_0$ and hence being analytic in $\overline{\mathbb{C}_+}$, we conclude that $s \equiv 0$. That is $g(x)d\mu(x) = 0$ and thus $g = 0$ μ a.e. Hence $g \equiv 0$ in $L^2(\mu)$ and thus $H = L^2(\mu)$. ❑

Let us end this section with an easy to check criteria for determinacy of the measure.

2.7 Two criteria for determinacy

First we show that if μ does not have a heavy tail, then μ corresponds to an determinate moment problem.
If μ is a finite measure on $\mathbb{R}$, we introduce its Fourier transform by

$$\hat{\mu}(\xi) = \int e^{-ix\xi} d\mu(x), \quad \xi \in \mathbb{R}.$$

Since $|e^{-ix\xi}| = 1$, it is clear that

$$|\hat{\mu}(\xi)| \leq \mu(\mathbb{R})$$

and $\hat{\mu}$ is continuous. Moreover, since

$$\partial_\xi^k e^{-ix\xi} = (-i)^k x^k$$

if μ has k finite moments then $\hat{\mu}$ is k-times differentiable and

$$\partial_\xi^k \hat{\mu}(\xi) = (-i)^k \int e^{-ix\xi} x^k d\mu(x).$$

In particular note that

$$i^k \partial_\xi^k \hat{\mu}(0) = s_k[\mu]. \tag{2.44}$$

2.7.1 Lemma. *Let μ, ν be finite measures on $\mathbb{R}$. If $\hat{\mu} = \hat{\nu}$, then $\mu = \nu$.*

Proof. Let f be a Schwartz function. Then, by the inversion formula for the classical Fourier transform

$$\int f(x)d\mu(x) = \int f^\vee(\xi)e^{-i\xi x} d\xi d\mu(x) = 2\pi \int f^\wedge(\xi)\hat{\mu}(\xi)d\xi.$$

Thus,

$$\int f(x)d\mu(x) = \int f(x)d\nu(x)$$

By density of the set of Schwartz function this holds for any $f \in C_0(\mathbb{R})$ and thus $\nu = \mu$. ❑

Let us introduce

$$|s_k|\,[\mu] = \int |x|^k d\mu(x).$$

2.7.2 Lemma. *It holds that*

$$\exists \epsilon > 0 : \int e^{\epsilon|x|} d\mu(x) < \infty \iff \exists C > 0 : \; |s_k|\,[\mu] \le C^{k+1} k!\,.$$

Proof. By monotone convergence,

$$\int e^{\epsilon|x|} d\mu(x) = \lim_{n\to\infty} \sum_{k=0}^{n} \frac{\epsilon^k |s_k|\,[\mu]}{k!}.$$

Now if the limit is finite, then eventually

$$\frac{\epsilon^k |s_k|\,[\mu]}{k!} < \frac{1}{2}$$

and thus, with $C = \max\{1/\epsilon, 1/2\}$ we have $|s_k|\,[\mu] \le C^{k+1} k!$. Likewise, if $|s_k|\,[\mu] \le C^{k+1} k!$ then

$$\frac{\epsilon^k |s_k|\,[\mu]}{k!} \le C(\epsilon C)^k.$$

Thus, the series converges for $\epsilon < 1/C$. ❑

2.7.3 Proposition. *If there exists* $\epsilon > 0$ *such that*

$$\int e^{\epsilon|x|} d\mu(x) < \infty,$$

then μ *corresponds to an determinate moment problem. In particular, this holds for all compactly supported measures.*

Proof. Since for $\xi \in \mathbb{C}$, $|e^{-i\xi x}| \le e^{|x|\,\mathrm{Im}\,\xi}$,

$$\hat{\mu}(\xi) = \int e^{-i\xi x} d\mu(x)$$

is analytic in a strip $I_\epsilon = \{\xi \in \mathbb{C} \mid |\mathrm{Im}\,\xi| < \epsilon\}$. If ν is a another measure with the same moments, then by Lemma 2.7.2 $\hat{\nu}$ is also analytic in a strip $I_{\epsilon'}$. By (2.44) we conclude that

$$\hat{\mu}^{(k)}(0) = \hat{\mu}^{(k)}(0), \quad \forall k \in \mathbb{N}_0.$$

By the identity principle, we conclude that $\hat{\mu} \equiv \hat{\nu}$ and hence by Lemma 2.7.1, $\nu = \mu$. This finishes the proof. ❑

The second criterion will be in terms of summability of the moments.

2.7.4 Lemma. *Let s be a moment sequence and a_n the associated Jacobi parameters by Proposition 2.1.12. If*

$$\sum_{n=1}^{\infty} \frac{1}{a_n} = \infty,$$

then s is determinate. This holds in particular if $\sup a_n < \infty$.

Proof. We show that s being indeterminate implies that $\frac{1}{a_n} \in \ell^1$. Fix $z_0 \in \mathbb{C}_+$ and assume that s is indeterminate. By the Wronski identity (2.12)

$$\frac{1}{a_n} = p_{n-1}(z_0)q_n(z_0) - q_{n-1}(z_0)p_n(z_0)$$

Theorem 2.4.8 implies that $(p_n(z_0))_n, (q_n(z_0))_n \in \ell^2$ and thus $\frac{1}{a_n} \in \ell^1$. ❑

We want to translate this into a condition on the moments s_k.

2.7.5 Lemma. *Let $(a_j)_{j=1}^n \in \mathbb{R}^n$. Then*

$$\sum_{j=1}^{n} \frac{1}{(a_1 \dots a_j)^{1/j}} \leq 2e \sum_{j=1}^{n} \frac{1}{a_j}.$$

Proof. We have $1 + x \leq e^x$ so $(1 + \frac{1}{n})^n \leq e$ and thus, inductively,

$$n^n \leq e^n n!.$$

Indeed,

$$(n+1)^{n+1} = (n+1)n^n\Big(1 + \frac{1}{n}\Big)^n \leq e^{n+1}(n+1)!.$$

Thus,

$$\frac{1}{(a_1 \dots a_j)^{1/j}} = \frac{1}{(j!)^{1/j}} \left(\prod_{k=1}^{j} \frac{k}{a_k}\right)^{1/j} \leq \frac{e}{j^2} \sum_{k=1}^{j} \frac{k}{a_k},$$

by the arithmetic-geometric mean inequality. Thus,

$$\sum_{j=1}^{n} \frac{1}{(a_1 \dots a_j)^{1/j}} \leq e \sum_{j=1}^{n} \sum_{k=1}^{j} \frac{1}{j^2} \frac{k}{a_k} = e \sum_{k=1}^{n} \frac{1}{a_k} \sum_{j=k}^{n} \frac{k}{j^2} \leq 2e \sum_{k=1}^{n} \frac{1}{a_k},$$

since

$$\sum_{j=k}^{n} \frac{k}{j^2} \leq 2k \sum_{j=k}^{\infty} \frac{1}{j(j+1)} = 2k \sum_{j=k}^{\infty} \Big(\frac{1}{j} - \frac{1}{j+1}\Big) = 2.$$

❑

2.7.6 Corollary (Carleman's condition)**.** *If*

$$\sum_{k=1}^{\infty} \frac{1}{s_{2k}^{1/2k}} = \infty, \tag{2.45}$$

then the moments problem is determinate.

Proof. By Proposition 2.1.12, $p_n(x) = \frac{x^n}{a_1 \dots a_n} + q(x)$, where $q \in \mathcal{P}_{n-1}$. Thus,

$$\left\langle \frac{x^n}{a_1 \dots a_n}, p_n(x) \right\rangle = 1.$$

Thus, by Cauchy-Schwarz

$$\frac{1}{s_{2n}^{1/2n}} \le \frac{1}{(a_1 \dots a_n)^{1/n}}.$$

By Lemma 2.7.5, (2.45) implies that $(\frac{1}{a_n}) \notin \ell^1$ and hence Lemma 2.7.4 shows that the moment problem is determinate. ❑

2.8 Krein's density theorem

In this section we prove a criterion of indeterminacy. Let μ be a probability measure on $\mathbb{R}$ and write $d\mu(x) = w(x)dx + d\mu_s$ its Lebesgue decomposition. Since $\log^+ t \le t$, for $t \ge 0$, we have

$$0 \le \int \log^+ w(x) \frac{dx}{1+x^2} \le \int w(x) \frac{dx}{1+x^2} \le 1.$$

Hence, $\frac{\log w(x)}{1+x^2}$ is integrable if and only if

$$\int \log^- w(t) \frac{dx}{1+x^2} < \infty$$

or equivalently, if

$$\frac{1}{\pi} \int \log w(x) \frac{dx}{1+x^2} > -\infty.$$

The integral

$$\frac{1}{\pi} \int \log w(x) \frac{dx}{1+x^2}$$

is often called the *entropy integral*. We will use the following Lemma from complex analysis, which can be concluded from residue's theorem.

2.8.1 Lemma. *Let P be a polynomials so that $P(z) \neq 0$ for $\operatorname{Im} z \ge 0$. Then*

$$\log|P(i)| = \frac{1}{\pi} \int \frac{\log|P(x)|}{1+x^2} dx.$$

Recall that

$$K_n(z,w) = \sum_{j=0}^{n-1} p_j(z)\overline{p_j(w)} = a_n \frac{p_n(z)\overline{p_{n-1}(w)} - p_{n-1}(z)\overline{p_n(w)}}{z - \overline{w}}.$$

We require one more lemma

2.8.2 Lemma. *All zeros of $z \mapsto K_n(z,i)$ belong to $\mathbb{C}_- = \{z \mid \operatorname{Im} z < 0\}$.*

Proof. Let $z \in \mathbb{C}_+ \cup \mathbb{R}$ and assume that $K_n(z,i) = 0$. This implies that

$$-\frac{p_n(z)}{p_{n+1}(z)} = -\frac{\overline{p_n(i)}}{\overline{p_{n+1}(i)}}$$

Since by Corollary 2.1.27 $\operatorname{Im} -\frac{p_n(z)}{p_{n+1}(z)} > 0$, for every $z \in \mathbb{C}_+$, this gives a contradiction. ❑

2.8.3 Theorem. *Let μ be a probability measure with density w such that*

$$\frac{1}{\pi}\int \log w(x)\frac{dx}{1+x^2} > -\infty.$$

If all moments of μ are finite, then the corresponding moment problem is indeterminate.

