Trace Formulas and Inverse Spectral Theory for Finite Jacobi Operators

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Einleitung

Diese Arbeit untersucht folgende Problemstellung: welche Spektraldaten eines endlichen Jacobioperators reichen aus, um den Operator eindeutig zu rekonstruieren.

Für $f \in \ell^2(\mathbb{Z})$ ist der Jacobioperator H definiert durch

$$(Hf)(n) = a_n f(n+1) + a_{n-1} f(n-1) + b_n f(n),$$

wobei

$$a_n \in \mathbb{R}\backslash\{0\}, \quad b_n \in \mathbb{R}, \quad n \in \mathbb{Z}.$$

Durch Dirichlet Randbedingungen (i.e. $f(n_0) = 0, f(n_1) = 0$) an die Definition von $(Hf)(n_0+1)$ und $(Hf)(n_1-1)$ erhalten wir den endlichen Jacobioperator auf $\ell^2[n_0+1, n_1-1]$, der zu folgender reellen, tridiagonalen, symmetrischen Matrix gehört:

$$\begin{pmatrix} b_{n_0+1} & a_{n_0+1} & & & \\ a_{n_0+1} & b_{n_0+2} & a_{n_0+2} & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n_1-3} & b_{n_1-2} & a_{n_1-2} \\ & & & a_{n_1-2} & b_{n_1-1} \end{pmatrix}.$$

Jacobioperatoren tauchen in einer Vielzahl von Anwendungen auf. Man kann sie als das diskrete Analogon zu Sturm-Liouville-Operatoren auffassen und ihre Behandlung weist viele Ähnlichkeiten mit der Theorie für Sturm-Liouville-Operatoren auf. Spektraltheorie und Inverse Spektraltheorie für Jacobioperatoren spielen eine große Rolle bei Untersuchungen von vollständig integrablen nichtlinearen Gittern, wie beispielsweise dem Toda Gitter ([14]).

Unser Ausgangspunkt war eine Arbeit von F. Gesztesy and B. Simon, [3]. Wir erweitern einige ihrer Resultate, zum Teil indem wir die Theorie, die von G. Teschl in [12] für Jacobioperatoren entwickelt wird, auf den endlichdimensionalen Fall übertragen.

Wir beweisen, dass N Eigenwerte einer $N \times N$ Jacobi Matrix J zusammen mit $N-1$ Eigenwerten von zwei Teilmatrizen die Jacobi Matrix eindeutig bestimmen. Die Teilmatrizen erhalten wir durch Streichen der n-ten Zeile und Spalte von J. Hinreichende und notwendige Bedingungen an die Eigenwerte werden gegeben, aus denen die Existenz einer zugehörigen Jacobi Matrix folgt. In der Physik beschreibt dieses Modell eine Kette von N Massenpunkten mit fixierten Enden, die durch Federn miteinander verbunden sind (siehe [12], Sektion 1.5). Aus den Eigenfrequenzen dieses Systems und des Systems, in dem ein

weiterer innerer Punkt festgehalten wird, können die Massen und die Federkonstanten des ursprünglichen Systems eindeutig rekonstruiert werden.

Die Koeffizienten a^2, b eines endlichen Jacobioperators können explizit durch die Spektraldaten angegeben werden, analog wie in [12] für reflektionslose Jacobioperatoren.

Kapitel 1 bis Kapitel 4 behandeln direkte und inverse Spektraltheorie für beschränkte Jacobioperatoren, um sie dann in Kapitel 5 auf den endlichdimensionalen Fall anzuwenden.

Kapitel 1 gibt eine Einführung in die Theorie der beschränkten Jacobioperatoren. Eigenschaften von Lösungen der Jacobi Differenzengleichung, Eigenschaften der Wronskideterminante und der Green Funktion werden untersucht. Jacobioperatoren mit Randwertbedingungen werden definiert.

Kapitel 2 stellt die Fundamente der Spektraltheorie für Jacobioperatoren vor. Wir studieren Weyl-m-Funktionen und ihre asymptotische Entwicklung, identifizieren diese als Herglotz Funktionen und zeigen den Zusammenhang zum Momentenproblem auf. Das Momentenproblem wird diskutiert, wie auch asymptotische Entwicklungen von Green Funktionen.

Kapitel 3 präsentiert eine einfache rekursive Methode, die Koeffizienten a^2, b zu rekonstruieren, wenn die Weylmatrix für ein fixes n bekannt ist.

Kapitel 4 führt die ξ-Funktion und Spurformeln für Jacobioperatoren ein.

Kapitel 5 sammelt nun alle Resultate für endliche Jacobioperatoren. Die explizite Darstellung der ξ-Funktion ist der Schlüssel zur Berechnung der Spurformeln. Wir präsentieren die Lösung des Inversen Spektralproblems, die in [3] gegeben wird, und unsere Erweiterung.

Im Appendix werden die benötigten Resultate aus der Theorie für Herglotz Funktionen zusammengefaßt, um in der Arbeit darauf verweisen zu können.

Danksagung

In vielen Teilen dieser Arbeit folgte ich der Monographie [12] meines Diplomarbeitsbetreuers, Prof. Gerald Teschl. Ich möchte mich bei ihm bedanken für seine hervorragende Betreuung, für das Thema meiner Diplomarbeit und den Zeitaufwand, den ihn seine Hilfestellungen und Erklärungen gekostet haben.

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Contents

Introduction

The goal of this thesis is to determine spectral data of finite Jacobi operators which are necessary and sufficient to reconstruct the operator uniquely.

For $f \in \ell^2(\mathbb{Z})$, the Jacobi operator H is defined by

$$(Hf)(n) = a_n f(n+1) + a_{n-1} f(n-1) + b_n f(n),$$

where

$$a_n \in \mathbb{R}\backslash\{0\}, \quad b_n \in \mathbb{R}, \quad n \in \mathbb{Z}.$$

If we impose Dirichlet boundary conditions (i.e. $f(n_0) = 0, f(n_1) = 0$) on the definition of $(Hf)(n_0+1)$ and $(Hf)(n_1-1)$, we obtain a finite dimensional Jacobi operator on $\ell^2[n_0+1, n_1-1]$ associated to the real tridiagonal symmetric matrix

$$\begin{pmatrix} b_{n_0+1} & a_{n_0+1} & & & \\ a_{n_0+1} & b_{n_0+2} & a_{n_0+2} & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n_1-3} & b_{n_1-2} & a_{n_1-2} \\ & & & a_{n_1-2} & b_{n_1-1} \end{pmatrix}.$$

Jacobi operators appear in a variety of applications. They can be viewed as the discrete analogue of Sturm-Liouville operators and their investigation has many similarities with Sturm-Liouville theory. Spectral and inverse spectral theory for Jacobi operators play a fundamental role in the investigation of completely integrable nonlinear lattices, in particular the Toda lattice ([14]).

Our work was motivated by the paper of F. Gesztesy and B. Simon, [3], and we extended some of their results, partially by applying the theory given in the monograph [12] of G. Teschl to the finite dimensional case.

We prove that N eigenvalues of a $N \times N$ Jacobi matrix J together with $N-1$ eigenvalues of two submatrices of J which we obtain by omitting the n-th line and column uniquely determine J. Necessary and sufficient restrictions on the sets of eigenvalues are given under which one obtains existence of J. From a physical point of view such a model describes a chain of N particles coupled via springs and fixed at both end points (see [12], Section 1.5). Determining the eigenfrequencies of this system and the one obtained by keeping one particle fixed, one can uniquely reconstruct the masses and spring constants.

The coefficients a^2, b of a finite Jacobi operator can be expressed explicitly in terms of the spectral data, in analogy to reflectionless Jacobi operators considered in [12].

Chapter 1 to Chapter 4 deal with spectral and inverse spectral theory for bounded Jacobi operators to apply them in Chapter 5 to the finite case.

Chapter 1 gives an introduction to the theory of bounded Jacobi operators. Properties of solutions of the Jacobi difference equation, properties of the Wronskian and the Green function are prepared. Jacobi operators with boundary conditions are defined.

Chapter 2 establishes the pillars of spectral theory for Jacobi operators. We study Weyl m-functions and their asymptotic expansions, identify them as Herglotz functions and show their connection with the Moment problem. The Moment problem is discussed, as well as asymptotic expansions of the Green function.

Chapter 3 presents a simple recursive method of reconstructing the sequences a^2, b, if the Weyl matrix is known for one fixed n.

Chapter 4 introduces to the ξ function and to trace formulas for Jacobi operators.

Chapter 5 collects then all our results for finite Jacobi operators. The explicit computation of the ξ function is the main tool to derive the trace formulas. We present the solution of the inverse spectral problem given in [3] and our extension.

The Appendix compiles the results from the theory of Herglotz functions we apply and is included for easy reference.

Acknowledgments

I followed to a great extend the monograph [12] of my master thesis advisor, Prof. Gerald Teschl. I thank him very much for his excellent advice, for the topic of this thesis and the time he devoted to this work.

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Chapter 1

Jacobi Operators

1.1 Preliminaries

We start with some notation. Denote by $\ell(\mathbb{Z},\mathbb{R})$ the set of real-valued sequences $(f(n))_{n\in\mathbb{Z}}$, by $\ell(\mathbb{Z},\mathbb{C}) =: \ell(\mathbb{Z})$ the set of complex-valued sequences. For $I \subseteq \mathbb{Z}$, $\ell(I) := \{(f(n))_{n\in I}\}$.

Definition 1.1.

$$\begin{aligned}\ell^p(\mathbb{Z}) &:= \{f \in \ell(\mathbb{Z}) |\, \|f\|_p = \sum_{n=-\infty}^{\infty} |f(n)|^p < \infty\}, \quad 1 \le p < \infty,\\ \ell^\infty(\mathbb{Z}) &:= \{f \in \ell(\mathbb{Z}) |\, \|f\|_\infty = \sup_{n\in\mathbb{Z}} |f(n)| < \infty\}.\end{aligned}$$

Let $a, b \in \ell(\mathbb{Z},\mathbb{R})$ satisfy

$$a_n \in \mathbb{R}\backslash\{0\},\ b_n \in \mathbb{R}.$$

We introduce the **second order, symmetric difference equation**

$$\begin{aligned}\tau: \quad \ell(\mathbb{Z}) &\to \ell(\mathbb{Z})\\ f(n) &\mapsto a_n f(n+1) + a_{n-1} f(n-1) + b_n f(n).\end{aligned} \tag{1.1}$$

Associated with τ is the tridiagonal matrix

$$\begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ & a_{n-2} & b_{n-1} & a_{n-1} & & & \\ & & a_{n-1} & b_n & a_n & & \\ & & & a_n & b_{n+1} & a_{n+1} & \\ & & & & \ddots & \ddots & \ddots \end{pmatrix}. \tag{1.2}$$

We consider the corresponding eigenvalue problem which is referred to as **Jacobi difference equation**

$$\tau u = zu, \quad u \in \ell(\mathbb{Z}), \quad z \in \mathbb{C}, \tag{1.3}$$

$$a_n u(n+1) + a_{n-1} u(n-1) + b_n u(n) = zu(n), \quad \forall n \in \mathbb{Z}. \tag{1.4}$$

The appropriate setting for this eigenvalue problem is the Hilbert space $\ell^2(\mathbb{Z})$, as we will consider it in the next section. But first we study the space of solutions and introduce fundamental solutions.

Since all $a_n \neq 0$, we see from (1.4) that a solution u of $\tau u = zu$ is uniquely determined by the values $u(n_0)$ and $u(n_0+1)$ at two consecutive points n_0, n_0+1. Thus we have exactly two linearly independent solutions. We introduce the following **fundamental solutions** c, $s \in \ell(\mathbb{Z})$

$$\tau c(z,.,n_0) = zc(z,.,n_0), \qquad \tau s(z,.,n_0) = zs(z,.,n_0), \tag{1.5}$$

fulfilling the **initial conditions**

$$\begin{aligned} c(z,n_0,n_0) &= 1, & c(z,n_0+1,n_0) &= 0, \\ s(z,n_0,n_0) &= 0, & s(z,n_0+1,n_0) &= 1. \end{aligned} \tag{1.6}$$

Now we can write any solution u as a linear combination of these two solutions

$$u(n) = u(n_0)c(z,n,n_0) + u(n_0+1)s(z,n,n_0).$$

Our next task will be to treat expansions of $c(z,n,n_0)$ and $s(z,n,n_0)$. Let J_{n_1,n_2} be the **Jacobi Matrix**

$$J_{n_1,n_2} = \begin{pmatrix} b_{n_1+1} & a_{n_1+1} & & & \\ a_{n_1+1} & b_{n_1+2} & a_{n_1+2} & & \\ & \ddots & \ddots & \ddots & \\ & & a_{n_2-3} & b_{n_2-2} & a_{n_2-2} \\ & & & a_{n_2-2} & b_{n_2-1} \end{pmatrix}. \tag{1.7}$$

Set $n_0 = 0$ for simplicity. For $n > 0$, $s(z,n,0)$ is a polynomial in z of degree $n-1$. By (1.6), $s(z,0,0) = 0$, $s(z,1,0) = 1$, and we see by induction on (1.4),

$$a_n s(z,n+1,0) = (z-b_n)s(z,n,0) - a_{n-1}s(z,n-1,0), \tag{1.8}$$

that $s(z,n+1,0)$ is a polynomial of degree n. Again, inductively we know the leading coefficient

$$s(z,n+1,0) = \frac{1}{a_1 \dots a_n} z^n + \cdots \tag{1.9}$$

since $s(z,1,0) = 1$,

$$s(z,2,0) = \frac{1}{a_1}\big((z-b_1)s(z,1,0) - a_0 s(z,0,0)\big) = \frac{z-b_1}{a_1},$$

and we use induction on (1.8).

Proposition 1.2. ([1], p. 542). *The following expansion holds for $s(z,n,n_0)$, $n > n_0$,*

$$s(z,n,n_0) = \frac{\det(z - J_{n_0,n})}{\prod_{j=n_0+1}^{n-1} a_j}. \tag{1.10}$$

Proof. By (1.9), $\big(\prod_{j=n_0+1}^{n-1} a_j\big)s(z,n,n_0)$ and $\det(z - J_{n_0,n})$ are monic polynomials of degree $(n-1)-n_0$. We have to show that they have the same zeros and multiplicities. But if z_0 is a zero of $s(.,n,n_0)$, then

$$\big(s(z_0,n_0+1,n_0),\dots,s(z_0,n-1,n_0)\big)$$

is an eigenvector of (1.7) corresponding to the eigenvalue z_0. The converse statement is also true since the eigenvalue condition is the defining equation for $s(z_0, n, n_0)$. Moreover, the eigenvalues are simple by Remark 1.15 below, so the multiplicities are all one. □

By the same reasoning,

$$c(z, n_0 - n, n_0) = \frac{\det(z - J_{n_0-n,n_0+1})}{\prod_{j=n_0-n}^{n_0-1} a_j} \tag{1.11}$$

is a polynomial of degree n. The fundamental solutions $c(z)$ and $s(z)$ are related by

$$c(z, n_0, n_1) = \frac{a_{n_1}}{a_{n_0}}\, s(z, n_1 + 1, n_0), \tag{1.12}$$

further considerations can be found in [12].

As a last preparation we introduce the (modified) **Wronskian** for two sequences u, v

$$W_n(u, v) = a_n\big(u(n)v(n+1) - v(n)u(n+1)\big). \tag{1.13}$$

Proposition 1.3. *For f, $g \in \ell(\mathbb{Z})$,*

$$\sum_{j=m}^{n} \Big(f(\tau g) - (\tau f)g\Big)(j) = W_n(f, g) - W_{m-1}(f, g). \tag{1.14}$$

This formula is referred to as **Green's formula**.

Proof. By simple calculation. In the case of two summands,

$$\begin{aligned} \big(f(\tau g) - (\tau f)g\big)(j) &= f(j)\big(a_j g(j+1) + a_{j-1} g(j-1) + b_j g(j)\big) \\ &\quad - \big(a_j f(j+1) + a_{j-1} f(j-1) + b_j f(j)\big) g(j) \end{aligned}$$

$$\begin{aligned} \big(f(\tau g) - (\tau f)g\big)(j+1) &= f(j+1)\big(a_{j+1} g(j+2) + a_j g(j) + b_{j+1} g(j+1)\big) \\ &\quad - \big(a_{j+1} f(j+2) + a_j f(j) + b_{j+1} f(j+1)\big) g(j+1). \end{aligned}$$

If we follow the cancellations, just $W_{j+1}(f, g) - W_{j-1}(f, g)$ survives. □

Remark 1.4. For any two solutions of the Jacobi difference equation $\tau u = zu$, (1.3), W is constant (i.e. W is independent of n) since (1.14) becomes

$$\sum_{j=m}^{n} \Big(f(\tau g) - (\tau f)g\Big)(j) = \sum_{j=m}^{n} \Big(fzg - zfg\Big)(j) = 0$$

and thus

$$W_n(f, g) = W_{m-1}(f, g).$$

The Wronskian also indicates linear independence of solutions.

Proposition 1.5. *Let u, v be solutions of $\tau f = zf$, then*

$$W_n(u, v) \neq 0 \quad \Leftrightarrow \quad u, v \text{ are lineary independent.} \tag{1.15}$$

1.2 Jacobi Operators

We will study operators on the Hilbert space $\ell^2(\mathbb{Z})$ associated with the symmetric difference equation (1.1). For f, $g \in \ell^2(\mathbb{Z})$, the scalar product and norm are given by

$$\langle f, g\rangle = \sum_{n\in\mathbb{Z}} f(n)g(n), \quad \|f\| = \sqrt{\langle f, f\rangle}.$$

For simplicity we will assume from now on that a, b are bounded sequences.

Hypothesis 1.6. Suppose

$$a, b \in \ell^\infty(\mathbb{Z}, \mathbb{R}), \qquad a_n \neq 0. \tag{1.16}$$

Definition 1.7. Associated with a, b is the **Jacobi operator** H

$$\begin{aligned} H: \quad \ell^2(\mathbb{Z}) &\to \ell^2(\mathbb{Z}) \\ f &\mapsto \tau f, \end{aligned}$$

where τ has been defined in (1.1)

$$\tau f(n) = a_n f(n+1) + a_{n-1} f(n-1) + b_n f(n), \quad \forall n \in \mathbb{Z}. \tag{1.17}$$

Remark 1.8. If we drop the assumption $a_n \neq 0$ for a fixed n in Hypothesis 1.6, H can be decomposed into the direct sum of two operators acting on $\ell^2(-\infty, n] \oplus \ell^2[n+1, \infty)$ (see [12]). Hence the analysis of H in the case $a_n = 0$ can be reduced to the analysis of restrictions of H. In addition, [12] (Lemma 1.6) shows that the case $a_n \neq 0$ for n fixed reduces to the case $a_n > 0$ or $a_n < 0$.

In the next theorems we collect some results from operator theory on Hilbert spaces. Let δ_n denote the standard basis of $\ell(\mathbb{Z})$

$$\delta_n(m) = \delta_{m,n} = \begin{cases} 0 & m \neq n \\ 1 & m = n. \end{cases}$$

Theorem 1.9. *Assume Hypothesis 1.6. Then H is a bounded self-adjoint operator. a, b bounded is equivalent to H bounded since $\|a\|_\infty \leq \|H\|$, $\|b\|_\infty \leq \|H\|$ and*

$$\|H\| \leq 2\|a\|_\infty + \|b\|_\infty, \tag{1.18}$$

where $\|H\|$ denotes the operator norm of H and $\|a\|_\infty = sup_n(|a_n|)$.

Proof. Clearly,

$$\lim_{n\to\pm\infty} W_n(f, g) = 0 \quad \text{for } f,\, g \in \ell^2(\mathbb{Z}). \tag{1.19}$$

Green's formula (1.14)

$$\sum_{j=m}^{n} \Big(f(\tau g) - (\tau f)g\Big)(j) = W_n(f, g) - W_{m-1}(f, g)$$

together with (1.19) shows that H is self-adjoint, so

$$\langle f, Hg\rangle = \langle Hf, g\rangle, \quad f, g \in \ell^2(\mathbb{Z}).$$

The second statement follows from $a_n^2 + a_{n-1}^2 + b_n^2 = \|H\delta_n\|^2 \leq \|H\|^2$ and $|\langle f, Hf\rangle| \leq (2\|a\|_\infty + \|b\|_\infty)\|f\|^2$. □

Theorem 1.10. *If H is a bounded self-adjoint operator on a Hilbert space, all eigenvalues of H are real and two eigenvectors of H corresponding to distinct eigenvalues are orthogonal.*

Proof. If $Hf = zf$ and $f \neq 0$, then

$$z\langle f, f\rangle = \langle Hf, f\rangle = \langle f, Hf\rangle = \langle f, zf\rangle = \overline{z}\langle f, f\rangle$$

and hence $z \in \mathbb{R}$. Suppose

$$Hf = zf, \quad Hf' = z'f', \quad z \neq z',$$

then

$$z\langle f, f'\rangle = \langle Hf, f'\rangle = \langle f, Hf'\rangle = \langle f, z'f'\rangle = \overline{z'}\langle f, f'\rangle,$$

so $\langle f, f'\rangle = 0$ and f, f' are orthogonal. □

The **spectrum** $\sigma(H)$ of H is defined to be the set of those $z \in \mathbb{C}$ where $(H - z\mathbb{I})^{-1}$ does not exist as a bounded operator on $\ell^2 \to \ell^2$.

Theorem 1.11. *The spectrum of a bounded operator is a nonempty compact subset of $\mathbb{C}$. If H is also self-adjoint, then the spectrum of H lies in the segment $[-\|H\|, \|H\|]$.*

Remark 1.12. A proof can be found in [8] or in any book on functional analysis. We even know that the spectrum $\sigma(H)$ of a bounded operator lies in the disk of radius $\|H\|$. If $|\lambda| > \|H\|$, then $H - \lambda\mathbb{I}$ has an inverse operator given by the series

$$(H - \lambda\mathbb{I})^{-1} = -\sum_{k=0}^{\infty} \lambda^{-k-1} H^k.$$

Therefore, $\sigma(H)$ is contained in the disk $|\lambda| \leq \|H\|$.

For Jacobi operators we know even more:

Lemma 1.13. ([12]). *Let*

$$c_{\pm}(n) = b_n \pm (|a_n| + |a_{n-1}|).$$

Then

$$\sigma(H) \subseteq [\inf_{n\in\mathbb{Z}} c_-(n), \sup_{n\in\mathbb{Z}} c_+(n)].$$

Proof. First we show that H is bounded from above by $\sup c_+$.

$$\begin{aligned}\langle f, Hf\rangle &= \sum_{n\in\mathbb{Z}} f(n)\Big(a_n f(n+1) + a_{n-1} f(n-1) + b_n f(n)\Big) \\ &= \sum_{n\in\mathbb{Z}} \Big(- a_n |f(n+1) - f(n)|^2 + (a_{n-1} + a_n + b_n)|f(n)|^2\Big),\end{aligned}$$

this equation follows from routine calculation. Write down three consecutive summands of the last sum and follow the cancellations.

By Remark 1.8 (cf. [12], Lemma 1.6), we can first choose $a_n > 0$ to obtain

$$\langle f, Hf\rangle \leq \sup_{n\in\mathbb{Z}} c_+(n)\, \|f\|^2$$

and if we let $a_n < 0$, we see that H is bounded from below by $\inf c_-$

$$\langle f, Hf\rangle \geq \inf_{n\in\mathbb{Z}} c_-(n)\,\|f\|^2.$$

□

One of the most important objects in spectral theory is the **resolvent** of H, $(H - z\mathbb{I})^{-1} =: (H - z)^{-1}$, where $z \in \rho(H) := \mathbb{C}\backslash\sigma(H)$ and $\rho(H)$ denotes the **resolvent set** of H.

Definition 1.14. The matrix elements of $(H-z)^{-1}$ are called **Green function**

$$G(z, m, n) = \langle \delta_m, (H - z)^{-1}\delta_n\rangle, \quad z \in \rho(H). \tag{1.20}$$

The symmetry of H implies that

$$G(z, m, n) = G(z, n, m) \tag{1.21}$$

and by definition $G(z, m, n)$ is the matrix of the resolvent

$$(H - z)\,G(z, ., n) = \delta_n(.). \tag{1.22}$$

We will now construct solutions $u_+(z)$ and $u_-(z)$ of the Jacobi difference equation (1.3) which are square summable near $+\infty$ respectively $-\infty$. Set

$$u(z, .) = (H - z)^{-1}\delta_0(.) = G(z, ., 0), \quad z \in \rho(H). \tag{1.23}$$

$u(z, .) \in \ell^2(\mathbb{Z})$ by construction, since $(H - z)^{-1}$ is bounded for $z \in \rho(H)$. But $u(z, .)$ fulfills the Jacobi difference equation (1.3) only for $n > 0$ and $n < 0$, since

$$(H - z)u(z, n) = \delta_0(n) = \begin{cases} 0 & n \neq 0 \\ 1 & n = 0. \end{cases} \quad \Leftrightarrow \quad (Hu)(z, n) = zu(z, n)$$

If we take $u(z, -2)$ and $u(z, -1)$ as initial conditions we obtain a solution $u_-(z, n)$ of $\tau u = zu$ on the whole of $\ell(\mathbb{Z})$. By (1.4),

$$u_-(z, 0) = \frac{1}{a_{-1}}\big((z - b_{-1})u(z, -1) - a_{-2}u(z, -2)\big)$$

and so on. $u_-(z, n)$ coincides with $u(z, n)$ for $n < 0$, so it is ℓ^2 near $-\infty$ as desired. A solution $u_+(z, n)$ being ℓ^2 near $+\infty$ is constructed in analogy.

Remark 1.15. The solutions $u_\pm(z)$ are unique up to constant multiples since the Wronskian of two such solutions vanishes if we evaluate it at $\pm\infty$. This implies that the point spectrum (i.e. the set of eigenvalues) of H and $H^\beta_{\pm,n_0}$ is always simple (cf. Section 1.3 for the definition of $H^\beta_{\pm,n_0}$).

With this solutions we get an explicit formula for $G(z, m, n)$.