Proof. We have

$$\frac{1}{\pi}\int |K_n(x,i)|^2 w(x)\frac{dx}{1+x^2} \le \frac{1}{\pi}\int |K_n(x,i)|^2 w(x)dx \le \frac{1}{\pi}\int |K_n(x,i)|^2 d\mu(x) = \frac{1}{\pi}K_n(i,i).$$

On the other hand, by Jensen's inequality applied to the probability measure $\frac{1}{\pi}\frac{dx}{1+x^2}$,

$$\frac{1}{\pi}\int \log(|K_n(x,i)|^2 w(x))\frac{dx}{1+x^2} \le \log\left(\frac{1}{\pi}\int |K_n(x,i)|^2 w(x)\frac{dx}{1+x^2}\right).$$

Combining this we find

$$\frac{2}{\pi}\int \log(|K_n(x,i)|)\frac{dx}{1+x^2} + \frac{1}{\pi}\int \log w(x)\frac{dx}{1+x^2} \le \log\left(\frac{1}{\pi}K_n(i,i)\right).$$

Since $x \mapsto K_n(x,i)$ has all zeros in $\mathbb{C}_-$, we conclude from Lemma 2.8.2 that

$$\frac{1}{\pi}\int \log(|K_n(x,i)|)\frac{dx}{1+x^2} = \log|K_n(i,i)| = \log K_n(i,i).$$

Therefore,

$$\log K_n(i,i) \le -\log\pi + \frac{1}{\pi}\int \log w(x)\frac{dx}{1+x^2}.$$

Recalling that

$$K_n(i,i) = \sum_{j=0}^{n-1}|p_j(i)|^2,$$

Theorem 2.4.8 proves the assertion. ❑

2.8.4 Example. For $\alpha > 0$, consider the family of measures

$$d\mu_\alpha(x) = c_\alpha e^{-|x|^\alpha}dx,$$

where c_α is a normalizing constant. Then, by Theorem 2.8.3, the moment problem for μ_α is intederminate, if $\alpha < 1$ and by Proposition 2.7.3 it is determinate for $\alpha \ge 1$. If $\alpha = 2$, then the corresponding orthogonal polynomials are the well-studied Hermite polynomials.

2.9 Connection to Operator Theory

We will see that the extremal solutions encountered in Theorem 2.6.1 appear as spectral measures of self-adjoint extensions of Jacobi operators associated to an indeterminate moment problem.

2.9.1 Unbounded operators

We give a short revision on unbounded operators.
In the following let $\mathcal{H}$ be a Hilbert space. An *unbounded operator*, A, is a linear map from a subspace $D(A) \subset \mathcal{H}$ into $\mathcal{H}$. The set $D(A)$ is called its *domain*. A is called densely defined, if $D(A)$ is dense in $\mathcal{H}$.
Its *graph* is denoted by

$$\Gamma(A) = \{(Au, u) \mid u \in D(A)\}.$$

Note that $\Gamma(A)$ is a subspace of $\mathcal{H} \oplus \mathcal{H}$, that is, a linear relation. We call A closed if $\Gamma(A)$ is closed. We call B an extension of A if $\Gamma(A) \subset \Gamma(B)$, that is, if $D(A) \subset D(B)$ and $B|_{D(A)} = A$. A is then called a restriction of B. We also write $A \subset B$. A is called *closeable*, if it has a closed extension.
It is not hard to see, that a linear relation, $\mathcal{S}$, is the graph of an operator, if and only if $(0, w) \in \mathcal{S}$ implies that $w = 0$. From this it then follows that A is closeable if and only if $\overline{\Gamma(A)}$ is the graph of an operator. The closure $\overline{A}$ is then defined by $\Gamma(\overline{A}) = \overline{\Gamma(A)}$.
Let A be a densely defined operator. The domain of its adjoint $D(A^*)$ is the defined as follows

$$v \in \mathcal{D}(A^*) \quad \iff \quad \exists w \in \mathcal{H} : \forall u \in D(A)\ \langle Au, v\rangle = \langle u, w\rangle.$$

It is now easy to see that since A is densely defined, w is unique and we set $A^* v := w$.
Let us introduce $\mathbf{J} : \mathcal{H} \oplus \mathcal{H} \to \mathcal{H} \oplus \mathcal{H} \to$, by $\mathbf{J}((u, v)) = (-v, u)$. Then it follows that

$$\Gamma(A^*) = (\mathbf{J}\Gamma(A))^{\perp}.$$

We collect some properties which are all not very hard to show.

2.9.1 Lemma. *Let A be an unbounded densly defined operator. Then it holds:*

(i) *A^* is closed;*

(ii) $\ker A^* = (\operatorname{ran} A)^{\perp}$*;*

(iii) *A is closeable $\iff$ A^* is densely defined;*

(iv) *If A is closeable, then $\overline{A} = A^{**}$;*

(v) *If A is closeable, then $(\overline{A})^* = A^*$;*

(vi) *If $A \subset B$, then $B^* \subset A^*$;*

We turn to symmetric and self-adjoint operators and von Neumann's extension theory.
An operator A is called *symmetric* if

$$\Gamma(A) \subset \Gamma(A^*) \iff \forall u, v \in D(A) : \langle Au, v\rangle = \langle u, Av\rangle.$$

An operator is called self-adjoint, if $A = A^*$.
If A is symmetric, $z \in \mathbb{C} \setminus \mathbb{R}$, $u \in D(A)$, then one can show that

$$\|(A - z)u\| \geq \operatorname{Im} z \|u\|.$$

In particular, $\ker(A - z) = \{0\}$, i.e., A has no nonreal eigenvalues.
If A is symmetric, than $A \subset A^*$. It is thus, desirable to look for self-adjoint extensions, B of A. In this case $A \subset B = B^* \subset A^*$.

Let A be a densely defined, closed symmetric operator. We define the defect spaces

$$K_\pm := \operatorname{ran}(A \pm i)^\perp = \ker(A^* \mp i)$$

and the deficiency indices

$$d_\pm = \dim K_\pm.$$

The Cayley transform, $C_A : \operatorname{ran}(A+i) \to \operatorname{ran}(A-i)$, of A, is defined by

$$C_A := (A-i)(A+i)^{-1}.$$

It is a convenient tool, since it maps, as we will see symmetric operators into isometries, which are bounded.

2.9.2 Lemma. *Let A be a densely defined, closed symmetric operator. Then C_A is an isometry from* $\operatorname{ran}(A+i)$ *onto* $\operatorname{ran}(A-i)$.

Proof. We only need to check that it is an isometry. Since A is symmetric we have for any $u \in D(A)$

$$\|(A-i)u\|^2 = \|Au\|^2 + \|u\|^2 = \|(A+i)u\|^2.$$

For $u \in D(A)$ and $w = (A+i)u$ we have

$$\|C_A w\| = \|(A-i)u\| = \|(A+i)u\| = \|w\|.$$

❑

Thus, we see that finding self-adjoint extensions of A is equivalent to finding unitary extensions of C_A. This is possible if $d_+ = d_-$. All self-adjoint extensions are found by all surjective isometries from K_+ to K_-. Let $\tilde{V} : K_+ \to K_-$ be such a map, then

$$\tilde{C}_A = C_A \oplus \tilde{V}$$

is a unitary map on $\mathcal{H} = \operatorname{ran}(A+i) \oplus K_+ = \operatorname{ran}(A-i) \oplus K_-$. The domain and and the action of the corresponding self-adjoint extension can explicitly computed.

2.9.3 Lemma. *Let A be a densely defined, closed symmetric operator with equal deficiency indices. Let B be a self-adjoint extension and $\tilde{C}_A$ its Cayley transform. Then*

$$D(B) = D(A) + (1 - \tilde{C}_A)K_+$$

and for $u \in D(A)$, $k_+ \in K_+$ we have

$$B(u + (1 - \tilde{C}_A)k_+) = Au + i(1 + \tilde{C}_A)k_+.$$

Note that since $k_+ \in K_+$ we have

$$\tilde{C}_A k_+ = \tilde{V} k_+,$$

where $\tilde{V}$ is as above.

2.9.2 Unbounded Jacobi matrices

Let s be a non trivial moment sequence an (p_n) the associated orthonormal polynomials. They satisfy

$$\begin{aligned} zp_n(z) &= a_{n+1}p_{n+1}(z) + b_n p_n(z) + a_n p_{n-1}(z), \quad n \geq 1 \\ zp_0(z) &= a_1 p_1(z) + b_0 p_0(z). \end{aligned}$$

This induces an operator on $\ell^2(\mathbb{N}_0)$. Recall that $\mathcal{J}$ acts on sequences $u \in \mathbb{C}^{\mathbb{N}_0}$ by

$$\begin{aligned} (\mathcal{J}u)_n &= a_{n+1}u_{n+1} + b_n u_n + a_n u_{n-1}, \quad n \geq 1 \\ (\mathcal{J}u)_0 &= a_1 u_1 + b_0 u_0. \end{aligned}$$

We define the *maximal operator*

$$D(J_{\max}) = \{u \in \ell^2(\mathbb{N}_0) \mid \mathcal{J}u \in \ell^2(\mathbb{N}_0)\}.$$

and

$$J_{\max} = \mathcal{J}|_{D(J_{\max})}.$$

For $n \geq 1$, the Wronskian of two sequences u, v us defined by

$$W_n(u, w) = a_n(u_n v_{n-1} - u_{n-1}v_n).$$

The following Lemma may be interpreted as a version of Green's formula.

2.9.4 Lemma. *For any $u, v \in D(J_{max})$*

$$\lim W_n(u, \overline{v}) = W_\infty(u, \overline{v}), \quad \textit{exists}$$

and

$$\langle J_{max}u, v\rangle - \langle u, J_{max}v\rangle = W_\infty(u, \overline{v}).$$

Proof. A direct computation shows that

$$(J_{\max}u)_n\overline{v}_n - u_n(J_{\max}v)_n = \begin{cases} W_{n+1}(u, \overline{v}) - W_n(u, \overline{v}), & n \geq 1, \\ W_1(u, \overline{v}), & n = 0. \end{cases}$$

Summing of n gives

$$\sum_{j=0}^{n}(J_{\max}u)_n\overline{v}_n - \sum_{j=0}^{n} u_n(J_{\max}v)_n = W_{n+1}(u, \overline{v}).$$

Since $u, v, J_{\max}u, J_{\max}v \in \ell^2(\mathbb{N}_0)$, we can send $n \to \infty$ on the left-hand side and obtain

$$\langle J_{\max}u, v\rangle - \langle u, J_{\max}v\rangle = \lim_{n\to\infty} = W_{n+1}(u, \overline{v}) = W_\infty(u, \overline{v}).$$

❑

To search for self-adjoint restrictions of $J_{\max}$, we look for its adjoint. Let $\ell_c^2(\mathbb{N}_0)$ denote the set of those elements of $\ell^2(\mathbb{N}_0)$ which are compactly supported. Let J_0 be the restriction of $J_{\max}$ to $D(J_0) = \ell_c^2(\mathbb{N}_0)$.