Proposition 1.16.

$$G(z, m, n) = \frac{1}{W(u_-(z), u_+(z))} \begin{cases} u_+(z, n)u_-(z, m) & \text{for } m \leq n \\ u_+(z, m)u_-(z, n) & \text{for } n \leq m. \end{cases} \tag{1.24}$$

Proof. We have to show that $G(z,m,n)$ satisfies (1.22)

$$(H-z)\,G(z,.,n) = \delta_n(.).$$

The m,n element is

$$\Big((H-z)\,G(z,.,n)\Big)_{m,n} = \sum_k (H_{m,k} - z\delta_{m,k})\,G(z,k,n) =$$

$$= a_{m-1}\,G(z,m-1,n) + (b_m - z)\,G(z,m,n) + a_m\,G(z,m+1,n).$$

Now we have to hunt down the different cases: if $m = n$

$$\begin{aligned} = \quad & \frac{1}{W}(a_{n-1}u_+(z,n)u_-(z,n-1) \\ & +(b_n - z)u_+(z,n)u_-(z,n) + a_n u_+(z,n+1)u_-(z,n)). \end{aligned} \tag{1.25}$$

By (1.4) we obtain for $u_+(z)$

$$(b_n - z)u_+(z,n) + a_n u_+(z,n+1) = -a_{n-1}u_+(z,n-1)$$

and (1.25) becomes

$$= \frac{1}{W}(a_{n-1}u_+(z,n)u_-(z,n-1) - a_{n-1}u_+(z,n-1)u_-(z,n)) = 1,$$

the last equation being the definition of the Wronskian (1.13). The other case is similar, one just uses relation (1.4). □

We introduce the following abbreviations

$$g(z,n) = G(z,n,n) = \frac{u_+(z,n)u_-(z,n)}{W(u_-(z),u_+(z))}, \tag{1.26}$$

$$\begin{aligned} h(z,n) &= 2a_n G(z,n,n+1) - 1 \\ &= \frac{a_n\big(u_+(z,n)u_-(z,n+1) + u_+(z,n+1)u_-(z,n)\big)}{W(u_-(z),u_+(z))}. \end{aligned} \tag{1.27}$$

1.3 Jacobi Operators with Boundary Conditions

We will consider finite and semi-infinite matrices associated with H which we obtain by restricting H to intervals and imposing boundary conditions at the endpoints. We will adopt the notation given in [12].

First we define restrictions H_{-,n_0} and H_{+,n_0} of the Jacobi operator H to the subspaces $\ell^2(-\infty, n_0-1]$ and $\ell^2[n_0+1,\infty)$. The operators $H_{\pm,n_0}$ can be thought of as imposing the boundary condition $f(n_0) = 0$ on the definition of $(Hf)(n_0 \pm 1)$. This case, $f(n_0) = 0$, will be referred to as **Dirichlet boundary condition** at n_0.

Definition 1.17.

$$(H_{+,n_0}f)(n) = \begin{cases} a_{n_0+1}f(n_0+2) + b_{n_0+1}f(n_0+1) & n = n_0+1 \\ (Hf)(n) & n > n_0+1 \end{cases}$$

$$(H_{-,n_0}f)(n) = \begin{cases} a_{n_0-2}f(n_0-2) + b_{n_0-1}f(n_0-1) & n = n_0-1 \\ (Hf)(n) & n < n_0-1. \end{cases}$$

For $m, n > n_0$ ($< n_0$), the corresponding Green functions are

$$G_{\pm,n_0}(z,m,n) = \langle \delta_m, (H_{\pm,n_0} - z)^{-1}\delta_n \rangle, \quad z \in \rho(H_{\pm,n_0}).$$

Their explicit formulas read in analogy to (1.24)

$$G_{+,n_0}(z,m,n) = \frac{1}{W(s(z),u_+(z))} \begin{cases} s(z,n,n_0)u_+(z,m) & \text{for } m \geq n \\ s(z,m,n_0)u_+(z,n) & \text{for } n \geq m \end{cases} \tag{1.28}$$

$$G_{-,n_0}(z,m,n) = \frac{-1}{W(s(z),u_-(z))} \begin{cases} s(z,n,n_0)u_-(z,m) & \text{for } m \leq n \\ s(z,m,n_0)u_-(z,n) & \text{for } n \leq m. \end{cases} \tag{1.29}$$

$s(z,.,n_0)$ is the fundamental solution of $\tau u = zu$ satisfying the Dirichlet boundary condition $s(z,n_0,n_0) = 0$ (cf. (1.6)). To show existence of $u_\pm(z,.)$ for $z \in \rho(H_{\pm,n_0})$ we use $(H_{\pm,n_0} - z)^{-1}$.

We can also consider half line operators $H^\beta_{\pm,n_0}$ on $\ell^2(n_0, \pm\infty)$ associated with the general boundary condition

$$f(n_0+1) + \beta f(n_0) = 0, \quad \beta \in \mathbb{R} \cup \{\infty\} \tag{1.30}$$

at n_0 rather than only the Dirichlet boundary condition $f(n_0) = 0$.

Definition 1.18.

$$H^0_{+,n_0} = H_{+,n_0+1}, \qquad H^\beta_{+,n_0} = H_{+,n_0} - a_{n_0}\beta^{-1}\langle \delta_{n_0+1}, . \rangle \delta_{n_0+1}, \quad \beta \neq 0,$$

$$H^\infty_{-,n_0} = H_{-,n_0}, \qquad H^\beta_{-,n_0} = H_{-,n_0+1} - a_{n_0}\beta\langle \delta_{n_0}, . \rangle \delta_{n_0}, \quad \beta \neq \infty.$$

The operators $H_{\pm,n_0}$ and $H^\beta_{\pm,n_0}$ are considered in detail in [12], [13].

Last, we define finite restrictions H_{n_1,n_2} to the subspaces $\ell^2(n_1,n_2)$ by imposing Dirichlet boundary conditions at the endpoints ($f(n_1) = 0$, $f(n_2) = 0$).

Definition 1.19.

$$(H_{n_1,n_2}f)(n) = \begin{cases} a_{n_1+1}f(n_1+2) + b_{n_1+1}f(n_1+1) & n = n_1+1 \\ (Hf)(n) & n_1+1 < n < n_2-1 \\ a_{n_2-2}f(n_2-2) + b_{n_2-1}f(n_2-1) & n = n_2-1. \end{cases}$$

The operator H_{n_1,n_2} is clearly associated with the Jacobi matrix J_{n_1,n_2} (cf. (1.7)). We will study H_{n_1,n_2} in Chapter 5.

All operators we defined here are bounded and self-adjoint, since they are restrictions of such operators.

Chapter 2

Spectral Theory for Jacobi Operators

2.1 Weyl m-Functions

Weyl m-functions are the quantities analogous to the Green function $g(z,n) = \langle \delta_n, (H-z)^{-1}\delta_n\rangle$ for the half line operators $H_{\pm,n_0}$ (cf. Definition 1.17).

Definition 2.1. For $z \in \rho(H_{\pm,n_0})$,

$$\begin{aligned} m_+(z,n_0) &= \langle \delta_{n_0+1}, (H_{+,n_0}-z)^{-1}\delta_{n_0+1}\rangle = G_{+,n_0}(z,n_0+1,n_0+1), \\ m_-(z,n_0) &= \langle \delta_{n_0-1}, (H_{-,n_0}-z)^{-1}\delta_{n_0-1}\rangle = G_{-,n_0}(z,n_0-1,n_0-1). \end{aligned}$$

The base point n_0 is of no importance and we will only consider $m_\pm(z) := m_\pm(z,0)$ most of the time. As in the previous chapter, $u_\pm(z)$ denote the solutions of (1.3) in $\ell(\mathbb{Z})$ which are square summable near $\pm\infty$. We also have a more explicit form of $m_\pm(z,n_0)$.

Proposition 2.2.

$$m_+(z,n_0) = -\frac{u_+(z,n_0+1)}{a_{n_0}u_+(z,n_0)}, \qquad m_-(z,n_0) = -\frac{u_-(z,n_0-1)}{a_{n_0-1}u_-(z,n_0)}. \tag{2.1}$$

Proof. (1.28) becomes

$$\begin{aligned} m_+(z,n_0) &= G_{+,n_0}(z,n_0+1,n_0+1) \\ &= \frac{s(z,n_0+1,n_0)u_+(z,n_0+1)}{a_{n_0}\big(s(z,n_0,n_0)u_+(z,n_0+1) - s(z,n_0+1,n_0)u_+(z,n_0)\big)} \end{aligned}$$

and the result follows since $s(z,n_0,n_0) = 0$ and $s(z,n_0+1,n_0) = 1$ (cf. (1.6)). Compute $m_-(z,n_0)$ from (1.29). □

Remark 2.3. All results for $m_-(z)$ can be obtained from the corresponding results for $m_+(z)$ using **reflection** at n_0. [12] (Lemma 1.7) shows how information obtained near one endpoint can be transformed into information near the other.

$m_\pm(z,n)$ satisfy the following recurrence relations

$$a_n^2 m_+(z,n) + \frac{1}{m_+(z,n-1)} = b_n - z \tag{2.2}$$

and

$$a_{n-1}^2 m_-(z,n) + \frac{1}{m_-(z,n+1)} = b_n - z \tag{2.3}$$

since we know by (2.1)

$$a_n^2 m_+(z,n) + \frac{1}{m_+(z,n-1)} = -a_n^2 \frac{u_+(z,n+1)}{a_n u_+(z,n)} - \frac{a_{n-1} u_+(z,n-1)}{u_+(z,n)} = b_n - z,$$

the last equality follows from (1.4).

Furthermore, we can regain $g(z,n) = G(z,n,n)$ from $m_\pm(z)$.

Lemma 2.4. ([3]).

$$\begin{aligned} g(z,n) &= -\frac{1}{a_n^2 m_+(z,n) + a_{n-1}^2 m_-(z,n) + z - b_n} && (2.4)\\ &= -\frac{1}{a_{n-1}^2 m_-(z,n) - \frac{1}{m_+(z,n-1)}}. && (2.5) \end{aligned}$$

Proof. First we prove (2.5). From the definition of $g(z,n)$ (cf. (1.26)) we infer

$$\begin{aligned} g(z,n) &= \frac{u_+(z,n)u_-(z,n)}{W(u_-(z),u_+(z))}\\ &= \frac{u_+(z,n)u_-(z,n)}{a_{n-1}\big(u_-(z,n-1)u_+(z,n) - u_-(z,n)u_+(z,n-1)\big)}\\ &= \frac{1}{\underbrace{a_{n-1}\frac{u_-(z,n-1)}{u_-(z,n)}}_{-a_{n-1}^2 m_-(z,n)} \underbrace{- a_{n-1}\frac{u_+(z,n-1)}{u_+(z,n)}}_{m_+(z,n-1)^{-1}}} \end{aligned}$$

by (2.1). (2.4) follows now from (2.2). □

Now that we saw some of the basic relations for $m_\pm(z)$ we will investigate the role of Weyl m-functions in spectral theory.

The definition of Weyl m-functions (we omit the base point $n_0 = 0$),

$$m_\pm(z) = \langle \delta_{\pm 1}, (H_\pm - z)^{-1}\delta_{\pm 1}\rangle, \quad z \in \rho(H_\pm),$$

implies that $m_\pm(z)$ are holomorphic in $\mathbb{C}\backslash\sigma(H_\pm)$. We also know the following properties.

Lemma 2.5. ([12]). *For $\delta_{\pm 1} \in \ell^2(\mathbb{Z})$ with $\|\delta_{\pm 1}\| = 1$,*

(i) $\operatorname{Im}(m_\pm(z)) = \operatorname{Im}(z)\,\|(H_\pm - z)^{-1}\delta_{\pm 1}\|^2$

(ii) $m_\pm(\overline{z}) = \overline{m_\pm(z)}$

(iii) $|m_\pm(z)| \le \|(H_\pm - z)^{-1}\| \le \frac{1}{|\operatorname{Im}(z)|}$.

Proof. (i)

$$(H_\pm - z)^{-1} - (H_\pm - \overline{z})^{-1} = \frac{H_\pm - \overline{z} - H_\pm + z}{(H_\pm - z)(H_\pm - \overline{z})} = (z - \overline{z})(H_\pm - z)^{-1}(H_\pm - \overline{z})^{-1},$$

take now the inner product with $\delta_{\pm 1}$, then

$$\begin{aligned} m_\pm(z) - m_\pm(\overline{z}) &= 2\mathrm{Im}(z)\langle \delta_{\pm 1}, (H_\pm - z)^{-1}(H_\pm - \overline{z})^{-1}\delta_{\pm 1}\rangle \\ \mathrm{Im}(m_\pm(z)) &= \mathrm{Im}(z)\langle (H_\pm - z)^{-1}\delta_{\pm 1}, (H_\pm - z)^{-1}\delta_{\pm 1}\rangle \\ &= \mathrm{Im}(z)\, \|(H_\pm - z)^{-1}\delta_{\pm 1}\|^2. \end{aligned}$$

We used that $(H_\pm - z)^{-1}$ and $(H_\pm - \overline{z})^{-1}$ commute.

(ii) $H_\pm$ is real symmetric.

(iii)

$$|m_\pm(z)| = |\langle \delta_{\pm 1}, (H_\pm - z)^{-1}\delta_{\pm 1}\rangle| \leq \|\delta_{\pm 1}\|\, \|(H_\pm - z)^{-1}\|$$

and

$$|\mathrm{Im}(z)| = \frac{|\mathrm{Im}(m_\pm(z))|}{\|(H_\pm - z)^{-1}\delta_{\pm 1}\|^2} \leq \frac{1}{\|(H_\pm - z)^{-1}\delta_{\pm 1}\|},$$

this holds for all δ with $\|\delta\| = 1$, so (iii) is proven. □

A holomorphic function $F : \mathbb{C}_+ \to \mathbb{C}_+$ is called a **Herglotz function**, where $\mathbb{C}_\pm = \{z \in \mathbb{C} | \pm \mathrm{Im}(z) > 0\}$ (see Appendix A). $m_\pm(z)$ are Herglotz functions since $m_\pm(z)$ are holomorphic on $\mathbb{C}_+$ and Lemma 2.5, (i), shows that they map the upper half plane to itself. Hence by Theorem A.1, $m_\pm(z)$ have the following representation

$$m_\pm(z) = \int_{\mathbb{R}} \frac{d\rho_\pm(\lambda)}{\lambda - z}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \tag{2.6}$$

where

$$\rho_\pm(\lambda) = \int_{(-\infty,\lambda]} d\rho_\pm$$

is a nondecreasing bounded function which is given by Stieltjes inversion formula (cf. Theorem A.1)

$$\rho_\pm(\lambda) = \lim_{\delta \downarrow 0} \lim_{\epsilon \downarrow 0} \frac{1}{\pi} \int_{-\infty}^{\lambda+\delta} \mathrm{Im}\big(m_\pm(x + i\,\epsilon)\big) dx.$$

Here we have normalized $\rho_\pm$ such that it is right continuous and obeys $\rho_\pm(\lambda) = 0$ for $\lambda < \sigma(H_\pm)$.

Let $P_\Lambda(H_\pm)$, $\Lambda \subseteq \mathbb{R}$, denote the family of spectral projections corresponding to $H_\pm$. Then $d\rho_\pm$ can be identified using the spectral theorem,

$$m_\pm(z) = \langle \delta_{\pm 1}, (H_\pm - z)^{-1}\delta_{\pm 1}\rangle = \int_{\mathbb{R}} \frac{d\langle \delta_{\pm 1}, P_{(-\infty,\lambda]}(H_\pm)\delta_{\pm 1}\rangle}{\lambda - z}. \tag{2.7}$$

Thus we see that $d\rho_\pm = d\langle \delta_{\pm 1}, P_{(-\infty,\lambda]}(H_\pm)\delta_{\pm 1}\rangle$ is the spectral measure of $H_\pm$ associated to the sequence $\delta_{\pm 1}$.

Lemma 2.6. ([13]). *$m_\pm(z,n)$ have the Laurent expansions*

$$m_\pm(z,n) = -\sum_{j=0}^{\infty} \frac{m_{\pm,j}(n)}{z^{j+1}}, \quad m_{\pm,0}(n) = 1. \tag{2.8}$$

The coefficients are given by

$$m_{\pm,j}(n) = \langle \delta_{n\pm1}, (H_{\pm,n})^j \delta_{n\pm1} \rangle, \quad j \in \mathbb{N}, \tag{2.9}$$

and satisfy

$$m_{\pm,0} = 1, \quad m_{\pm,1}(n) = b_{n\pm1},$$
$$m_{+,2}(n) = b_{n+1}^2 + a_{n+1}^2, \quad m_{-,2}(n) = b_{n-1}^2 + a_{n-2}^2,$$
$$m_{+,j+1}(n) = b_{n+1} m_{+,j}(n) + a_{n+1}^2 \sum_{l=0}^{j-1} m_{+,j-l-1}(n) m_{+,l}(n+1), \quad j \in \mathbb{N}, \tag{2.10}$$
$$m_{-,j+1}(n) = b_{n-1} m_{-,j}(n) + a_{n-2}^2 \sum_{l=0}^{j-1} m_{-,j-l-1}(n) m_{-,l}(n+1), \quad j \in \mathbb{N}. \tag{2.11}$$

Remark 2.7. Note that $m_\pm(z,n)$ only depend on a^2.

Proof. We invoke **Neumann's expansion** for the resolvent

$$(H_{\pm,n} - z)^{-1} = -z^{-1} \left(1 - \frac{H_{\pm,n}}{z}\right)^{-1} = -\sum_{j=0}^{\infty} \frac{(H_{\pm,n})^j}{z^{j+1}}, \quad |z| > \|H_{\pm,n}\|.$$

Thus we infer

$$m_\pm(z,n) = \langle \delta_{n\pm1}, (H_{\pm,n} - z)^{-1} \delta_{n\pm1} \rangle = -\sum_{j=0}^{\infty} \frac{\langle \delta_{n\pm1}, (H_{\pm,n})^j \delta_{n\pm1} \rangle}{z^{j+1}}$$

for $|z| > \|H_{\pm,n}\|$. To prove the recurrence relations we take (2.2) at $m_+(z,n+1)$

$$a_{n+1}^2 m_+(z,n+1) + \frac{1}{m_+(z,n)} = b_{n+1} - z,$$

multiply with $m_+(z,n)$ and insert the Laurent expansion (2.8)

$$a_{n+1}^2 \sum_{k,l=0}^{\infty} \frac{m_{+,k}(n) m_{+,l}(n+1)}{z^{k+l+2}} + (b_{n+1} - z) \sum_{j=0}^{\infty} \frac{m_{+,j}(n)}{z^{j+1}} + 1 = 0.$$

Set $k + l = j$, rewrite the first sum

$$a_{n+1}^2 \sum_{j=0}^{\infty} \frac{1}{z^{j+2}} \sum_{l=0}^{j} m_{+,j-l}(n) m_{+,l}(n+1) + (b_{n+1} - z) \sum_{j=0}^{\infty} \frac{m_{+,j}(n)}{z^{j+1}} + 1 = 0$$

and collect the coefficients of z^{j+1}

$$a_{n+1}^2 \sum_{l=0}^{j-1} m_{+,j-l-1}(n) m_{+,l}(n+1) + b_{n+1} m_{+,j}(n) - m_{+,j+1}(n) = 0.$$

□

Remark 2.8. For arbitrary expectations of resolvents of self-adjoint operators similar results as Lemma 2.5, Lemma 2.6, and the considerations about spectral measures hold. We will discuss them in Section 2.3.

If we combine (2.6)

$$m_\pm(z) = \int_{\mathbb{R}} \frac{d\rho_\pm(\lambda)}{\lambda - z} = -\int_{\mathbb{R}} \frac{d\rho_\pm(\lambda)}{z(1-\lambda z^{-1})} = -\sum_{j=0}^{\infty} \frac{1}{z^{j+1}} \int_{\mathbb{R}} \lambda^j d\rho_\pm(\lambda)$$

with Lemma 2.6 (at the base point $n = 0$), we see that the **moments** $m_{\pm,j}$ of $d\rho_\pm$ are finite and given by

$$m_{\pm,j} := \int_{\mathbb{R}} \lambda^j d\rho_\pm(\lambda) = \langle \delta_{\pm 1}, (H_\pm)^j \delta_{\pm 1} \rangle. \tag{2.12}$$

There is a close connection between the so called moment problem (i.e. determining $d\rho_\pm$ from all its moments $m_{\pm,j}$) and the reconstruction of $H_\pm$ from $d\rho_\pm$. Since by Lemma 2.6

$$m_{\pm,0} = 1, \quad m_{\pm,1} = b_{\pm 1}, \quad m_{+,2} = b_1^2 + a_1^2, \quad m_{-,2} = b_{-1}^2 + a_{-2}^2, \quad \text{etc.}$$

we infer

$$b_{\pm 1} = m_{\pm,1}, \quad a_1^2 = m_{+,2} - (m_{+,1})^2, \quad a_{-2}^2 = m_{-,2} - (m_{-,1})^2, \quad \text{etc..} \tag{2.13}$$

We will consider this topic in the next section. Before that we want to modify $m_\pm(z, n)$ a bit, since when it comes to calculations, the following pair of Weyl m-functions

$$\tilde{m}_\pm(z, n) = \mp \frac{u_\pm(z, n+1)}{a_n u_\pm(z, n)}, \quad \tilde{m}_\pm(z) = \tilde{m}_\pm(z, 0) \tag{2.14}$$

is often more convenient than the original one. The connection is given by

$$m_+(z, n) = \tilde{m}_+(z, n), \quad m_-(z, n) = \frac{a_n^2 \tilde{m}_-(z, n) - z + b_n}{a_{n-1}^2}, \tag{2.15}$$

and

$$\frac{1}{m_-(z, n+1)} = -a_n^2 \tilde{m}_-(z, n). \tag{2.16}$$

The corresponding spectral measures (for $n = 0$) are related by

$$d\rho_+ = d\tilde{\rho}_+, \quad d\rho_- = \frac{a_0^2}{a_{-1}^2} d\tilde{\rho}_-. \tag{2.17}$$

2.2 The Moment Problem

We want to investigate how the sequences a^2 and b can be reconstructed from the measure ρ_+ and we will see that the moments $m_{+,j}$, $j \in \mathbb{N}$, are sufficient for this task. This is generally known as **(Hamburger) moment problem**.

Suppose we have a given sequence m_j, $j \in \mathbb{N}_0$, such that

$$C(k) = \det \begin{pmatrix} m_0 & m_1 & \cdots & m_{k-1} \\ m_1 & m_2 & \cdots & m_k \\ \vdots & \vdots & \ddots & \vdots \\ m_{k-1} & m_k & \cdots & m_{2k-2} \end{pmatrix} > 0 \quad \text{for all } k \in \mathbb{N}. \tag{2.18}$$

Without restriction we assume $m_0 = 1$. Now we can define a sesquilinear form (linear in the first entry and complex linear in the second entry) on the set of polynomials as follows

$$\langle P(\lambda), Q(\lambda) \rangle_{L^2} = \sum_{j,k=0}^{\infty} m_{j+k} \overline{p_j} q_k, \tag{2.19}$$

where $P(z) = \sum p_j z^j$ and $Q(z) = \sum q_k z^k$. It has the property that

$$\langle P, z\, Q \rangle_{L^2} = \sum_{j,k=0}^{\infty} m_{j+k} \overline{p_j} q_{k-1} = \sum_{j,k=0}^{\infty} m_{j+k+1} \overline{p_j} q_k = \langle z\, P, Q \rangle_{L^2}. \tag{2.20}$$

Next we consider the polynomials (set $C(0) = 1$)

$$s(z,k) = \frac{1}{\sqrt{C(k-1)C(k)}} \det \begin{pmatrix} m_0 & m_1 & \cdots & m_{k-1} \\ m_1 & m_2 & \cdots & m_k \\ \vdots & \vdots & \ddots & \vdots \\ m_{k-2} & m_{k-1} & \cdots & m_{2k-3} \\ 1 & z & \cdots & z^{k-1} \end{pmatrix}, \quad k \in \mathbb{N}. \tag{2.21}$$

$\{s(z,k), k \in \mathbb{N}\}$ forms a basis for the set of polynomials which is clear if we compute $s(z,k)$ explicitly

$$\begin{aligned} s(z,k) &= \frac{1}{\sqrt{C(k-1)C(k)}} \left(z^{k-1} C(k-1) + z^{k-2} D(k-1) + O(z^{k-3}) \right) \\ &= \sqrt{\frac{C(k-1)}{C(k)}} \left(z^{k-1} + \frac{D(k-1)}{C(k-1)} z^{k-2} + O(z^{k-3}) \right), \end{aligned} \tag{2.22}$$

where $D(0) = 0$, $D(1) = m_1$, and

$$D(k) = \det \begin{pmatrix} m_0 & m_1 & \cdots & m_{k-2} & m_k \\ m_1 & m_2 & \cdots & m_{k-1} & m_{k+1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ m_{k-1} & m_k & \cdots & m_{2k-3} & m_{2k-1} \end{pmatrix}, \; k \in \mathbb{N}. \tag{2.23}$$

Moreover, this basis is orthonormal

$$\langle s(\lambda,k), s(\lambda,l) \rangle_{L^2} = \delta_{k,l}. \tag{2.24}$$

To prove this claim, let $k \geq j$, say, then

$$\langle s(\lambda,k), \lambda^j \rangle_{L^2} = \sum_{l=0}^{k-1} m_{j+l} \, (\text{coeff of } (\lambda^l) \text{ in } s(\lambda,k))$$

$$= \frac{1}{\sqrt{C(k-1)C(k)}} \det \begin{pmatrix} m_0 & m_1 & \cdots & m_{k-1} \\ m_1 & m_2 & \cdots & m_k \\ \vdots & \vdots & \ddots & \vdots \\ m_{k-2} & m_{k-1} & \cdots & m_{2k-3} \\ m_j & m_{j+1} & \cdots & m_{j+k-1} \end{pmatrix}$$

$$= \begin{cases} 0, & 0 \le j \le k-2 \\ \sqrt{\frac{C(k)}{C(k-1)}}, & j = k-1. \end{cases} \tag{2.25}$$

So $\langle s(\lambda,k), s(\lambda,k)\rangle_{L^2} = 1$ since the additional coefficient of λ^{k-1} is $\sqrt{\frac{C(k-1)}{C(k)}}$. The sesquilinear form (2.19) is positive definite and hence an inner product ($C(k) > 0$ is also necessary for this).