2.9.5 Theorem. *It holds that $J_0^* = J_{max}$ and $\overline{J_0}$ is the restriction of J_{max} to*

$$D(\overline{J_0}) = \{v \in D(J_{max}) \mid W_\infty(u, \overline{v}) = 0, \forall u \in D(J_{max})\}. \tag{2.46}$$

Proof. First note that J_0 is densely defined. We start by computing its adjoint. Assume that $v, w \in \ell^2(\mathbb{N}_0)$ satisfy

$$\langle J_0 u, v\rangle = \langle u, w\rangle, \quad \forall u \in \ell^2_c(\mathbb{N}_0).$$

Since $\ell^2_c(\mathbb{N}_0)$ is the span of $(e_n)_{n\in\mathbb{N}_0}$ this is equivalent to

$$\langle J_0 e_n, v\rangle = \langle e_n, w\rangle, \quad \forall n \in \mathbb{N}_0$$

which is equivalent to

$$a_{n+1}v_n + b_n v_n + a_n v_{n-1} = w_n, \forall n \in \mathbb{N}_0,$$

(with the convention that $v_{-1} = 0$). Thus, this holds if and only if $(v, w) \in \Gamma(J_{\max})$. This shows that $J_0^* = J_{\max}$. In particular $J_{\max}$ is a closed extension of J_0 and thus, $\overline{J_0}$ is also a restriction of $J_{\max}$. It remains to show (2.46). Let the set in (2.46) be denoted by D_1. Note that $\overline{J_0} = (J_0^*)^* = J_{\max}^*$. The definition of the adjoint together with Lemma 2.9.4 implies that $D_1 \subset D(J_m ax^*)$. To show the opposite, note that $J_{\max}^* = \overline{J_0}$ is a restriction of $J_{\max}$. Thus, for any $v \in D(J_{\max}^*)$ and $u \in J_{\max}$ we have

$$\langle J_{\max} u, v\rangle = \langle u, J_{\max}^* v\rangle = \langle u, J_{\max} v\rangle.$$

Again, Lemma 2.9.4 now implies that $W_\infty(u, \overline{v}) = 0$ and thus $v \in D_1$.

❑

2.9.3 Concrete realizations

We will now apply the above theory to obtain self-adjoint extensions of J_0, whose spectral measures will be solution of the moment problem. Let us define

$$\mathcal{F} = \begin{cases} (\ell^2_c(\mathbb{N}_0), \langle\cdot,\cdot\rangle) & \to \quad (\mathcal{P}, \langle\cdot,\cdot\rangle_s) \\ (c_k)_{k=0}^n & \mapsto \quad (x \mapsto \sum_{k=0}^n c_k p_k(x)). \end{cases}$$

Note that for $u, v \in \ell^2_c(\mathbb{N}_0)$

$$\langle \mathcal{F}u, \mathcal{F}v\rangle_s = \langle u, v\rangle.$$

Since $\ell^2(\mathbb{N}_0)$ is complete and $\ell^2_c(\mathbb{N}_0)$ forms a dense subset, we see that $\iota = \mathcal{F}^{-1}$ provides a completion for $(\mathcal{P}, \langle\cdot,\cdot\rangle_s)$. Note that by construction we have that for any $v \in \ell^2(\mathbb{N}_0)$

$$\mathcal{F} J_0 v = x\mathcal{F} v.$$

Thus, by induction and linearity it follows that for any polynomial p,

$$\mathcal{F} p(J_0) v = p(x)\mathcal{F} v.$$

Now assume that J is a self-adjoint extension of J_0 with spectral measure E, i.e.,

$$J = \int x dE.$$

Then, since $\mathcal{F} e_0 = 1$, it follows that

$$\int x^n dE_{e_0,e_0}(x) = \langle J^n e_0, e_0\rangle = \langle \mathcal{F} J^n e_0, \mathcal{F} e_0\rangle_s = \langle x^n \mathcal{F} e_0, \mathcal{F} e_0\rangle_s = \langle x^n 1, 1\rangle_s = s_n.$$

That is dE_{e_0,e_0} is a solution of the moment problem. We will now assume that s corresponds to an indeterminate moment problem. Then we can extend $\mathcal{F}$ to $\ell^2(\mathbb{N}_0)$ and by Proposition 2.4.11

$$\mathcal{F}u = \sum_{k=0}^{\infty} u_k p_k$$

defines an entire function.

Let us now compute $K_\pm$ for $\overline{J_0}$. That is $K_\pm = \ker(\overline{J_0}^* \mp i)$. Since $(\overline{J_0})^* = J_0^* = J_{\max}$, we are looking for $v \in \ell^2$ such that

$$\mathcal{J}v = \mp iv.$$

Note that the solution space is 1 dimensional and since $(p_n(\mp i))_{n\in\mathbb{N}_0} \in \ell^2(\mathbb{N}_0)$, it follows that

$$K_\pm = \operatorname{span}\{(p_n(\mp i))_{n\in\mathbb{N}_0}\} = \operatorname{span}\{(\overline{p_n(\pm i)})_{n\in\mathbb{N}_0}\}$$

Let

$$k_\pm = (\overline{p_n(\pm i)})_{n\in\mathbb{N}_0}.$$

Note that

$$\mathcal{F}(k_\pm) = \sum_{n=0}^{\infty} p_n(z)\overline{p_n(i)} = \lim_{n\to\infty} K_n(z,i).$$

Since $K_\pm$ are only one dimensional, the unitary maps correspond to multiplication by a unimodular constant. Thus, we can find all self adjoint extensions of $\overline{J_0}$, via the unitary maps

$$V_\gamma k_+ = \gamma k_-, \quad |\gamma| = 1.$$

Let J_γ be the corresponding self adjoint extension and C_γ its Cayley transform. Then, by Lemma 2.9.3 we have

$$D(J_\gamma) = D(\overline{J}_0) + (I - C_\gamma)K_+$$

and for $u = u_0 + ck_+$, $c \in \mathbb{C}$,

$$J_\gamma u = \mathcal{J}u_0 + ic(k_+ + \gamma k_-).$$

2.9.6 Theorem. *Let $|\gamma| = 1$ and J_γ be the corresponding self adjoint extension with spectral measure E^γ. Then $\mu_\gamma = E^\gamma_{e_0,e_0}$ is a solution of the moment problem which is extremal in the sense of Theorem 2.6.1.*

Proof. We already know that μ_γ is a solution for the moment problem. Thus, it suffices to show that for some $z \in \mathbb{C}_+$

$$\frac{\operatorname{Im} w_{\mu_\gamma}(z)}{\operatorname{Im} z} = \sum_{k=0}^{\infty} |w_{\mu_\gamma}(z)p_k(z) + w_k(z)|^2. \tag{2.47}$$

For $z \in \mathbb{C}\setminus\mathbb{R}$, let $R_\gamma(z) = (J_\gamma - z)^{-1}$. Note that by the functional calculus,

$$w_{\mu_\gamma}(z) = \int \frac{dE_{e_0,e_0}(\gamma)}{x - z} = \langle R_\gamma(z)e_0, e_0\rangle.$$

Let us set

$$v(z) = \mathcal{F}_x^{-1}\left(\frac{p_k(x) - p_k(z)}{x - z}\right).$$

Then we see by linearity of $\mathcal{F}$ that

$$(J_\gamma - z)v(z) = \mathcal{F}_x^{-1}\,(p_k(x) - p_k(z)) = e_k - p_k(z)e_0,$$

i.e.,

$$R_\gamma(z)(e_k - p_k(z)e_0) = v(z).$$

Thus, we get

$$\begin{aligned}\langle R_\gamma(z)e_0, e_k\rangle &= \langle R_\gamma(z)e_0, e_k - p_k(\overline{z})e_0\rangle + \langle R_\gamma(z)e_0, p_k(\overline{z})e_0\rangle \\ &= \langle e_0, R_\gamma(\overline{z})(e_k - p_k(\overline{z})e_0)\rangle + p_k(z)\langle R_\gamma(z)e_0, e_0\rangle \quad = \langle e_0, v(\overline{z})e_0\rangle + p_k(z)w_{\mu_\gamma}(z) \\ &= q_k(z) + p_k(z)w_{\mu_\gamma}(z).\end{aligned}$$

By Parseval's identity, we have

$$\|R_\gamma(z)e_0\|^2 = \sum_{k=0}^{\infty} |\langle R_\gamma(z)e_0, e_k\rangle|^2.$$

On the other hand, applying the resolvent identity, we get

$$\|R_\gamma(z)e_0\|^2 = \langle R_\gamma(z)e_0, R_\gamma(z)e_0\rangle = \langle R_\gamma(\overline{z})R_\gamma(z)e_0, e_0\rangle = \left\langle \frac{R_\gamma(z) - R_\gamma(\overline{z})}{z - \overline{z}} e_0, e_0 \right\rangle = \frac{\operatorname{Im} w_{\mu_\gamma}(z)}{\operatorname{Im} z}.$$

That is, (2.47) holds. ❑

2.9.7 Remark. In fact, one can show that any measure, extremal in the sense of Theorem 2.6.1 is obtained in this way.

Chapter 3

Spectral theory of periodic Jacobi matrices

From now on we will restrict to the case that all coefficients are bounded, i.e., $\sup_n(|a_n| + |b_n|) < \infty$. By Lemma 2.1.17 this implies that J is a bounded self-adjoint operator. By Theorem 2.1.16 this corresponds to a unique moment sequence, which is determinate, say by Carleman's condition. Let μ denote the solution of the moment problem. Recall that we defined $\mathcal{F} : \ell^2_n(\mathbb{N}_0) \to \mathcal{P}$ by

$$\mathcal{F}((c_k)_{k=1}^n) = \sum_{k=1}^n c_k p_k(x),$$

where p_k denote the orthogonal polynomials associated to J. In particular $\mathcal{F}e_0 = 1$. Moreover, since the moment problem is determinate, $\mathcal{P}$ is dense and we can extend $\mathcal{F}$ to a unitary operator from $\ell^2(\mathbb{N}_0)$ to $L^2(\mathbb{R}, \mu)$. Let E denote the spectral measure for J. Then we have seen that

$$\int x^n dE_{e_0,e_0} = \langle J^n e_0, e_0 \rangle_{\ell^2} = \langle \mathcal{F} J^n e_0, \mathcal{F} e_0 \rangle_{L^2} = \langle x^n 1, 1 \rangle = \int x^n d\mu(x).$$

By determinacy of the moment problem, we conclude that $E_{e_0,e_0} = \mu$. Finally, we note that

$$e_n = \mathcal{F}^{-1} p_n(x) \cdot 1 = p_n(J)\mathcal{F}^{-1}1 = p_n(J)e_0.$$

Thus,

$$\mathrm{span}\{p(J)e_n \mid p \in \mathcal{P}\}$$

is dense in $\ell^2(\mathbb{N}_0)$. That is, e_0 is a cyclic vector for J. Since J is unitarily equivalent to the multiplication operator in $L^2(\mathbb{R}, \mu)$ it follows that

$$\sigma(J) = \mathrm{supp}\,\mu.$$

Thus, in order to study the spectrum of J it suffices to study μ, respectively the corresponding Herglotz function. By the functional calculus, we have

$$m_+(z) := \langle (J - z)^{-1} e_0, e_0 \rangle = \int \frac{d\mu(x)}{x - z}.$$