Expanding the polynomial $zs(z,k)$ in terms of $s(z,j)$, $j \in \mathbb{N}$, we infer

$$\begin{aligned} zs(z,k) &= \sum_{j=0}^{k+1} \langle s(\lambda,j), \lambda s(\lambda,k)\rangle_{L^2} s(z,j) \\ &= \sum_{j=0}^{k+1} \langle \lambda s(\lambda,j), s(\lambda,k)\rangle_{L^2} s(z,j) \\ &= a_k s(z,k+1) + b_k s(z,k) + c_{k-1} s(z,k-1), \end{aligned} \tag{2.26}$$

by (2.25) we only get values for $j \ge k-1$. Here we have set $s(z,0) = 0$ and

$$a_k = \langle s(\lambda,k+1), \lambda s(\lambda,k)\rangle_{L^2}, \quad b_k = \langle s(\lambda,k), \lambda s(\lambda,k)\rangle_{L^2}, \quad k \in \mathbb{N}, \tag{2.27}$$

$$c_{k-1} = \langle s(\lambda,k-1), \lambda s(\lambda,k)\rangle_{L^2} = \langle s(\lambda,k), \lambda s(\lambda,k-1)\rangle_{L^2} = a_{k-1}.$$

Now we can compare powers of z in (2.26) to determine a_k, b_k explicitly. By (2.22),

$$zs(z,k) = \sqrt{\frac{C(k-1)}{C(k)}} z^k + \frac{D(k-1)}{\sqrt{C(k-1)C(k)}} z^{k-1} + O(z^{k-2})$$

and if we compute the coefficients of z^k and z^{k-1} in (2.26) we obtain

$$\sqrt{\frac{C(k-1)}{C(k)}} z^k = a_k \sqrt{\frac{C(k)}{C(k+1)}} z^k$$

$$\Rightarrow \quad a_k = \frac{\sqrt{C(k-1)C(k+1)}}{C(k)}, \tag{2.28}$$

$$\frac{D(k-1)}{\sqrt{C(k-1)C(k)}} z^{k-1} = a_k \frac{D(k)}{\sqrt{C(k)C(k+1)}} z^{k-1} + b_k \sqrt{\frac{C(k-1)}{C(k)}} z^{k-1}$$

$$\Rightarrow \quad b_k = \frac{D(k)}{C(k)} - \frac{D(k-1)}{C(k-1)}. \tag{2.29}$$

This says that given the measure $d\rho_+$ (or its moments $m_{+,j}$, $j \in \mathbb{N}$) we can compute $s(\lambda,n)$, $n \in \mathbb{N}$, via orthonormalization of the set $\{\lambda^n, n \in \mathbb{N}_0\}$. This fixes $s(\lambda,n)$ up to a sign if we require $s(\lambda,n)$ real-valued. Then we can compute a_n, b_n as above up to the sign of a_n which changes if we change the sign of $s(\lambda,n)$.

So $d\rho_+$ uniquely determines a_n^2 and b_n for $n \in \mathbb{N}$. Since knowing $d\rho_+(\lambda)$ is equivalent to knowing $m_+(z)$, $m_+(z)$ uniquely determines a_n^2 and b_n for $n \in \mathbb{N}$.

2.3 Asymptotic Expansions

Our aim is to derive asymptotic expansions for $g(z,n)$, $h(z,n)$ and to describe their associated spectral measures. This treatment will of course be similar to that of Weyl m-functions in Section 2.1.

First we recall the definition of $g(z,n)$ and $h(z,n)$ given in (1.26) and (1.27)

$$\begin{aligned} g(z,n) &= G(z,n,n) = \langle \delta_n, (H-z)^{-1}\delta_n\rangle, \\ h(z,n) &= 2a_n G(z,n,n+1) - 1 = 2a_n\langle \delta_n, (H-z)^{-1}\delta_{n+1}\rangle - 1. \end{aligned}$$

As a consequence of the spectral theorem we have the following result.

Lemma 2.9. ([12]). *Suppose $\delta \in \ell^2(\mathbb{Z})$ with $\|\delta\| = 1$. Then*

$$g(z) = \langle \delta, (H-z)^{-1}\delta\rangle$$

is Herglotz, so $g(z)$ has the following representation

$$g(z) = \int_{\mathbb{R}} \frac{d\rho_\delta(\lambda)}{\lambda - z},$$

where $d\rho_\delta(\lambda) = d\langle \delta, P_{(-\infty,\lambda]}(H)\delta\rangle$ is the spectral measure of H associated to the sequence δ. Moreover,

(i) $g(z) = -\sum_{j=0}^{\infty} \frac{\langle \delta, H^j\delta\rangle}{z^{j+1}}$

(ii) $\mathrm{Im}(g(z)) = \mathrm{Im}(z)\,\|(H-z)^{-1}\delta\|^2$

(iii) $\overline{g(z)} = g(\overline{z})$

(iv) $|g(z)| \le \|(H-z)^{-1}\| \le \frac{1}{|\mathrm{Im}(z)|}$.

Proof. (i) We use again **Neumann's expansion** for the resolvent

$$(H-z)^{-1} = -z^{-1}\left(1 - \frac{H}{z}\right)^{-1} = -\sum_{j=0}^{\infty}\frac{H^j}{z^{j+1}}, \quad |z| > \|H\|.$$

(ii), (iii) and (iv) are proven in an analogous manner as in Lemma 2.5. □

Lemma 2.9 implies the following **asymptotic expansions** for $g(z,n)$ and $h(z,n)$.

Lemma 2.10. ([13]). *The quantities $g(z,n)$ and $h(z,n)$ have the Laurent expansions*

$$\begin{aligned} g(z,n) &= -\sum_{j=0}^{\infty}\frac{g_j(n)}{z^{j+1}}, \quad g_0 = 1, \\ h(z,n) &= -1 - \sum_{j=0}^{\infty}\frac{h_j(n)}{z^{j+1}}, \quad h_0 = 0, \end{aligned} \tag{2.30}$$

and the coefficients are given by

$$\begin{aligned} g_j(n) &= \langle \delta_n, H^j\delta_n\rangle, \\ h_j(n) &= 2a_n\langle \delta_n, H^j\delta_{n+1}\rangle, \quad j \in \mathbb{N}_0. \end{aligned} \tag{2.31}$$

Remark 2.11. [12], Lemma 1.6, shows that $g_j(n)$, $h_j(n)$ do not depend on the sign of a_n, they only depend on a_n^2.

In the next lemma we show how to compute g_j, h_j recursively.

Lemma 2.12. ([2], Lemma 2.1). *The coefficients $g_j(n)$ and $h_j(n)$ for $j \in \mathbb{N}_0$ satisfy the following recursion relations*

$$\begin{aligned} g_{j+1}(n) &= \frac{h_j(n) + h_j(n-1)}{2} + b_n g_j(n), && (2.32)\\ h_{j+1}(n) - h_{j+1}(n-1) &= 2\big(a_n^2 g_j(n+1) - a_{n-1}^2 g_j(n-1)\big) \\ &\quad + b_n\big(h_j(n) - h_j(n-1)\big). && (2.33) \end{aligned}$$

Proof. The first equation follows from

$$\begin{aligned} g_{j+1}(n) &= \langle H\delta_n, H^j\delta_n\rangle \\ &= a_{n-1}\langle \delta_{n-1}, H^j\delta_n\rangle + b_n\langle \delta_n, H^j\delta_n\rangle + a_n\langle \delta_{n+1}, H^j\delta_n\rangle \\ &= \frac{h_j(n-1)}{2} + b_n g_j(n) + \frac{h_j(n)}{2} \end{aligned}$$

using $H\delta_n = a_{n-1}\delta_{n-1} + b_n\delta_n + a_n\delta_{n+1}$. Similarly,

$$\begin{aligned} h_{j+1}(n) &= 2a_n\langle H\delta_n, H^j\delta_{n+1}\rangle \\ &= 2a_n\big(a_{n-1}\langle \delta_{n-1}, H^j\delta_{n+1}\rangle + b_n\langle \delta_n, H^j\delta_{n+1}\rangle + a_n\langle \delta_{n+1}, H^j\delta_{n+1}\rangle\big) \\ &= 2a_n a_{n-1}\langle \delta_{n-1}, H^j\delta_{n+1}\rangle + b_n h_j(n) + 2a_n^2 g_j(n+1), \end{aligned}$$

$$\begin{aligned} h_{j+1}(n-1) &= 2a_{n-1}\langle H\delta_n, H^j\delta_{n-1}\rangle \\ &= 2a_{n-1}\big(a_{n-1}\langle \delta_{n-1}, H^j\delta_{n-1}\rangle \\ &\quad + b_n\langle \delta_n, H^j\delta_{n-1}\rangle + a_n\langle \delta_{n+1}, H^j\delta_{n-1}\rangle\big) \\ &= 2a_{n-1}^2 g_j(n-1) + b_n h_j(n-1) + 2a_n a_{n-1}\langle \delta_{n-1}, H^j\delta_{n+1}\rangle. \end{aligned}$$

Subtraction yields the result. In the last step we used $G(z,m,n) = G(z,n,m)$. □

The system in Lemma 2.12 does not determine $g_j(n)$, $h_j(n)$ uniquely since it requires solving a first order recurrence relation at each step, producing an unknown summation constant each time. One can determine this constant (cf. [12], p. 107) but since this procedure is not very straightforward, we advocate a different approach. If we take (3.6) from below

$$4a_n^2 g(z,n)g(z,n+1) = h(z,n)^2 - 1,$$

insert the Laurent expansions for $g(z,.)$, $h(z,n)$ and compare powers of z^{j+2} we infer

$$h_{j+1}(n) = 2a_n^2\sum_{l=0}^{j} g_{j-l}(n)g_l(n+1) - \frac{1}{2}\sum_{l=0}^{j} h_{j-l}(n)h_l(n), \quad j \in \mathbb{N}. \tag{2.34}$$

This determines g_j, h_j recursively together with (2.32). Explicitly we obtain

$$\begin{aligned} g_0 &= 1, \quad g_1(n) = b_n, \quad g_2(n) = a_n^2 + a_{n-1}^2 + b_n^2, \\ h_0 &= 0, \quad h_1(n) = 2a_n^2, \quad h_2(n) = 2a_n^2\big(b_n + b_{n+1}\big), \quad \text{etc..} \end{aligned} \tag{2.35}$$

Remark 2.13. A third approach producing a recursion for g_j only is given in [12], Remark 6.5.

Chapter 3

Inverse Spectral Theory

We already discovered in our survey of the moment problem, Section 2.2, that $m_+(z)$ uniquely determines a_n^2 and b_n for $n \in \mathbb{N}$.

Now we want to present a simple recursive method of reconstructing the sequences a^2, b from $g(z,n)$ and $h(z,n)$. When the **Weyl matrix** is known for one fixed $n_0 \in \mathbb{Z}$, this is a well known result which is sharpened in [13]. We will see for example that $g(z,n_0)$ and $h(z,n_0)$ are sufficient for this task.

Definition 3.1. The Weyl matrix $M(z)$ is given by

$$\begin{aligned} M(z) &= \int_{-\infty}^{\infty} \frac{d\rho(\lambda)}{\lambda - z} - \frac{1}{2a_0} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} g(z,0) & \frac{h(z,0)}{2a_0} \\ \frac{h(z,0)}{2a_0} & g(z,1) \end{pmatrix}, \quad z \in \mathbb{C}\backslash\sigma(H). \end{aligned}$$

Suppose we know

$$M(z,n) = \begin{pmatrix} g(z,n) & \frac{h(z,n)}{2a_n} \\ \frac{h(z,n)}{2a_n} & g(z,n+1) \end{pmatrix}, \quad z \in \mathbb{C}\backslash\sigma(H), \tag{3.1}$$

for one fixed $n \in \mathbb{Z}$. By Lemma 2.10 we obtain

$$g(z,n) = -\sum_{j=0}^{\infty} \frac{\langle \delta_n, H^j \delta_n \rangle}{z^{j+1}} = -\frac{1}{z} - \frac{b_n}{z^2} + O\left(z^{-3}\right), \tag{3.2}$$

$$h(z,n) = -1 - \sum_{j=0}^{\infty} \frac{2a_n \langle \delta_n, H^j \delta_{n+1} \rangle}{z^{j+1}} = -1 - \frac{2a_n^2}{z^2} + O\left(z^{-3}\right). \tag{3.3}$$

All $O\left(z^{-l}\right)$ terms apply for $|z| \to \infty$. Hence a_n^2 and b_n can be recovered as follows

$$b_n = -\lim_{z\to\infty} z(1 + zg(z,n)), \tag{3.4}$$

$$a_n^2 = -\frac{1}{2} \lim_{z\to\infty} z^2(1 + h(z,n)). \tag{3.5}$$

Moreover, we derive useful identities

$$4a_n^2 g(z,n)g(z,n+1) = h(z,n)^2 - 1, \tag{3.6}$$

$$h(z,n+1) + h(z,n) = 2\big(z - b_{n+1}\big)g(z,n+1), \tag{3.7}$$

if we combine (1.26) and (1.27)

$$\begin{aligned} g(z,n) &= \frac{u_+(z,n)u_-(z,n)}{W(u_-(z),u_+(z))}, \\ h(z,n) &= \frac{a_n\big(u_+(z,n)u_-(z,n+1)+u_+(z,n+1)u_-(z,n)\big)}{W(u_-(z),u_+(z))}. \end{aligned}$$

The identities show that $g(z,n)$ and $h(z,n)$ together with a_n^2 and b_n can be determined recursively. If, say, $g(z,n_0)$ and $h(z,n_0)$ are given, we obtain b_{n_0} and $a_{n_0}^2$ by taking the limit in (3.4) and (3.5). Then we know $g(z,n_0+1)$ by (3.6) and thus b_{n_0+1}. Inserting them in (3.7) gives $h(z,n_0+1)$ and so on.

In addition, we see that a_n^2, $g(z,n)$, $g(z,n+1)$ determine $h(z,n)$ up to its sign,

$$h(z,n)=\sqrt{1+4a_n^2g(z,n)g(z,n+1)},$$

since $h(z,n)$ is holomorphic with respect to $z\in\mathbb{C}\backslash\sigma(H)$. The remaining sign can be determined from the asymptotic behavior $h(z,n)=-1+O(z^{-2})$.

Hence we have proven the following result.

Theorem 3.2. ([13]). *One of the following set of data for a fixed $n_0\in\mathbb{Z}$ determines the sequences a^2 and b:*

(i) *$g(.\,,n_0)$ and $h(.\,,n_0)$*

(ii) *$g(.\,,n_0+1)$ and $h(.\,,n_0)$*

(iii) *$g(.\,,n_0)$, $g(.\,,n_0+1)$ and $a_{n_0}^2$.*

Remark 3.3. Remark 2.11 shows that the sign of a_n cannot be determined from either $g(z,n_0)$, $h(z,n_0)$ or $g(z,n_0+1)$.

The off diagonal Green function can be recovered as follows

$$G(z,n,n+k)=g(z,n)\prod_{j=n}^{n+k-1}\frac{1+h(z,j)}{2a_jg(z,j)},\quad k>0, \tag{3.8}$$

since by (1.27) and (1.24)

$$\begin{aligned} g(z,n)\prod_{j=n}^{n+k-1}\frac{1+h(z,j)}{2a_jg(z,j)} &= g(z,n)\prod_{j=n}^{n+k-1}\frac{G(z,j,j+1)}{G(z,j,j)} \\ &= \frac{1}{W}\,u_+(z,n)u_-(z,n)\prod_{j=n}^{n+k-1}\frac{u_+(z,j+1)}{u_+(z,j)} \\ &= \frac{1}{W}\,u_-(z,n)u_+(z,n+k)=G(z,n,n+k). \end{aligned}$$

A similar procedure works for H_+. The asymptotic expansion

$$m_+(z,n)=-\frac{1}{z}-\frac{b_{n+1}}{z^2}-\frac{a_{n+1}^2+b_{n+1}^2}{z^3}+O(z^{-4}) \tag{3.9}$$

shows that a_{n+1}^2, b_{n+1} can be recovered from $m_+(z,n)$. In addition,

$$a_n^2 m_+(z,n) + \frac{1}{m_+(z,n-1)} = b_n - z \tag{3.10}$$

shows that $m_+(z,n_0)$ determines a_n^2, b_n, and $m_+(z,n)$ for $n > n_0$. By the same considerations, $m_-(z,n_0)$ determines a_{n-1}^2, b_n, and $m_-(z,n-1)$ for $n < n_0$. Thus both $m_\pm(z,n_0)$ determine the sequences a^2 and b except for $a_{n_0-1}^2$, $a_{n_0}^2$, b_{n_0}. But if we consider (cf. (2.15))

$$\tilde{m}_-(z,n) = \frac{z - b_n + a_{n-1}^2 m_-(z,n)}{a_n^2},$$

we see that $a_{n_0-1}^2$, $a_{n_0}^2$, b_{n_0}, and $m_-(z,n_0)$ can be computed from $\tilde{m}_-(z,n_0)$. We conclude

Theorem 3.4. ([13]). *The quantities $\tilde{m}_+(z,n_0)$ and $\tilde{m}_-(z,n_0)$ for one fixed $n_0 \in \mathbb{Z}$ uniquely determine the sequences a^2 and b.*

Furthermore, we have the following relations between $g(z)$, $h(z)$, and $\tilde{m}_\pm(z)$

$$\begin{aligned} g(z,n) &= -\frac{1}{a_n^2\big(\tilde{m}_+(z,n) + \tilde{m}_-(z,n)\big)}, \\ g(z,n+1) &= \frac{\tilde{m}_+(z,n)\tilde{m}_-(z,n)}{\tilde{m}_+(z,n) + \tilde{m}_-(z,n)}, \\ h(z,n) &= \frac{\tilde{m}_+(z,n) - \tilde{m}_-(z,n)}{\tilde{m}_+(z,n) + \tilde{m}_-(z,n)}. \end{aligned} \tag{3.11}$$

Conversely,

$$\tilde{m}_\pm(z,n) = \frac{1 \pm h(z,n)}{2a_n^2 g(z,n)} = -\frac{2g(z,n+1)}{1 \mp h(z,n)}. \tag{3.12}$$

Chapter 4

Trace Formulas

In this chapter we will investigate trace formulas for bounded Jacobi operators H, for a treatment of unbounded Jacobi operators and Jacobi operators with boundary conditions we refer the reader to [12] or [13]. The most basic example of a trace formula is

$$\operatorname{tr}(H - H_n) = b_n,$$

where $H_n = H_{-,n} \oplus H_{+,n}$.

Our main tool will be the exponential Herglotz representation of $g(z,n) = \langle \delta_n, (H-z)^{-1}\delta_n \rangle$. $g(z,n)$ is a Herglotz function by Lemma 2.9 and its exponential representation (cf. Theorem A.2) reads

$$g(z,n) = |g(i,n)| \exp\left(\int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) \xi(\lambda,n) d\lambda \right), \quad z \in \mathbb{C}\backslash\sigma(H), \tag{4.1}$$

where the ξ function $\xi(\lambda,n)$ (see [4]) is defined by

$$\xi(\lambda,n) = \frac{1}{\pi} \lim_{\epsilon \downarrow 0} \arg g(\lambda + i\epsilon, n) \quad \text{for a.e. } \lambda \in \mathbb{R}. \tag{4.2}$$

$\arg(.) \in (-\pi, \pi]$ and $\xi(\lambda,n)$ satisfies $0 \leq \xi(\lambda,n) \leq 1$. By [12], p. 112,

$$\int_{\mathbb{R}} \frac{\xi(\lambda,n)}{1+\lambda^2} d\lambda = \arg g(i,n). \tag{4.3}$$

For a bounded Jacobi operator H we know by Lemma 1.13 that

$$\sigma(H) \subseteq [\inf_{n\in\mathbb{Z}} c_-(n), \sup_{n\in\mathbb{Z}} c_+(n)],$$

where $c_\pm(n) = b_n \pm (|a_n| + |a_{n-1}|)$. So we can abbreviate

$$E_0 = \min \sigma(H), \quad E_\infty = \max \sigma(H).$$

We claim that

$$\xi(\lambda,n) = \begin{cases} 0 & \text{for } \lambda < E_0 \\ 1 & \text{for } \lambda > E_\infty. \end{cases} \tag{4.4}$$

To show this, we have to derive the sign of $g(\lambda,n)$ for $\lambda < E_0$ and $\lambda > E_\infty$. $(H-\lambda) > 0$ for $\lambda < E_0$, so $(H-\lambda)^{-1} > 0$ and $g(\lambda,n) = \langle \delta_n, (H-\lambda)^{-1}\delta_n \rangle > 0$,

this implies $\xi(\lambda, n) = 0$. Similarly, we infer $\xi(\lambda, n) = 1$ for $\lambda > E_\infty$ since in this case $(H - \lambda) < 0$ and thus $g(\lambda, n) < 0$. For this argumentation we need of course that $g(\lambda, n)$ is continuous and real for $\lambda \in \mathbb{R}$.

(4.1) reads now

$$g(z, n) = \frac{1}{E_\infty - z} \exp\left(\int_{E_0}^{E_\infty} \frac{\xi(\lambda, n) d\lambda}{\lambda - z} \right), \tag{4.5}$$

we will give an analogous proof in Proposition 5.4 below.

Theorem 4.1. ([12]). *Let $\xi(\lambda, n)$ be defined as above and let $H_n = H_{-,n} \oplus H_{+,n}$. Then we have the following trace formulas*

$$b_n^{(l)} = \operatorname{tr}\left(H^l - H_n^l\right) = E_\infty^l - l \int_{E_0}^{E_\infty} \lambda^{l-1} \xi(\lambda, n) d\lambda, \tag{4.6}$$

where

$$b_n^{(1)} = b_n,$$

$$b_n^{(l)} = l g_l(n) - \sum_{j=1}^{l-1} g_{l-j}(n) b_n^{(j)}, \quad l \geq 2. \tag{4.7}$$

Proof. The claim follows after expanding both sides of

$$\ln\left((E_\infty - z) g(z, n)\right) = \int_{E_0}^{E_\infty} \frac{\xi(\lambda, n) d\lambda}{\lambda - z} \tag{4.8}$$

and comparing coefficients. The right side becomes

$$\begin{aligned} \int_{E_0}^{E_\infty} \frac{\xi(\lambda, n) d\lambda}{\lambda - z} &= -\int_{E_0}^{E_\infty} \frac{\xi(\lambda, n) d\lambda}{z(1 - \lambda z^{-1})} \\ &= -\sum_{l=1}^{\infty} \frac{1}{z^l} \int_{E_0}^{E_\infty} \lambda^{l-1} \xi(\lambda, n) d\lambda. \end{aligned}$$

Using the asymptotic expansion of $g(z, n)$ we expand the left side

$$\begin{aligned} \ln\left((E_\infty - z) g(z, n)\right) &= \ln\left(-z \left(1 - \frac{E_\infty}{z}\right) \left(-\sum_{j=0}^{\infty} \frac{g_j(n)}{z^{j+1}} \right) \right) \\ &= \ln\left(1 - \frac{E_\infty}{z}\right) + \ln\left(1 + \sum_{j=1}^{\infty} \frac{g_j(n)}{z^j}\right) \\ &= -\sum_{k=1}^{\infty} \frac{E_\infty^k}{k z^k} + \sum_{l=1}^{\infty} \frac{c_l(n)}{z^l}, \end{aligned}$$

where

$$c_1(n) = g_1(n), \quad c_l(n) = g_l(n) - \sum_{j=1}^{l-1} \frac{j}{l} g_{l-j}(n) c_j(n), \quad l \geq 2.$$

Set $l c_l(n) = b_n^{(l)}$ and compare coefficients of z^l. □

Remark 4.2. The special case $l = 1$ of (4.6),

$$\begin{aligned} b_n &= E_\infty - \int_{E_0}^{E_\infty} \xi(\lambda, n) d\lambda \\ &= \frac{E_0 + E_\infty}{2} + \frac{1}{2} \int_{E_0}^{E_\infty} (1 - 2\xi(\lambda, n)) d\lambda, \end{aligned} \tag{4.9}$$

has first been given in [4].

Chapter 5

Finite Jacobi Operators

In this chapter we will study finite restrictions H_{n_1,n_2} of H to the subspaces $\ell^2(n_1, n_2)$ as introduced in Section 1.3. We set $n_1 = 0$, $n_2 = N + 1$ and $H_{0,N+1} = H_N$ for simplicity. H_N has been obtained from H by imposing Dirichlet boundary conditions at the endpoints ($f(0) = 0$, $f(N + 1) = 0$).

First we recall the definition of H_N.

$$(H_N f)(n) = \begin{cases} a_1 f(2) + b_1 f(1) & n = 1 \\ (Hf)(n) & 1 < n < N \\ a_{N-1} f(N-1) + b_N f(N) & n = N. \end{cases} \tag{5.1}$$

The tridiagonal Jacobi matrix $J_{0,N+1}$ is associated with H_N:

$$J_{0,N+1} = \begin{pmatrix} b_1 & a_1 & & & \\ a_1 & b_2 & a_2 & & \\ & \ddots & \ddots & \ddots & \\ & & a_{N-2} & b_{N-1} & a_{N-1} \\ & & & a_{N-1} & b_N \end{pmatrix}. \tag{5.2}$$

One immediately obtains that the eigenvalues of H_N are simple. Suppose u, v are two different eigenfunctions of $H_N f = zf$ corresponding to the same eigenvalue $z \in \mathbb{C}$, then

$$\begin{aligned} W_1(u, v) &= a_1\big(u(1)v(2) - u(2)v(1)\big) \\ &= u(1)(z - b_1)v(1) - v(1)(z - b_1)u(1) = 0, \end{aligned}$$

by Proposition 1.5 this implies that u and v are not linearly independent. We used

$$a_1 f(2) + b_1 f(1) = zf(1) \tag{5.3}$$

for $v(2)$ and $u(2)$. Our choice of evaluating $W_n(u, v)$ at $n = 1$ is no restriction since the Wronskian is constant in n by Remark 1.4.

Next we consider the special solution $s(z, n, 0)$ characterized by the initial conditions $s(z, 0, 0) = 0$, $s(z, 1, 0) = 1$ (cf. (1.5)). For $n \in \mathbb{N}$, $s(z, n, 0)$ has precisely $n - 1$ distinct real zeros. To prove this, we consider the expansion

(1.10) for $s(z,n,0)$, $n>0$,

$$s(z,n,0)=\frac{\det(z-J_{0,n})}{\prod_{j=1}^{n-1}a_j}.$$

$s(\lambda_0,n,0)=0$ implies that λ_0 is an eigenvalue of $H_{0,n}$, thus λ_0 must be real and simple. Summarizing, we have the following classical result from the theory of orthogonal polynomials.