We will clarify the meaning of the sub-+ in the next section. From now on we will restrict our consideration to Jacobi parameters that are periodic, i,e, there exists some $p \geq 1$ so that for all $n \in \mathbb{Z}$

$$a_{n+p} = a_n, \quad b_{n+p} = b_n.$$

3.1 Two-sided Jacobi matrices

For periodic Jacobi matrices, it turns out that for several reasons it is more natural to extend a_n, b_n by periodicity to sequences on $\mathbb{Z}$. Thus, given periodic Jacobi parameters $(a_n)_{n\geq 1}, (b_n)_{n\geq 0}$, we consider there extension to $\mathbb{Z}$ be demanding that

$$a_{n+p} = a_n, \quad b_{n+p} = b_n.$$

for all $n \in \mathbb{Z}$. In the following, let J act on sequences in $\mathbb{C}^{\mathbb{Z}}$ by

$$(Ju)_n = a_{n+1}u_{n+1} + b_n u_n + a_n u_{n-1}.$$

Since all coefficients are bounded, one can show as in Lemma 2.1.17 that J defines an bounded self-adjoint operator in $\ell^2(\mathbb{Z})$. In the following let e_n denote the standard basis of $\ell^2(\mathbb{N}_0)$ or $\ell^2(\mathbb{Z})$, which should always be clear from the context. Let $\ell^2_+ = \ell^2(\mathbb{N}_0)$, $\ell^2_- = \ell^2(\mathbb{Z}_{<0})$ and $P_\pm$ denote the orthogonal projections from $\ell^2(\mathbb{Z})$ onto $\ell^2_\pm$. Moreover, define the finite range operator $F : \ell^2(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ by

$$F(v) = \langle v, e_0\rangle e_{-1} + \langle v, e_{-1}\rangle e_0.$$

Define

$$J_\pm = P_\pm J P_\pm.$$

Then we have

$$J = J_+ + J_- + a_0 F. \tag{3.1}$$

Thus, J is a finite dimensional perturbation of the diagonal operator $J_- + J_+$. We will now prove an analogo of $p_n(J_+)e_0 = e_n$ for two-sided Jacobi matrices. We call $(y_n)_{n\in\mathbb{Z}}$ a formal eigensolution for J if it solves

$$a_{n+1}y_{n+1} + b_n y_n + a_n y_{n-1} = z y_n.$$

The phrasing formal, highlights the fact that we do not require that y belongs to the domain of J. Let $(u_n), (v_n)$ be formal eigensolutions for J with initiall conditions

$$u_{-1} = 0, \quad u_0 = 1, \quad v_{-1} = 1, \quad u_0 = 0.$$

Thus, for positive n, u_n, v_n are essentially the orthonormal polynomials of first and second kind for J_+. Then we have

3.1.1 Lemma. *For any $z \in \mathbb{Z}$,*

$$e_n = v_n(J)e_{-1} + u_n(J)e_0.$$

Proof. Let

$$\psi_n = v_n(J)e_{-1} + u_n(J)e_0.$$

Then $\psi_j = e_j$, for $j = 0, -1$. Thus, it suffices to show that

$$J\psi_n = a_{n+1}\psi_{n+1} + b_n\psi_n + a_n\psi_{n-1}.$$

Since u, v are formal eigensolutions, by the functional calculus for J, we have that

$$Ju_n(J) = a_{n+1}u_{n+1}(J) + b_n u_n(J) + a_n u_{n-1}(J),$$

and the same holds for v. Thus, the claim follows. ❑

This motivates, that for J it is more natural to work with e_{-1}, e_0. We define the matrix valued Green function

$$M(z) = \begin{pmatrix} G_{-1,-1}(z) & G_{-1,0}(z) \\ G_{0,-1}(z) & G_{0,0}(z) \end{pmatrix} = \begin{pmatrix} \langle (J-z)^{-1} e_{-1}, e_{-1}\rangle & \langle (J-z)^{-1} e_0, e_{-1}\rangle \\ \langle (J-z)^{-1} e_{-1}, e_0\rangle & \langle (J-z)^{-1} e_0, e_0\rangle \end{pmatrix}.$$

We also introduce

$$m_-(z) = \langle (J_- - z)^{-1} e_{-1}, e_{-1}\rangle, \quad m_+(z) = \langle (J_+ - z)^{-1} e_0, e_0\rangle.$$

By means of (3.1) we can express M in terms of $m_\pm$ and a_0.

3.1.2 Lemma. *For $z \in \mathbb{C} \setminus \mathbb{R}$ we have*

$$M(z) = \begin{pmatrix} m_-(z)^{-1} & a_0 \\ a_0 & m_+(z)^{-1} \end{pmatrix}^{-1}.$$

In particular, the diagonal of the Green function are given by

$$-\frac{1}{G_{-1,-1}(z)} = a_0^2 m_+(z) - \frac{1}{m_-(z)},$$
$$-\frac{1}{G_{0,0}(z)} = a_0^2 m_-(z) - \frac{1}{m_+(z)}.$$

Proof. We have

$$J - z = J_+ + J_- - z + a_0 F.$$

Thus, applying the second resolvent identity we get

$$(J-z)^{-1} = (J_+ + J_- - z)^{-1} - a_0 (J-z)^{-1} F (J_+ + J_- - z)^{-1}.$$

Now taking scalar products with respect to e_{-1} and e_0 and using the diagonal structure of $J_- + J_+$ we get

$$\begin{aligned} G_{-1,-1} &= m_- - a_0 m_- G_{-1,0}, \\ G_{-1,0} &= -a_0 m_+ G_{-1,-1}, \\ G_{0,-1} &= -a_0 m_- G_{0,0}, \\ G_{0,0} &= m_+ - a_0 m_+ G_{0,-1}. \end{aligned}$$

That is

$$\begin{aligned} 1 &= m_-^{-1} G_{-1,-1} + a_0 G_{-1,0}, \\ 0 &= m_+^{-1} G_{-1,0} + a_0 G_{-1,-1}, \\ 0 &= m_-^{-1} G_{0,-1} + a_0 G_{0,0}, \\ 1 &= m_+^{-1} G_{0,0} + a_0 G_{0,-1}. \end{aligned}$$

and thus

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} G_{-1,-1} & G_{-1,0} \\ G_{0,-1} & G_{0,0} \end{pmatrix} \begin{pmatrix} m_-^{-1} & a_0 \\ a_0 & m_+^{-1} \end{pmatrix},$$

which finishes the proof. The formulae for the diagonal entries now follow easily. ❑

3.2 Coefficient stripping and periodic discriminant

Let $J_+^{(1)}$ denote the Jacobi matrix that is obtained from J_+ by deleting the first row and column. That is

$$J_+ = J_+^{(1)} + b_0\langle\cdot, e_0\rangle e_0 + a_1 F_+,$$

where

$$F_+ = \langle\cdot, e_0\rangle e_1 + \langle\cdot, e_1\rangle e_0$$

Let

$$m_+^{(1)}(z) = \langle (J_+^{(1)} - z)^{-1} e_1, e_1\rangle.$$

3.2.1 Lemma. *For $z \in \mathbb{C} \setminus \mathbb{R}$ we have*

$$m(z) = -\frac{1}{z - b_0 + a_1^2 m^{(1)}(z)}.$$

Proof. Let $H = \langle\cdot, e_0\rangle e_0$. Then, as in the proof of Lemma 3.1.2 we get by the resolvent identity that

$$(J_+ - z)^{-1} = (J_+^{(1)} + b_0 H)^{-1} - a_1 (J_+ - z)^{-1} F_+ (J_+^{(1)} + b_0 H)^{-1}.$$

We get

$$\langle (J_+ - z)^{-1} e_0, e_0\rangle = \frac{1}{b_0 - z} - a_1 \frac{1}{b_0 - z}\langle (J_+ - z)^{-1} e_1, e_0\rangle,$$
$$\langle (J_+ - z)^{-1} e_1, e_0\rangle = -a_1 m^{(1)}(z) m(z).$$

Inserting the second equation into the first yields the Lemma. ❑

Note that this can be written as

$$m(z) = \begin{pmatrix} 0 & -\frac{1}{a_1} \\ a_1 & \frac{z-b_0}{a_1} \end{pmatrix} \star m^{(1)}(z),$$

that is

$$m^{(1)}(z) = \begin{pmatrix} \frac{z-b_0}{a_1} & \frac{1}{a_1} \\ -a_1 & 0 \end{pmatrix} \star m(z) = A(z, a_1, b_0) \star m(z), \tag{3.2}$$

where

$$A(z, a, b) = \begin{pmatrix} \frac{z-b}{a} & \frac{1}{a} \\ -a & 0, \end{pmatrix}$$

was defined in (2.8). By periodicity, we clearly have that

$$m_\pm^{(p)}(z) = m_\pm(z).$$

Recall, that we assumed that the Jacobi parameters are p-periodic. We use the representatives

$$a_1, \cdots a_p, \quad \text{and,} \quad b_0, \cdots b_{p-1}.$$

Then, we have

$$T_p^+(z) = A(z, a_p, b_{p-1}) \cdots A(z, a_1, b_0)$$

and

$$T_p^-(z) = A(z, a_0, b_0) \cdots A(z, a_{p-1}, b_{p-1}).$$

Let $p_j^\pm$ denote the orthonormal polynomials associated to $J_\pm$. Then we have

$$T_p^+(z) = \begin{pmatrix} p_p^+(z) & q_p^+(z) \\ -a_p p_{p-1}^+(z) & -a_p q_{p-1}^+(z) \end{pmatrix}, \quad T_p^-(z) = \begin{pmatrix} p_p^-(z) & q_p^-(z) \\ -a_p p_{p-1}^-(z) & -a_p q_{p-1}^-(z) \end{pmatrix}.$$

3.2.2 Proposition. *We have*

$$p_p^+ = p_p^-, \quad a_p q_p^+ = p_{p-1}^-, \quad p_{p-1}^+ = a_p q_p^-, \quad q_{p-1}^+ = q_{p-1}^-.$$

Proof. We have the factorization

$$\begin{pmatrix} \frac{z-b}{a} & \frac{1}{a} \\ -a & 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{a} & 0 \\ 0 & a \end{pmatrix} \begin{pmatrix} z-b & 1 \\ -1 & 0 \end{pmatrix}.$$

Let

$$j = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}.$$

We get that for general a, b, α, β

$$A(z,a,b)^\intercal A(z,\alpha,\beta)^\intercal = \begin{pmatrix} z-b & -1 \\ 1 & 0 \end{pmatrix} jA(z,a,\beta)j \begin{pmatrix} \frac{1}{\alpha} & 0 \\ 0 & \alpha \end{pmatrix}$$

Applying this to all factors of $T_p^-(z)^\intercal$ and multiplying from the left with $B = j\begin{pmatrix} \frac{1}{a_p} & 0 \\ 0 & a_p \end{pmatrix}$ and from the right with B^{-1} shows that

$$j\begin{pmatrix} \frac{1}{a_p} & 0 \\ 0 & a_p \end{pmatrix} T_p^-(z)^\intercal \begin{pmatrix} a_p & 0 \\ 0 & \frac{1}{a_p} \end{pmatrix} j = T_p^+(z). \tag{3.3}$$

Looking at the entries of this identity proves the claim. ❑

3.2.3 Theorem. *The function $m_+(z)$ is a solution to the quadratic equation*

$$0 = \alpha(z)m(z)^2 + \beta(z)m(z) + \gamma(z), \tag{3.4}$$

where

$$\alpha(z) = a_p p_{p-1}^+(z), \quad \beta(z) = p_p^+(z) + a_p q_{p-1}^+(z), \quad \gamma(z) = q_p^+(z).$$

The second solution to this equation is $(a_p^2 m_-(z))^{-1}$.