Theorem 5.1. *The polynomial $s(z,n,0)$, $n\in\mathbb{N}$, has $n-1$ real and distinct roots denoted by*

$$\lambda_{1,n}<\lambda_{2,n}<\ldots<\lambda_{n-1,n}.$$

The zeros of $s(z,n,0)$ and $s(z,n+1,0)$ are interlacing, that is,

$$\lambda_{1,n+1}<\lambda_{1,n}<\lambda_{2,n+1}<\ldots<\lambda_{n-1,n}<\lambda_{n,n+1}. \tag{5.4}$$

Moreover,

$$\sigma(H_{0,n})=\{\lambda_{j,n}\}_{j=1}^{n-1}.$$

Proof. A proof of (5.4) using Prüfer variables can be found in [12], p. 77. □

So $H_N=H_{0,N+1}$ has real eigenvalues $\lambda_1<\ldots<\lambda_N$ (we set $\lambda_{j,N}=\lambda_j$) and associated orthonormal eigenvectors $\varphi_1,\ldots,\varphi_N$ with $\varphi_j(1)\neq 0$ (if $\varphi_j(1)=0$, then φ_j would be identical 0 by (5.3)).

For the Green function of H_N $(1\leq m,n\leq N)$

$$G_{0,N+1}(z,m,n)=\langle\delta_m,(H_N-z)^{-1}\delta_n\rangle$$

we obtain

$$G_{0,N+1}(z,m,n)=\frac{1}{W(s(z),c(z))}\begin{cases}s(z,n,0)c(z,m,N) & \text{for } m\geq n\\ s(z,m,0)c(z,n,N) & \text{for } n\geq m.\end{cases} \tag{5.5}$$

$s(z,.,0)$ and $c(z,.,N)$ are the fundamental solutions satisfying the boundary conditions $s(z,0,0)=0$, $c(z,N+1,N)=0$.

5.1 The ξ Function

We saw in Chapter 4 that the ξ function plays an important role, knowing its precise form is the key ingredient to compute trace formulas explicitly. Indeed, in the case of finite Jacobi operators, the ξ function behaves very nicely.

Our starting point is the following result for the Weyl m-function $m_+(z)=m_+(z,0)=\langle\delta_1,(H_+-z)^{-1}\delta_1\rangle$.

Theorem 5.2. ([3]). *If $\lambda_1<\ldots<\lambda_N$ denote the eigenvalues of H_N and $\nu_1<\ldots<\nu_{N-1}$ the eigenvalues of $H_{1,N+1}$, then*

$$m_+(z)=-\frac{\prod_{l=1}^{N-1}(z-\nu_l)}{\prod_{j=1}^{N}(z-\lambda_j)}. \tag{5.6}$$

Proof. By (5.5),

$$\begin{aligned} m_+(z) &= G_{0,N+1}(z,1,1) \\ &= \frac{s(z,1,0)c(z,1,N)}{a_0\big(s(z,0,0)c(z,1,N) - s(z,1,0)c(z,0,N)\big)} \\ &= -\frac{c(z,1,N)}{a_0 c(z,0,N)} \end{aligned}$$

and (1.11)

$$c(z, n_0 - n, n_0) = \frac{\det(z - J_{n_0-n,n_0+1})}{\prod_{j=n_0-n}^{n_0-1} a_j}$$

becomes

$$c(z,1,N) = \frac{\det(z - J_{1,N+1})}{\prod_{j=1}^{N-1} a_j}, \quad c(z,0,N) = \frac{\det(z - J_{0,N+1})}{\prod_{j=0}^{N-1} a_j}$$

$$\Rightarrow \quad m_+(z) = -\frac{\prod_{l=1}^{N-1}(z-\nu_l)}{\prod_{j=1}^{N}(z-\lambda_j)}.$$

□

The ξ function is defined by

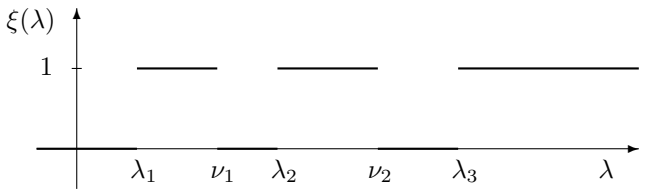
$$\xi(\lambda, n) = \frac{1}{\pi} \lim_{\epsilon \downarrow 0} \arg m_+(\lambda + i\epsilon, n) \quad \text{for a.e. } \lambda \in \mathbb{R}, \tag{5.7}$$

where $\arg(.) \in (-\pi, \pi]$. We set $\xi(\lambda, 0) = \xi(\lambda)$. Again we have to study the sign changes of $m_+(z)$ as $z \in \mathbb{R}$ moves along the real line. Remember that $m_+(z)$ is continuous and real for $z \in \mathbb{R}$. For $z < \lambda_1$, $m_+(z) > 0$ by (5.6), this implies $\xi(z) = 0$. After the first pole, $z = \lambda_1$, $m_+(z)$ becomes negative and thus $\xi(z) = 1$. At $z = \nu_1$, the sign changes again and so on. For $z > \lambda_N$, $m_+(z) < 0$ and therefore $\xi(z) = 1$. We conclude

Lemma 5.3.

$$\xi(\lambda) = \sum_{j=1}^{N-1} \chi_{(\lambda_j, \nu_j)}(\lambda) + \chi_{(\lambda_N, \infty)}(\lambda) \quad \textit{for a.e. } \lambda \in \mathbb{R}, \tag{5.8}$$

where $\chi_\Omega(.)$ denotes the characteristic function of the set $\Omega \subseteq \mathbb{R}$, $\lambda_1 < \ldots < \lambda_N$ are the eigenvalues of H_N and $\nu_1 < \ldots < \nu_{N-1}$ the eigenvalues of $H_{1,N+1}$. $\xi(\lambda)$ for H_3 is depicted below.



5.2 Trace Formulas for Finite Jacobi Operators

In [3], trace formulas for finite Jacobi operators are derived. We will give another proof based on the results for arbitrary Jacobi operators in Chapter 4 and we will extend the results in [3] to higher order trace relations.

For our investigations we will need the exponential Herglotz representation of $m_+(z)$.

Proposition 5.4.

$$m_+(z) = \frac{1}{\lambda_N - z} \exp\left(\int_{\lambda_1}^{\nu_{N-1}} \frac{\xi(\lambda) d\lambda}{\lambda - z} \right). \tag{5.9}$$

Proof. $m_+(z)$ is a Herglotz function by the conclusions of Lemma 2.5 and its exponential Herglotz representation reads by Theorem A.2 ($c = \ln|m_+(i)|$)

$$\begin{aligned} m_+(z) &= \exp\left(c + \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) \xi(\lambda) d\lambda \right) \\ &= \exp\left(c + \int_{\lambda_1}^{\lambda_N} \frac{1}{\lambda - z} \xi(\lambda) d\lambda + \int_{\lambda_N}^{\infty} \frac{1}{\lambda - z} d\lambda - \int_{\mathbb{R}} \frac{\lambda}{1+\lambda^2} \xi(\lambda) d\lambda \right) \\ &= \exp\left(\tilde{c} + \int_{\lambda_1}^{\nu_{N-1}} \frac{1}{\lambda - z} \xi(\lambda) d\lambda \right) \frac{1}{\lambda_N - z}, \end{aligned}$$

where we collected the terms which are independent of z in $\tilde{c}$,

$$\tilde{c} = \ln|m_+(i)| - \int_{\lambda_1}^{\nu_{N-1}} \frac{\lambda}{1+\lambda^2} \xi(\lambda) d\lambda + \frac{\ln(1+\lambda_N^2)}{2}.$$

Fortunately, we do not have to show directly that $\tilde{c} = 0$ since we infer by the asymptotic expansion of $m_+(z)$

$$\begin{aligned} m_+(z) &= -\frac{1}{z} + O(z^{-2}) \\ &= \exp\left(\tilde{c} + O(z^{-1}) \right) \frac{1}{\lambda_N - z} \\ &= \frac{\exp(\tilde{c})}{\lambda_N - z} \left(1 + O(z^{-1}) \right) \\ &= -\frac{\exp(\tilde{c})}{z} \left(1 + O(z^{-1}) \right) \\ \Rightarrow \quad \exp(\tilde{c}) &= 1 \quad \Rightarrow \quad \tilde{c} = 0. \end{aligned}$$

□

Theorem 5.5. ([3]). *Assume $N \in \mathbb{N}$ and let $\lambda_1 < \ldots < \lambda_N$ be the eigenvalues of $H_N = H_{0,N+1}$ and $\nu_1 < \ldots < \nu_{N-1}$ the eigenvalues of $H_{1,N+1}$. Then*

$$b_1 = \lambda_N - \int_{\lambda_1}^{\nu_{N-1}} \xi(\lambda) d\lambda = \sum_{j=1}^{N} \lambda_j - \sum_{l=1}^{N-1} \nu_l, \tag{5.10}$$

$$2a_1^2 + b_1^2 = \lambda_N^2 - 2 \int_{\lambda_1}^{\nu_{N-1}} \lambda \, \xi(\lambda) d\lambda = \sum_{j=1}^{N} \lambda_j^2 - \sum_{l=1}^{N-1} \nu_l^2. \tag{5.11}$$

Proof. If we know that

$$b_1 = \lambda_N - \int_{\lambda_1}^{\nu_{N-1}} \xi(\lambda) d\lambda, \tag{5.12}$$

the second claim follows if we insert the explicit form of the ξ function (5.8)

$$\lambda_N - \int_{\lambda_1}^{\nu_{N-1}} \xi(\lambda) d\lambda = \lambda_N - \sum_{j=1}^{N-1} \lambda_j - \sum_{l=1}^{N-1} \nu_l,$$

this holds also for (5.11). To prove (5.12), we use (5.9), the exponential representation of $m_+(z)$,

$$\begin{aligned} m_+(z) &= \frac{1}{\lambda_N - z} \exp\left(\int_{\lambda_1}^{\nu_{N-1}} \frac{\xi(\lambda, n) d\lambda}{\lambda - z} \right) \\ &= \frac{1}{\lambda_N - z} \exp\left(-\sum_{k=0}^{\infty} \frac{1}{z^{k+1}} \int_{\lambda_1}^{\nu_{N-1}} \lambda^k \xi(\lambda) d\lambda \right). \end{aligned}$$

Abbreviate now $c_k = \int \lambda^k \xi(\lambda) d\lambda$, then

$$\begin{aligned} m_+(z) &= \frac{1}{\lambda_N - z} \exp\left(-\sum_{k=0}^{\infty} \frac{c_k}{z^{k+1}} \right) \\ &= \frac{1}{\lambda_N - z} \prod_{k=0}^{\infty} \exp\left(-\frac{c_k}{z^{k+1}} \right) \\ &= \frac{1}{-z(1 - \lambda_N z^{-1})} \prod_{k=0}^{\infty} \left(\sum_{j=0}^{\infty} \left(-\frac{c_k}{z^{k+1}} \right)^j \frac{1}{j!} \right) \\ &= \left(-\frac{1}{z} - \frac{\lambda_N}{z^2} - \frac{\lambda_N^2}{z^3} - \cdots \right) \left(1 - \frac{c_0}{z} + \frac{c_0^2}{2!\, z^2} \pm \cdots \right) \\ &\quad \left(1 - \frac{c_1}{z^2} + \frac{c_1^2}{2!\, z^4} \pm \cdots \right) \cdots \\ &= -\frac{1}{z} - \frac{\lambda_N - c_0}{z^2} - \frac{\lambda_N^2 - \lambda_N c_0 + \frac{c_0^2}{2} - c_1}{z^3} + O(z^{-4}). \end{aligned}$$

The asymptotic expansion of $m_+(z)$ reads

$$m_+(z) = -\frac{1}{z} - \frac{b_1}{z^2} - \frac{a_1^2 + b_1^2}{z^3} + O(z^{-4})$$

and comparing coefficients yields

$$\begin{aligned} b_1 &= \lambda_N - c_0 = \lambda_N - \int_{\lambda_1}^{\nu_{N-1}} \xi(\lambda) d\lambda \\ a_1^2 + b_1^2 &= (\lambda_N - c_0)^2 + \lambda_N c_0 - \frac{c_0^2}{2} - c_1 \\ \Rightarrow \quad a_1^2 &= \lambda_N c_0 - \frac{c_0^2}{2} - c_1 \\ \Rightarrow \quad 2a_1^2 + b_1^2 &= \lambda_N^2 - 2c_1 = \lambda_N^2 - 2 \int_{\lambda_1}^{\nu_{N-1}} \lambda\, \xi(\lambda) d\lambda. \end{aligned}$$

□

The trace formulas in Theorem 5.5 are of course just the tip of the iceberg. In analogy to Theorem 4.1 we obtain the following result for finite operators.