Proof. By periodicity and (3.2) we have

$$m_+(z) = T_p^+(z) \star m_+(z).$$

That is

$$-a_p m_+(z) = \frac{p_p(z)m_+(z) + q_p(z)}{p_{p-1}(z)m_+(z) + q_{p-1}(z)}.$$

To show that $(a_p^2 m_-(z))^{-1}$ is the second solution, we first note that

$$m_-(z) = T_p^-(z) \star m_-(z).$$

Using $(T_p^-(z))^{-1} = JT_p^-(z)^\intercal J^{-1}$ and (3.3) we obtain that

$$T_p^+(z)\begin{pmatrix} \frac{1}{a_p} & 0 \\ 0 & a_p \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \star m_-(z) = \begin{pmatrix} \frac{1}{a_p} & 0 \\ 0 & a_p \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \star m_-(z).$$

This shows that $\tilde{m}(z) = (a_p^2 m_-(z))^{-1}$ is a solution to the quadratic equation. Since $\tilde{m}(z)$ maps $\mathbb{C}_+$ onto $\mathbb{C}_-$ it cannot be equal to m_+ and thus it is necessarily the second solution. ❑

Let us define the discriminant by

$$\Delta(z) := \operatorname{tr} T_p(z) = p_p^+(z) - a_p q_{p-1}^+(z)$$

Then using the Wronskian identity (2.12) we see that

$$\begin{aligned}\beta(z)^2 - 4\alpha(z)\gamma(z) &= (p_p^+(z) + a_p q_{p-1}^+(z))^2 2 - 4a_+ p_{p-1}^+(z) q_p^+(z)\\ &= (p_p^+(z) - a_p q_{p-1}^+(z))^2 - 4a_p(p_{p-1}^+(z)q_p^+(z) - p_p^+(z)q_{p-1}^+(z)) = \Delta(z)^2 - 4.\end{aligned}$$

Thus, we get that the two solutions of (3.4) are obtained by

$$m(z) = -\frac{\beta(z) \pm \sqrt{\Delta(z)^2 - 4}}{a_p p_{p-1}^+(z)}.$$

This motivates why we will study properties of the discriminant Δ.
Let us introduce the auxiliary function

$$g(z) = \frac{\Delta(z)}{a_p p_{p-1}^+(z)}.$$

3.2.4 Lemma. *The function $g(z)$ is a Herglotz function. Moreover, zeros of Δ and p_{p-1}^+ strictly interlace. In particular, all zeros of Δ are real and simple.*

Proof. We have

$$g(z) = \frac{p_p^+(z)}{a_p p_{p-1}^+(z)} - \frac{q_{p-1}^+(z)}{a_p p_{p-1}^+(z)}$$

Thus, by Corollary 2.1.27 and (2.16) it is the sum of two Herglotz functions and thus a Herglotz function. Let us now show that $\Delta(z)$ and $p_{p-1}^+(z)$ can have no common zeros. Assume that $x_0 \in \mathbb{R}$ is a zero of $p_{p-1}^+(z)$ and of Δ. Then by the Wronskian identity, we have

$$-1 = a_p p_p^+(x_0) q_{p-1}^+(x_0).$$

That is, $p_p^+(x_0)$ and $q_{p-1}^+(x_0)$ have opposite sign. On the other hand, $0 = \Delta(x_0)$ implies $p_p^+(x_0) = a_p q_{p-1}^+(x_0)$. A contradiction. As in the proof of Corollary 2.1.27 we see that the zeros of Δ and p_{p-1}^+ strictly interlace. Since p_{p-1}^+ has p_-1 simple real zeros and $g(z) \sim z$ as $z \to \infty$ we get that Δ has at least p zeros, one between each zero of p_{p-1}^+ and one to the left of the first and one to the right of the last zero of p_{p-1}^+. Since Δ is a polynomial of degree p, we conclude that it has p real simple zeros. ❑

In the following, we collect the characteristic properties of Δ. A point c is called critical point of a function f, if $f'(c) = 0$.

3.2.5 Theorem. *Δ has the following properties:*

(i) Δ is real;

(ii) All zeros are real and simple;

(iii) All critical points are real and if c is a critical point, then $|\Delta(c)| \geq 2$.

Proof. (i) is clear since p_p^+ and q_{p-1}^+ are real. (*ii*) was already shown in (3.2.4). It remains to show (*iii*). Let first x_0 be a zero of p_{p-1}^+. As in the previous proof, we conclude that $p_p^+(x_0)$ and $-a_p q_{p-1}^+(x_0)$ have the same sign and $-a_p q_{p-1}^+(x_0) p_p^+(x_0) = 1$. Thus, we conclude from the AM-GM inequality, that

$$\frac{|p_p^+(x_0) - a_p q_{p-1}^+(x_0)|}{2} \geq \sqrt{-a_p q_{p-1}^+(x_0)} = 1.$$

Let y_1, y_2 be two consecutive zeros of Δ. By simple counting, there is exactly one critical point c of Δ. Due to interlacing, there is also a zero, x_0 of p_{p-1}^+. Thus, we conclude that

$$|\Delta(c)| \geq |\Delta(x_0)| \geq 2.$$

This shows the last claim. ❑

Let us define the set

$$\mathsf{E} = \Delta^{-1}([-2,2]) = \{z \in \mathbb{C} \mid \Delta(z) \in -2, 2\}.$$

Then there exist $\mathbf{b}_0 < \mathbf{a}_1 \leq \mathbf{b}_1 < \mathbf{a}_2 \leq \mathbf{b}_2 < \cdots < \mathbf{a}_{p-1} \leq \mathbf{b}_{p-1} < \mathbf{a}_0$ such that

$$\mathsf{E} = \Delta^{-1}([-2,2]) = [\mathbf{b}_0, \mathbf{a}_0] \setminus \bigcup_{j=1}^{p-1} (\mathbf{a}_j, \mathbf{b}_j),$$

with the convention that $(\mathbf{a}, \mathbf{a}) = \emptyset$. Moreover, there is exactly one critical point λ_j of Δ in each gap $(\mathbf{a}_j, \mathbf{b}_j)$. Note that $\mathbf{a}_j = \mathbf{b}_j$ if and only if $|\Delta(\lambda_j)| = 2$. The sets $[b_j, a_{j+1}]$ are called bands of the spectrum. The open intervals $(\mathbf{a}_j, \mathbf{b}_j)$ are called gaps and the sets $[\mathbf{b}_j, \mathbf{a}_{j+1}]$ bands. A gap is called closed if $\mathbf{a}_j = \mathbf{b}_j$. We call the points $\mathbf{a}_j, \mathbf{b}_j$, $0 \leq j \leq p-1$ gap edges.
By definition of E, we can take an analytic square root of $\Delta(z)^2 - 4$ in $\mathbb{C}_+$. That is, there exists a function g, which is analytic in $\mathbb{C}_+$ such that $g(z)^2 = \Delta(z)^2 - 4$. Denote $g(z) = \sqrt{\Delta(z)^2 - 4}$.
Let us fix a branch of the square root and then analyze the argument of $\sqrt{\Delta(z)^2 - 4}$ as z approaches $\mathbb{R}$. Let us recall that powers of analytic functions are defined using the logarithm, and in its turn the logarithm of a nonvanishing function f, is defined as the primitive of f'/f. This allows us to analyze the argument of the boundary values of $\sqrt{\Delta(z)^2 - 4}$ along $\mathbb{R}$. We choose the branch of the square root so that $\sqrt{\Delta(z)^2 - 4}$ for $z \in [\mathbf{b}_0, \infty]$. By considering the integral

$$\int \frac{(\Delta(u)^2 - 4)'}{\Delta(u)^2 - 4} du$$

locally around a zero of $\Delta(z)^2 - 4$, we see that at every zero (counting mulitplicity) of $\Delta(z)^2 - 4$ the argument of $\sqrt{\Delta(z)^2 - 4}$ increases by $\pi/2$.
Note also that for any $(c, d) \subset \mathbb{R}$ which contains no zero of $\Delta(z)^2 - 4$, $\sqrt{\Delta(z)^2 - 4}$ has an analytic extension to $\mathbb{C}_+ \cup (c, d) \cup \mathbb{C}_-$. In particular, for $(c, d) \subset \mathbb{R} \setminus \mathsf{E}$, $g(z) = \sqrt{\Delta^2 - 4}$ is real valued, and thus, by the reflection principle, the analytic extension obeys, $\overline{g(\overline{z})} = g(z)$. This, shows that $\sqrt{\Delta(z)^2 - 4}$ has an analytic continuation to $\mathbb{C} \setminus E$.
We need to recall certain facts from complex analysis. Let Ω_1, Ω_2 be two connected open subsets of $\overline{\mathbb{C}}$, where $\overline{\mathbb{C}}$ denotes the Riemann sphere. We call a function $f : \Omega_1 \to \Omega_2$ conformal, if f is holomorphic and has a holomorphic inverse. The map

$$f : \begin{cases} \mathbb{D} & \to & \overline{\mathbb{C}} \setminus [-2,2] \\ \zeta & \mapsto & \zeta + \frac{1}{\zeta} \end{cases} \tag{3.5}$$

is conformal and is called the Zhukovsky map. Recall also that if Ω is simply connected and $f : \Omega \to \mathbb{C}$ so that f does not vanish on Ω, then there exists an analytic $g : \Omega \to \mathbb{C}$ such that $f = e^g$.

3.2.6 Proposition. *There exists analytic $B : \overline{\mathbb{C}} \setminus E \to \mathbb{D}$ such that*

$$\Delta(z) = B(z) + \frac{1}{B(z)}.$$

Morover, there exists $\Theta : \mathbb{C}_+ \to \mathbb{C}_+$ such that $B(z) = e^{ip\Theta(z)}$. Thus, for $z \in \mathbb{C}_+$ we have

$$\Delta(z) = 2\cos(p\Theta(z)).$$

Proof. By definition Δ maps $\overline{\mathbb{C}} \setminus E$ onto $\overline{\mathbb{C}} \setminus [-2, 2]$. Thus, if f is the Zhukovsky map, we can define $B(z) = f^{-1}(\Delta(z))$. From this all claims about B follow. Since f maps 0 to ∞ and Δ is finite on $\mathbb{C}_+$, it follows that B does not vanish on $\mathbb{C}_+$. Hence we can define

$$\Theta(z) = -\frac{i}{p} \log B(z)$$

Since $|B(z)| < 1$ in $\mathbb{C}_+$, it follows that $\operatorname{Im} \Theta(z) > 0$. ❑

3.2.7 Remark. Let us recall that the branch of log is only unique up to adding $2\pi i k$ for some $k \in \mathbb{Z}$. Thus, any

$$\tilde{\Theta} = \Theta + \frac{2\pi k}{p}, \quad k \in \mathbb{Z},$$

would also be a suitable choice. We will fix the choice of the branch of log later.

Θ has the interesting property, that not only Θ, but also $i\Theta'$ is a Herglotz function. Factorizing Δ' and $\Delta^2 - 4$ we have

$$\Delta(z)^2 - 4 = \frac{1}{(a_1 \dots a_p)^2} \prod_{j=0}^{p-1} (z - \mathbf{a}_j)(z - \mathbf{b}_j),$$

$$\Delta'(z) = \frac{q}{a_1 \dots a_p} \prod_{j=1}^{p-1} (z - \lambda_j)$$

This will be a consequence of the following formula.

3.2.8 Lemma. *For $z \in \mathbb{C}_+$ we have*

$$\Theta'(z) = \frac{i\Delta'(z)}{q\sqrt{\Delta(z)^2 - 4}} = \frac{i \prod_{j=1}^{p-1} (z - \lambda_j)}{\sqrt{\prod_{j=0}^{p-1} (z - \mathbf{a}_j)(z - \mathbf{b}_j)}}$$

This function has an extension to $\mathbb{C} \setminus \mathsf{E}$, which obeys $\overline{\Theta'(\overline{z})} = -\Theta'(z)$ and $-i\Theta'(z) > 0$ for $z \in (\mathbf{b}_0, \infty)$.

Proof. Since $\Delta = 2\cos(p\Theta)$ and $\Delta^2 - 4$ does not vanish in $\mathbb{C}_+$ we can fix a branch of the square root so that

$$\sqrt{\Delta^2 - 4} = -2i \sin(p\Theta).$$

Differentiating gives the first identity. The product formula follows from those for Δ' and $\Delta^2 - 4$. Since $\sqrt{\Delta^2 - 4}$ has an analytic extension to $\mathbb{C} \setminus \mathsf{E}$ the same holds for Θ'. Again from the sign of Θ' and $\sqrt{\Delta^2 - 4}$ it follows that $-i\Theta'(z) > 0$ is positive in $(\mathbf{b}_0, \infty)$. $\overline{\Theta'(\overline{z})} = -\Theta'(z)$ now follows by Schwarz reflection principle applied on $(\mathbf{b}_0, \infty)$. ❑

For our data λ_j, a_j, b_j, let us define

$$\xi(t) = \begin{cases} 0, & x \in (-\infty, \mathbf{b}_0), \\ \frac{1}{2}, & t \in \mathsf{E}, \\ 1, & t \in (\mathbf{a}_j, \lambda_j), \\ 0, & t \in (\lambda_j, \mathbf{b}_j), \\ 1, & t \in (\mathbf{a}_0, \infty) \end{cases}$$

3.2.9 Proposition. *$i\Theta'(z)$ is a Herglotz funnction. There exists $C > 0$ such that*

$$i\Theta'(z) = Ce^{\int \left(\frac{1}{t-z} - \frac{t}{1+t^2}\right)\xi(t)dt}. \tag{3.6}$$

Moreover, for

$$d\nu(t) = \chi_{\mathsf{E}}(t)\frac{1}{\sqrt{|(t-\mathbf{a}_0)(t-\mathbf{b}_0)|}}\prod_{j=1}^{p-1}\frac{t-\lambda_j}{\sqrt{|(t-\mathbf{a}_j)(t-\mathbf{b}_j)|}}dt, \tag{3.7}$$

we have

$$i\Theta'(z) = \int \frac{d\nu(t)}{t-z} \tag{3.8}$$

and $\nu(\mathbb{R}) = 1$.

Proof. Let ξ be as above and define

$$g(z) = e^{\int \left(\frac{1}{t-z} - \frac{t}{1+t^2}\right)\xi(t)dt}.$$

Note that since $\xi \leq 1$ for $z = x + iy$ we have

$$\operatorname{Im}\int \left(\frac{1}{t-z} - \frac{t}{1+t^2}\right)\xi(t)dt = y\int \frac{\xi(t)dt}{(t-x^2)+y^2} \leq y\int \frac{dt}{(t-x^2)+y^2} = \pi,$$

which implies that g is a Herglotz function. Since a primitive for $\frac{1}{t-z} - \frac{t}{1+t^2}$ is $\log((t-z)/\sqrt{1+t^2})$ we get

$$\exp\left(\int_{\mathbf{a}_0}^{\infty}\left(\frac{1}{t-z} - \frac{t}{1+t^2}\right)dt\right) = \frac{\sqrt{1+\mathbf{a}_0^2}}{\mathbf{a}_0 - z}$$

Similarly we see that there is C_1 such that

$$\exp\left(\frac{1}{2}\int_{\mathbf{b}_j}^{\mathbf{a}_{j+1}}\left(\frac{1}{t-z} - \frac{t}{1+t^2}\right)dt\right) = C_1\sqrt{\frac{\mathbf{a}_{j+1}-z}{\mathbf{b}_j - z}}$$

and C_2 such that

$$\exp\left(\frac{1}{2}\int_{\mathbf{a}_j}^{\lambda_j}\left(\frac{1}{t-z} - \frac{t}{1+t^2}\right)dt\right) = C_2\frac{\lambda_j - z}{\mathbf{a}_j - z}.$$

Combing this, we find that there is C_3 such that

$$g(z) = C_3\frac{\prod_{j=1}^{p}(z-\lambda_j)}{\sqrt{\prod_{j=0}^{p-1}(z-\mathbf{a}_j)(z-\mathbf{b}_j)}}.$$

Since $\xi = 1$ on $(\mathbf{a}_0, \infty)$, $g < 0$, there. Thus, we conclude that $C_3 = -C$, for some $C > 0$. Combining this with Lemma 3.2.8, we conclude (3.6). Since $i\Theta'(z)$ is real valued on $(-\infty, \mathbf{b}_0)$ and $(\mathbf{a}_0, \infty)$, by the Stieltjes inversion formula, the measure ν in the integral representation of $i\Theta'$ is compactly supported. Moreover, since $i\Theta'(z) \sim -z^{-1}$ for $z \to \infty$, $\beta = 0$ and we conclude that there is $\alpha \in \mathbb{R}$ such that

$$i\Theta'(z) = \alpha + \int \frac{d\nu(t)}{t - z}.$$

Since ν is compactly supported, sending $z \to \infty$ on both sides shows that $\alpha = 0$. Finally, Stieljes inversion shows that ν is of the form (3.7).
Since

$$\int \frac{d\nu(t)}{t-z} \sim -\frac{\nu(\mathbb{R})}{z} + o\left(\frac{1}{z}\right), \quad z \to \infty,$$

we conclude that $\nu(\mathbb{R}) = 1$. ❑

3.2.10 Remark. From the represenation (3.6), it is easy to derive, that with the appropriate choice of the square root,

$$i\Theta'(z) = \frac{-1}{\sqrt{(z - \mathbf{a}_0)(z - \mathbf{b}_0)}} e^{\int_{[\mathbf{b}_0, \mathbf{a}_0] \setminus \mathsf{E}} \frac{1}{t-z} \tilde{\xi}(t) dt},$$

where $\tilde{\xi}(t) = \frac{1}{2}$ if $t \in (\mathbf{a}_j, \lambda_j)$ and $\tilde{\xi}(t) = -\frac{1}{2}$ if $t \in (\lambda_j, \mathbf{b}_j)$.
We will now derive an integrated version of (3.8).

3.2.11 Lemma. *There exists a branch of* $\log B$ *such that on* $\mathbb{C}_+$*,*

$$\Theta(z) = -i \log((a_1 \dots a_p)^{1/p}) + i \int \log(z - t) d\nu(t). \tag{3.9}$$

Proof. Both sides of the above equality are analytic functions in $\mathbb{C}_+$, whose derivative coincide by (3.8). Thus, there is $c \in \mathbb{C}$ such that

$$\Theta(z) = c + i \int \log(z - t) d\nu(t).$$

To find c we will compare the asymptotics as $z \to \infty$ in $\mathbb{C}_+$, with the branch of the log with $-\pi < \operatorname{Im} \log < \pi$.
Since ν is supported on E and uniformly for $\theta \in \mathsf{E}$, $\log(z - t) - \log z = \log(1 - t/z) \to 0$ as $z \to \infty$ and $\nu(\mathbb{R}) = 1$, we have

$$i \int \log(z - t) d\nu(t) = i \log z + o(1). \tag{3.10}$$

We have

$$\Delta(z) = e^{ip\Theta(z)} + e^{-ip\Theta(z)} = e^{-ip\Theta(z)}(1 + e^{2ip\Theta(z)})$$

and

$$\Delta(z) \sim \frac{z^p}{a_1 \dots a_p}, \quad z \to \infty. \tag{3.11}$$

Since by construction $e^{i\Theta(z)} \to 0$ as $z \to \infty$, $z \in \mathbb{C}_+$, $(1 + e^{2ip\Theta(z)}) \to 1$ as $z \to \infty$. By (3.10),

$$-i\Theta(z) = \log z - ic + o(1).$$

Hence

$$e^{-ip\Theta(z)} \sim e^{-ipc} z^p$$

Comparing this with (3.11) shows that $c = -i/p \log(a_1 \dots a_p) + 2\pi k/p$, for some $k \in \mathbb{Z}$. At this place we choose the branch of $\log \Theta$, so that $k = 0$. This proves the claim. ❑

From now on, we will choose the branch of Θ, that corresponds to (3.9).

3.2.12 Proposition. *Θ extends continuously to $\mathbb{C}_+ \cup \mathbb{R}$ This extension obeys the following:*

(i) $\operatorname{Im}\Theta = 0$, *on* E,

(ii) $\operatorname{Re}\Theta = -\pi + \frac{j}{p}\pi$, *on* $[\mathbf{a}_j, \mathbf{b}_j]$ *for* $1 \le j \le p-1$,

(iii) $\operatorname{Re}\Theta = -\pi$ *on* $(-\infty, \mathbf{b}_0)$,

(iv) $\operatorname{Re}\Theta = 0$ *on* $[\mathbf{a}_0, \infty)$.

Proof. We start with proving that Θ has a continuous extension. Since Θ' is analytic at $\mathbb{R}$ except at $\mathbf{a}_j, \mathbf{b}_j$, it is clear that Θ can be continuously extended to $\mathbb{R} \setminus \{\mathbf{a}_0, \mathbf{b}_0, \dots, \mathbf{a}_{p-1}, \mathbf{b}_{p-1}\}$. Let κ be one of those points. Then for some $\epsilon > 0$ small enough, we can write $\Theta'(z) = \frac{1}{\sqrt{z-\kappa}} f(z)$, where $f(z)$ is analytic in $U := (B_\epsilon(\kappa) \cap (\mathbb{C}_+ \cap \mathbb{R})) \setminus \{\kappa\}$. Hence, for $z \in U$ and $a \in U$ fixed we can write

$$\Theta(z) = \Theta(a) + \int_a^z \frac{1}{\sqrt{u-\kappa}} f(u) du.$$

Integration by parts now shows that the right-hand side can be continuously extended to κ.

By continuity, this extension obeys $\Delta(z) = 2\cos(p\Theta(z))$. We have $\Delta(z) \in [-2, 2]$ on E, so $\Theta(z) \in \mathbb{R}$. Since Θ' is purely imaginary in gaps $(\mathbf{a}_j, \mathbf{b}_j)$, we conclude $\Theta(\mathbf{a}_j) = \Theta(\mathbf{b}_j)$. Meanwhile, $p\Theta(z) \in \pi\mathbb{Z}$ if and only if z is a band edge. Since $\Theta' > 0$ at band interiors, this implies that $\Theta(\mathbf{a}_{j+1}) - \Theta(\mathbf{b}_j) = \frac{\pi}{p}$, for each j. It follows that $\Theta(\mathbf{a}_0) - \Theta(\mathbf{b}_0) = \pi$. From (3.9) it follows that for $z > \mathbf{a}_0$ $\operatorname{Re}\Theta(z) = 0$. This proves all claimed statements. ❑

From the reflection principle, we get analytic extensions for Θ to $\mathbb{C} \setminus \mathsf{E}$.

3.2.13 Corollary. *The analytic extension of Θ through $\mathbb{C}_+ \cup (\mathbf{a}_j, \mathbf{b}_j) \cup \mathbb{C}_-$ obey*

$$\overline{\Theta(\overline{z})} = -\Theta(z) - 2\pi(1 - \frac{j}{p}).$$

3.2.14 Remark. Define on $\mathbb{C}_+$

$$L(z) = \operatorname{Im}\Theta(z).$$

Then

$$L(z) = -\log((a_1 \dots a_p)^{1/p}) + \int \log(|t - z|) d\nu(t).$$

In fact, one can show that this defines a positive harmonic function in $\mathbb{C}_+ \setminus \mathsf{E}$, that extends continuously $\mathbb{C}$ which is zero on E. From this one can connect it to two functions appearing in the literature. First of all L is the potential theoretic Green function of the domain $\overline{\mathbb{C}} \setminus \mathsf{E}$ with logarithmic pole at ∞ and ν is the equilibrium measure of the set E. Secondly, in spectral theory, L is called the Lyapunov exponent and the distribution function of ν is called the integrated density of states.

3.2.15 Lemma. *If $f : \mathbb{C}_+ \to \mathbb{C}$ is analytic with $\operatorname{Re} f' > 0$ on $\mathbb{C}_+$, then f is injective.*

Proof. For any $a, b \in \mathbb{C}_+$, $a \neq b$, by the mean value theorem

$$\operatorname{Re} \frac{f(a) - f(b)}{a - b} = \operatorname{Re} f'(a + t(b - a)) > 0, \quad t \in (0, 1).$$

So $f(a) \neq f(b)$. ❑

For any injective analytic map f on $\mathbb{C}_+$ let us denote $\Pi = f(\mathbb{C}_+)$. Clearly Π is connected and by the open mapping theorem, Π is open. Thus $f : \mathbb{C}_+ \to \Pi$ is a conformal map.

3.2.16 Lemma. *Let $f : \mathbb{C}_+ \to \mathbb{C}$ be analytic, injective and extends to a continuous map on the closure of $\mathbb{C}_+$ in $\overline{\mathbb{C}}$. Then $f(\partial\mathbb{C}_+) = \partial\Pi$.*

Proof. All toplogical notions are used in the topology of the Riemann sphere. Since f is continuous, we have $f(\overline{\mathbb{C}_+}) \subset \overline{f(\mathbb{C}_+)}$. Moreover, $f(\overline{\mathbb{C}_+})$ is compact as the continuous image of a compact set. In particular, it is closed. Thus,

$$\overline{\Pi} = \overline{f(\mathbb{C}_+)} \subset f(\overline{\mathbb{C}_+}) \subset \overline{f(\mathbb{C}_+)},$$

and hence $f(\overline{\mathbb{C}_+}) = \overline{\Pi}$.
Let $z_0 \in \mathbb{C}_+$ and $w_0 = f(z_0)$. Let $\delta > 0$ such that $\overline{B_\delta(z_0)} \subset \mathbb{C}_+$. The set $U = f(B_\delta(z_0))$ is open, so for $\epsilon > 0$ small enough, it contains $B_\epsilon(w_0)$. Since f is injective, it follows that for all $z \in \mathbb{C}_+ \setminus B_\delta(z_0)$, $|f(z) - w| \geq \epsilon$. By continuity, the same holds for z in the boundary of $\mathbb{C}_+$. Thus $f(\partial\mathbb{C}_+) \cap f(\mathbb{C}_+) = \emptyset$. Thus,

$$f(\partial\mathbb{C}_+) = f(\overline{\mathbb{C}_+}) \setminus f(\mathbb{C}_+) = \overline{\Pi} \setminus \Pi = \partial\Pi.$$

❑

Let

$$h_j = \operatorname{Im} \Theta(\lambda_j)$$

and

$$\Pi = \{z \in \mathbb{C} \mid -\pi < \operatorname{Re} z < 0\} \setminus \bigcup_{j=1}^{p-1} \left\{ -\pi + \frac{j}{p}\pi + it \mid 0 < t \leq h_j \right\}.$$

By Lemma 3.2.15, the function Θ is a conformal map. This map was first applied in spectral theory in the setting of continuum Schrödinger operators by V.A. Marchenko and I.V. Ostrovskii and thus bears the name Marchenko–Ostrovskii map.

3.2.17 Corollary. *The Marchenko-Ostrovskii map Θ is a conformal map from $\mathbb{C}_+$ to Π.*

3.3 Direct spectral theory of periodic Jacobi matrices

We will now investigate spectral properties if periodic Jacobi matrices.

3.3.1 Definition. e say that $z \in \mathbb{C}$ is a Dirichlet eigenvalue, if $p_{p-1}(z) = 0$. ◊

Let J_{p-1} be the truncation of J onto $\mathbb{C}^{p-1}$, that is

$$J_{p-1} = \begin{pmatrix} b_0 & a_1 & & & \\ a_1 & b_1 & a_2 & & \\ & a_2 & \ddots & \ddots & \\ & & \ddots & \ddots & a_{p-1} \\ & & & a_{p-1} & b_{p-2} \end{pmatrix} \tag{3.12}$$

3.3.2 Lemma. *Dirichlet eigenvalues are real and $x_0 \in \mathbb{R}$ is a Dirichlet eigenvalue, if and only if it is an eigenvalue of J_{p-1}.*

Proof. By Corollary 2.1.27, p_{p-1} has real and simple zeros. Let x_0 be a zero of p_{p-1}. Then, it holds that $p_{-1}(x_0) = 0, p_0(x_0) = 1$ and

$$\begin{aligned} x_0 p_0(x_0) &= b_0 p_0(x_0) + a_1 p_1(x_0), \\ x_0 p_j(x_0) &= a_{j+1} p_{j+1}(x_0) + b_j p_j(x_0) + a_j p_{j-1}(x_0), \quad 1 \le j \le p-3 \end{aligned}$$

and using that $p_{p-1}(x_0) = 0$

$$x_0 p_{p-2}(x_0) = b_{p-2} p_{p-2}(x_0) + a_{p-2} p_{j-3}(x_0).$$

That is, $(p_0(x_0), \ldots, p_{p-2}(x_0))^\intercal$ is an eigenvector of J_{p-1} to the eigenvalue x_0. Now let A be the set of Dirichlet eigenvalues and B the set of eigenvalues of J_{p-1}. Since $|A| = p-1$ and $|B| \le p-1$ and $A \subset B$, it follows that $A = B$. ❑

Recall that

$$m_+(z) = -\frac{\beta(z) - \sqrt{\Delta(z)^2 - 4}}{2a_p p^+_{p-1}(z)}, \tag{3.13}$$

where $\beta(z) = p^+_p(z) + a_p q^+_{p-1}(z)$ and $\Delta(z) = p^+_p(z) - a_p q^+_{p-1}(z)$. It is now clear that with the choice of the square root such that $\sqrt{\Delta(z)^2 - 4} > 0$ for $z > \mathbf{a}_0$, that $m_+(z)$ corresponds to the solution of (3.4) with a minus sign. For the other choice of the sign leads to a behavior $m(z) \sim z$ as $z \to \infty$. Hence we also have

$$-\frac{1}{a_p^2 m_-(z)} = \frac{\beta(z) + \sqrt{\Delta(z)^2 - 4}}{2a_p p^+_{p-1}(z)}. \tag{3.14}$$

3.3.3 Lemma. *If t_0 is a Dirichlet eigenvalue and $\Delta(t_0) = \pm 2$, then $\beta(t_0) = 0$.*

Proof. We claim that $p^+_p(t_0) = -a_p q^+_{p-1}(t_0) = \pm 1$, which clearly implies that $\beta(t_0) = 0$. Assume that $\Delta(t_0) = p^+_p(t_0) - a_p q^+_{p-1}(t_0) = \pm 2$. By the Wronskian identity we have $-1 = a_p p^+_p(t_0) q^+_{p-1}(t_0)$. Hence,

$$p^+_{p-1}(t_0)^2 \pm 2p^+_{p-1}(t_0) - 1 = 0,$$

implying that $p^+_{p-1}(t_0) = \pm 1$ and hence $-a_p q^+_{p-1}(t_0) = \pm 1$. ❑

3.3.4 Lemma. *If t_0 is a Dirichlet eigenvalue, then $|\beta(t_0)| = |\sqrt{\Delta(t_0)^2 - 4}|$.*

Proof. Again by the Wronskian identity, we have

$$\begin{aligned} \Delta(x_0)^2 - 4 = (p^+_p(x_0) - a_p q^+_{p-1}(x_0))^2 - 4 &= (p^+_p(x_0) - a_p q^+_{p-1}(x_0))^2 + 4p^+_p(x_0) a_p q^+_{p-1}(x_0) \\ &= (p^+_p(x_0) + a_p q^+_{p-1}(x_0))^2 = \beta(x_0)^2. \end{aligned}$$

❑

We can now fully characterize the spectrum of J_+. Let μ_+ be the measure in the integral representation of m_+. Let us write μ_+ into its Lebsgue decomposition with respect to Lebesgue measure, i.e., $d\mu_+(t) = w_+(t)dt + d\mu_s(t)$, where μ_s is singular with respect to Lebesgue measure.

3.3.5 Theorem. *The operator J_+ has essential spectrum E. On E, μ_+ is purely absolutely continuous with density*

$$\chi_{\mathsf{E}}(t)w_+(t) = \chi_{\mathsf{E}}(t)\frac{1}{\pi}\frac{\sqrt{4-\Delta(t)^2}}{a_p|p_{p-1}(t)|}dt \tag{3.15}$$

The discrete spectrum of J_+ corresponds to those Dirichlet eigenvalues which lie in open gaps (a_j, b_j) and for which

$$\beta(t_0) = -\sqrt{\Delta(t_0)^2-4}.$$

That is

$$d\mu_+(t) = \chi_{\mathsf{E}}(t)w_+(t)dt + \sum_{p_{p-1}(t)=0}\kappa_t\delta_t,$$

where $\kappa_t > 0$ if and only if t lies in an open gap and $\beta(t) = -\sqrt{\Delta(t)^2-4}$.

Proof. Note that $\operatorname{Im} m_+$ has a continuous extension to any interval of $\mathbb{R}$, which does not contain a Dirichlet eigenvalue. Thus, μ_+ cannot have a singular continuous part. By Corollary 1.4.3, the abolutely continuous part is supported on E and given by (3.15). By (1.4.4), the pure point part of μ_+ must be supported at the set of Dirichlet eigenvalues. If t_0 is a gap edge, then by Lemma 3.3.3, $\mu_+(\{t_0\}) = 0$. Likewise, if t_0 is a Dirichlet eigenvalue which is not a gap edge, then by Lemma 3.3.4, $\sqrt{\Delta(t_0)} = \pm\beta(t_0)$, and we see that $\sqrt{\Delta(t_0)} = \beta(t_0)$ corresponds to $\mu(\{t_0\}) = 0$ and $\sqrt{\Delta(t_0)} = -\beta(t_0)$ corresponds to $\mu_+(\{t_0\}) > 0$. ❑

Recall that

$$-\frac{1}{G_{-1,-1}(z)} = a_p^2\left(m_+(z) - \frac{1}{a_p^2 m_-(z)}\right). \tag{3.16}$$

Hence, by (3.13) and (3.14) we have

$$-\frac{1}{G_{-1,-1}(z)} = \frac{a_p^2\sqrt{\Delta(z)^2-4}}{a_p p_{p-1}^+(z)}.$$

Since, $G_{-1,-1}(z) \sim -\frac{1}{z}$ as $z \to \infty$ this implies that

$$G_{-1,-1}(z) = \frac{\prod_{j=1}^{p-1}(z-t_j)}{\sqrt{\prod_{j=0}^{p-1}(z-\mathbf{a}_j)(z-\mathbf{b}_j)}}. \tag{3.17}$$

Completely analogous to the proof of Proposition 3.2.9 one can show that

$$G_{-1,-1}(z) = \frac{-1}{\sqrt{(z-\mathbf{a}_0)(z-\mathbf{b}_0)}}e^{\int_{[\mathbf{b}_0,\mathbf{a}_0]\setminus\mathsf{E}}\frac{1}{t-z}\tilde{\xi}(t)dt}, \tag{3.18}$$

where $\tilde{\xi}(t) = \frac{1}{2}$ if $t \in (\mathbf{a}_j, t_j)$ and $\tilde{\xi}(t) = -\frac{1}{2}$ if $t \in (t_j, \mathbf{b}_j)$.
If $f : \mathbb{C}_+ \to \mathbb{C}$ is a function such that for $x \in \mathbb{R}$, $\lim_{\epsilon\to 0} f(x+i\epsilon)$ exists, in $\overline{\mathbb{C}}$, then we write

$$f(x+i0) := \lim_{\epsilon\to 0} f(x+i\epsilon).$$

3.3.6 Lemma. *For all $z \in \operatorname{int} E$ we have*

$$\frac{1}{a_0^2 \overline{m_-(x+i0)}} = m_+(x+i0). \tag{3.19}$$

Moreover, $G_{-1,-1}$ is purely imaginary on $\operatorname{int} E$

Proof. This follows immediately from the explict formulae for $m_\pm$ and from (3.17). ❑

For reasons that go beyond the scope of these lecture notes, the property (3.19) is called reflectionless property. We are now able to characterize the full spectral data, that allows us to recover m_- and m_+. Let $0 \le g \le p-1$ be the number of open gaps and let $\tilde{a}_j, \tilde{b}_j$, $0 \le j \le g$ be the gap edges that correspond to these open gaps. Likewise, let $\tilde{t}_j$ denote Dirichlet eigenvalues belonging to $[\tilde{a}_j, \tilde{b}_j]$. Moreover, for $1 \le j \le g$, we set

$$\varepsilon_j := \begin{cases} 1, & \tilde{t}_j \text{ is pole of } m_+, \\ -1, & \text{otherwise} \end{cases}.$$

We will see that the full spectral data is the set E and the collection of points $((\tilde{t}_j, \varepsilon_j)_{j=1}^g)$. Note again by the explicit formulae for $m_\pm$, if $\tilde{t}_j \in (\tilde{\mathbf{a}}_j, \tilde{\mathbf{b}}_j)$, then $\tilde{t}_j$ is either a pole of m_+ or a pole of $-m_-^{-1}$. However, there is a certain ambiguity, since at gap edges it is a pole of neither of these functions. Thus, to set $\varepsilon_j = -1$, in this case is somewhat arbitrary. It would be correct to identify in this case $(\tilde{t}_j, 1)$ and $(\tilde{t}_j, -1)$. With this identification, the set $\{(t, \varepsilon_j) \mid t \in [\tilde{\mathbf{a}}_j, \tilde{\mathbf{b}}_j], \varepsilon_j \in \{-1, 1\}\}$, can be identified with the torus $\mathbb{R}/\mathbb{Z}$.

3.3.7 Theorem. *For $z \in \mathbb{C}_+$ it holds*

$$a_p^2 m_+(z) = \frac{1}{2}\left(-\frac{1}{G_{-1,-1}(z)} - (z+\alpha) + \sum_{j=1}^{g} \frac{\varepsilon_j \sigma_j}{\tilde{t}_j - z}\right)$$

$$-\frac{1}{m_-(z)} = \frac{1}{2}\left(-\frac{1}{G_{-1,-1}(z)} + (z+\alpha) + \sum_{j=1}^{g} \frac{\varepsilon_j \sigma_j}{\tilde{t}_j - z}\right)$$

where

$$\sigma_k = \frac{\sqrt{\prod_{j=0}^g (\tilde{t}_k - \tilde{\mathbf{a}}_j)(\tilde{t}_k - \tilde{\mathbf{b}}_j)}}{\prod_{k \ne j} (\tilde{t}_k - \tilde{t}_j)}, \quad \text{and,} \quad \alpha = \frac{1}{2}\left(\mathbf{a}_0 + \mathbf{b}_0 + \sum_{j=1}^{g} (\tilde{\mathbf{a}}_j + \tilde{\mathbf{b}}_j - 2\tilde{t}_j)\right).$$

Proof. We have

$$-\frac{1}{G_{-1,-1}(z)} = a_p^2 m_+(z) - \frac{1}{m_-(z)}.$$

All involved functions are Herglotz functions with integral representations. The explicit formulae show that all measures in the integral representations are purely absolutely continuous on E and possibly mass points at $\tilde{t}_j$. Let us first discuss the absolutely continuous part. The reflectionless property (3.19) shows that, $a_p^2 \operatorname{Im} m_+(x+iO)$ and $\operatorname{Im} -\frac{1}{m_-(x+i0)}$ coincide on $\operatorname{int} \mathsf{E}$. Thus, the absolutely continuous part in the integral representations of both functions coincide. If $w_{-1,-1}$ and $w_\pm$ denote the densities of $-\frac{1}{G_{-1,-1}(z)}$, $a_0^2 m_+$, and $-m_-^{-1}$, then (3.16) shows that $w_- = w_+ = \frac{1}{2} w_{-1,-1}$. Now the measure of $-\frac{1}{G_{-1,-1}(z)}$ has point masses exactly at the Dirichlet eigenvalues belonging to open gaps. Since we have already seen that in this case it is either a pole of $a_0^2 m_+$ or of $-m_-^{-1}$, the point masses must coincide in this case. By Corollary 1.3.7, the point mass can be computed by

$$\sigma_k = \lim_{z \to \tilde{t}_k} -\frac{(\tilde{t}_k - z)}{G_{-1,-1}(z)} = \frac{\sqrt{\prod_{j=0}^{g} (\tilde{t}_k - \tilde{\mathbf{a}}_j)(\tilde{t}_k - \tilde{\mathbf{b}}_j)}}{\prod_{k \neq j} (\tilde{t}_k - \tilde{t}_j)}.$$

Note that $\sigma_k = 0$, if $\tilde{t}_k$ is a gap edge.
Consider the function

$$\frac{1}{2}\left(-\frac{1}{G_{-1,-1}}(z) + \sum_{j=1}^{g} \frac{\varepsilon_j \sigma_j}{\tilde{t}_j - z} \right)$$

By what we have argued, the measure in the integral representation of this function has the same absolutely continuous part as $a_0^2 m_+$. Also the mass point coincide, because if $\varepsilon_j = 1$ then the mass is $1/2(\sigma_j + \sigma_j) = \sigma_j$ and if $\varepsilon_j = -1$, then it is $1/2(\sigma_j - \sigma_j) = \sigma_j$. Thus, it remains to discuss the linear term $\alpha + \beta z$.
Expanding $-\frac{1}{G_{-1,-1}(z)}$ at ∞, using
Since $-\frac{1}{G_{-1,-1}(z)} \sim z$, $-m_-^{-1}(z) \sim z$ and $m_+(z) \sim -z^{-1}$ as $z \to \infty$, we see that z must be subtracted from $-\frac{1}{G_{-1,-1}(z)}$ in order to fit the behavior of $m_+(z)$. Finally, expanding $-\frac{1}{G_{-1,-1}(z)}$ at ∞ with the help of (3.18), we find that

$$-\frac{1}{G_{-1,-1}(z)} = z + \alpha + o(1).$$

Since $m_+(z) \sim -z^{-1}$ at ∞ we see that this term must be subtracted form $-\frac{1}{G_{-1,-1}(z)}$ to get $a_p^2 m_+(z)$. Likewise, due to (3.16) it must be added to $m_-(z)$. This finishes the proof. ❑