Theorem 5.6. *Assume $N \in \mathbb{N}$. We have the following trace formulas for H_N*

$$b_1^{(l)} = \sum_{j=1}^{N} \lambda_j^l - \sum_{k=1}^{N-1} \nu_k^l, \tag{5.13}$$

where

$$b_1^{(1)} = b_1,$$

$$b_1^{(l)} = l\, m_{+,l} - \sum_{j=1}^{l-1} m_{+,l-j} b_1^{(j)}, \quad l \geq 2. \tag{5.14}$$

Proof. As in the proof of Theorem 4.1 we expand

$$\ln\left((\lambda_N - z) m_+(z)\right) = \int_{\lambda_1}^{\nu_{N-1}} \frac{\xi(\lambda, n) d\lambda}{\lambda - z}$$

using the Laurent expansion of $m_+(z)$

$$m_+(z) = -\sum_{j=0}^{\infty} \frac{m_{+,j}}{z^{j+1}}$$

and infer

$$\begin{aligned} b_1^{(l)} &= E_\infty^l - l \int_{E_0}^{E_\infty} \lambda^{l-1} \xi(\lambda) d\lambda \\ &= \lambda_N^l - l \int_{\lambda_1}^{\lambda_N} \lambda^{l-1} \xi(\lambda) d\lambda \\ &= \lambda_N^l - \lambda\Big|_{\lambda_1}^{\nu_1} - \cdots - \lambda^l\Big|_{\lambda_{N-1}}^{\nu_{N-1}} \\ &= \sum_{j=1}^{N} \lambda_j^l - \sum_{k=1}^{N-1} \nu_k^l. \end{aligned}$$

□

We can give a different proof for Theorem 5.2, that

$$m_+(z) = -\frac{\prod_{l=1}^{N-1}(z - \nu_l)}{\prod_{j=1}^{N}(z - \lambda_j)}, \tag{5.15}$$

if we insert the ξ function (5.8) in the representation (5.9) of $m_+(z)$. Be aware that this is a circular reasoning, since we derived the ξ function from Theorem 5.2, but there are of course other possible ways to calculate $\xi(\lambda)$. So this proof might be of interest on its own.

Proof of Theorem 5.2. By (5.9),

$$\begin{aligned} m_+(z) &= \frac{1}{\lambda_N - z} \exp\left(\int_{\lambda_1}^{\nu_{N-1}} \frac{\xi(\lambda, n) d\lambda}{\lambda - z} \right) \\ &= \frac{1}{\lambda_N - z} \exp\left(\int_{\lambda_1}^{\nu_1} \frac{1}{\lambda - z} d\lambda + \cdots + \int_{\lambda_{N-1}}^{\nu_{N-1}} \frac{1}{\lambda - z} d\lambda \right) \\ &= \frac{1}{\lambda_N - z} \exp\left(\ln\left(\frac{\nu_1 - z}{\lambda_1 - z} \right) + \cdots + \ln\left(\frac{\nu_{N-1} - z}{\lambda_{N-1} - z} \right) \right) \\ &= \frac{1}{\lambda_N - z} \prod_{j=1}^{N-1} \frac{\nu_j - z}{\lambda_j - z}. \end{aligned}$$

□

Corollary 5.7. ([3]). $\{\lambda_j\}_{j=1}^N \cup \{\nu_l\}_{l=1}^{N-1}$ *uniquely determine* H_N. *Any set of real* λ *and* ν *is allowed as long as*

$$\lambda_1 < \nu_1 < \lambda_2 < \nu_2 < \ldots < \lambda_N.$$

Proof. By (5.6), λ and ν determine $m_+(z)$ and by (3.10),

$$a_1^2 m_+(z, 1) + \frac{1}{m_+(z, 0)} = b_1 - z,$$

we see that $m_+(z, 0)$ determines a_n^2, b_n, and $m_+(z, n)$ for $n > 0$ (cf. Theorem 3.4 and the considerations for (3.9) and (3.10)).

By Theorem 5.1 the eigenvalues of H_N and $H_{1,N+1}$ are interlacing. □

5.3 The Inverse Spectral Problem

We already saw how spectral information determines H, H_N (cf. Theorem 3.2, Theorem 3.4 and Corollary 5.7). Now we will focus on the actual reconstruction of a_n^2, b_n from given spectral data for H_N and present an explicit expression of a_n^2, b_n in terms of the spectral data.

In Section 2.2 we derived an explicit expression of a_n^2, b_n in terms of the moments $m_{+,l}$. So it remains to express $m_{+,l}$ in terms of the spectral data.

The spectral measure of $m_+(z)$ is

$$d\rho_+(\lambda) = \sum_j h(\lambda_j)\, \delta(\lambda - \lambda_j) d\lambda \tag{5.16}$$

and if we insert $d\rho_+(\lambda)$ in (2.6) we infer

$$m_+(z) = \int_{\mathbb{R}} \frac{d\rho_+(\lambda)}{\lambda - z} = \sum_{j=1}^N \frac{h(\lambda_j)}{\lambda_j - z}. \tag{5.17}$$

We claim that $h(\lambda_j)$ is the residuum of $m_+(z)$ in λ_j. By (5.6),

$$m_+(z) = -\frac{\prod_{l=1}^{N-1}(z - \nu_l)}{\prod_{k=1}^{N}(z - \lambda_k)}.$$

Since λ_j is a pole of first order, the residuum in λ_j is

$$\begin{aligned} \mathrm{Res}_{\lambda_j} m_+(z) &= \lim_{z\to\lambda_j} (\lambda_j - z)\, m_+(z) \\ &= \frac{\prod_{l=1}^{N-1}(\lambda_j - \nu_l)}{\prod_{k\neq j}^{N}(\lambda_j - \lambda_k)} =: \alpha_j. \qquad (5.18) \\ \Rightarrow \quad m_+(z) &= \sum_{j=0}^{N} \frac{\alpha_j}{\lambda_j - z} \qquad (5.19) \\ \Rightarrow \quad \alpha_j &= h(\lambda_j). \end{aligned}$$

$\alpha_j > 0$ for all j since the eigenvalues are interlacing, $\lambda_1 < \nu_1 < \lambda_2 < \ldots < \lambda_N$. The condition $\alpha_j > 0$ would also follow from the Herglotz property of $m_+(z)$.

The moments $m_{+,j}$ of $d\rho_+$ (cf. (2.12)) are thus given by

$$m_{+,0} = \langle \delta_1, (H_+)^0 \delta_1 \rangle = 1 = \int_{\mathbb{R}} d\rho_+(\lambda) = \sum_{j=1}^{N} \alpha_j, \qquad (5.20)$$

$$m_{+,l} = \langle \delta_1, (H_+)^l \delta_1 \rangle = \int_{\mathbb{R}} \lambda^l d\rho_+(\lambda) = \sum_{j=1}^{N} \lambda_j^l \alpha_j. \qquad (5.21)$$

If we combine now (5.21) with (2.28) and (2.29), we obtain the following result.

Theorem 5.8. *Let $N \in \mathbb{N}$. Suppose the spectral data $\{\lambda_j\}_{j=1}^N$ and $\{\nu_l\}_{l=1}^{N-1}$, $\lambda_1 < \nu_1 < \lambda_2 < \ldots < \lambda_N$, corresponding to H_N are given and $\sum_j \alpha_j = 1$. Then the coefficients a^2, b of H_N can be expressed explicitly in terms of the spectral data*

$$a_k^2 = \frac{C(k-1)C(k+1)}{C(k)^2}, \qquad (5.22)$$

$$b_k = \frac{D(k)}{C(k)} - \frac{D(k-1)}{C(k-1)}, \qquad (5.23)$$

where $C(k)$ and $D(k)$ are defined as in (2.18) and (2.23) using

$$m_{+,l} = \sum_{j=1}^{N} \lambda_j^l \alpha_j.$$

Remark 5.9. Theorem 5.8 is a special case of [12], Theorem 8.5, where a certain class of reflectionless bounded Jacobi operators is considered. A Jacobi operator H is called **reflectionless** if for all $n \in \mathbb{Z}$,

$$\xi(\lambda, n) = \frac{1}{2} \quad \text{for a.e. } \lambda \in \sigma_{ess}(H). \qquad (5.24)$$

$\sigma_{ess}(H_N) = 0$ for finite Jacobi operators H_N, so [12], Theorem 8.5, holds for H_N as well.

In our results for finite Jacobi operators so far we saw that the eigenvalues $\{\lambda_j\}_{j=1}^N$ of H_N together with the eigenvalues $\{\nu_l\}_{l=1}^{N-1}$ of $H_{1,N+1}$ uniquely determine H_N.

Now we want to generalize this situation in the following way. If we split $H_N = H_{0,N+1}$ at n $(0 < n < N+1)$ into $H_{-,n}$ and $H_{+,n}$ by omitting the n-th line and column, is it possible to reconstruct H_N from the set $\{\lambda_j\}_{j=1}^N$ and the eigenvalues $\{\mu_k^-\}_{k=1}^{n-1}$, $\{\mu_l^+\}_{l=1}^{N-n}$ of $H_{-,n}$ and $H_{+,n}$? From this point of view our results above cover the case $n = 1$ (and by reflection the case $n = N$).

$$H_N = \left(\begin{array}{c|c|c} H_{-,n} & & \\ & a_{n-1} & \\ \hline & a_{n-1} \quad b_n & a_n \\ \hline & a_n & \\ & & H_{+,n} \end{array}\right)$$

For the proof we will need the following representation of the Green function $g(z,n) = G_{0,N+1}(z,n,n)$ of H_N $(0 < n < N+1)$.

Proposition 5.10.

$$g(z,n) = -\frac{\prod_{k=1}^{n-1}(z-\mu_k^-)\prod_{l=1}^{N-n}(z-\mu_l^+)}{\prod_{j=1}^{N}(z-\lambda_j)}. \tag{5.25}$$

Proof. By (5.5),

$$\begin{aligned} g(z,n) &= \frac{s(z,n,0)c(z,n,N)}{W(s(z),c(z))} \\ &= \frac{s(z,n,0)c(z,n,N)}{a_0\big(s(z,0,0)c(z,1,N) - s(z,1,0)c(z,0,N)\big)}. \end{aligned}$$

$s(z,0,0) = 0$, $s(z,1,0) = 1$ and we obtain from (1.10) and (1.11)

$$\begin{aligned} s(z,n,0) &= \frac{\det(z-J_{0,n})}{\prod_{j=1}^{n-1} a_j}, \\ c(z,n,N) &= \frac{\det(z-J_{n,N+1})}{\prod_{j=n}^{N-1} a_j}, \\ c(z,0,N) &= \frac{\det(z-J_{0,N+1})}{\prod_{j=0}^{N-1} a_j} \\ \Rightarrow \quad g(z,n) &= -\frac{\det(z-J_{0,n})\det(z-J_{n,N+1})}{\det(z-J_{0,N+1})} \\ &= -\frac{\prod_{k=1}^{n-1}(z-\mu_k^-)\prod_{l=1}^{N-n}(z-\mu_l^+)}{\prod_{j=1}^{N}(z-\lambda_j)}. \end{aligned}$$

□

Thus we gained an expression for $g(z,n)$ involving only the desired data. From (2.4) we know that

$$-\frac{1}{g(z,n)} = z - b_n + a_n^2 m_+(z,n) + a_{n-1}^2 m_-(z,n), \tag{5.26}$$

$m_-(z,n)$ and $m_+(z,n)$ uniquely determine $H_{-,n}$ and $H_{+,n}$ (cf. (3.9), (3.10)). ¿From our previous considerations we know the form of $m_\pm(z)$ (cf. (5.19)), so we make the following ansatz for $m_\pm(z,n)$

$$m_-(z,n) = \sum_{k=1}^{n-1} \frac{\alpha_k^-}{\mu_k^- - z}, \qquad \alpha_k^- > 0, \tag{5.27}$$

$$m_+(z,n) = \sum_{l=1}^{N-n} \frac{\alpha_l^+}{\mu_l^+ - z}, \qquad \alpha_l^+ > 0, \tag{5.28}$$

where α_k^-, α_l^+ denote the unknown residues. We assume $\{\mu_k^-\}_k \cap \{\mu_l^+\}_l = \emptyset$ and consider the general case later.

Evaluation of the first moments (cf. (5.20)) shows that

$$\sum_{k=1}^{n-1} \alpha_k^- = 1, \qquad \sum_{l=1}^{N-n} \alpha_l^+ = 1. \tag{5.29}$$

Inserting our ansatz in (5.26) we obtain

$$\begin{aligned} \frac{\prod_{j=1}^{N}(z-\lambda_j)}{\prod_{k=1}^{n-1}(z-\mu_k^-)\prod_{l=1}^{N-n}(z-\mu_l^+)} &= z - b_n - a_n^2 \sum_{l=1}^{N-n} \frac{\alpha_l^+}{z-\mu_l^+} \\ &\quad - a_{n-1}^2 \sum_{k=1}^{n-1} \frac{\alpha_k^-}{z-\mu_k^-}. \end{aligned} \tag{5.30}$$

$$\begin{aligned} \prod_{j=1}^{N}(z-\lambda_j) &= (z-b_n)\prod_{k=1}^{n-1}(z-\mu_k^-)\prod_{l=1}^{N-n}(z-\mu_l^+) \\ &\quad - a_n^2 \sum_{l=1}^{N-n} \alpha_l^+ \prod_{k=1}^{n-1}(z-\mu_k^-)\prod_{m\neq l}(z-\mu_m^+) \\ &\quad - a_{n-1}^2 \sum_{k=1}^{n-1} \alpha_k^- \prod_{m\neq k}(z-\mu_m^-)\prod_{l=1}^{N-n}(z-\mu_l^+). \end{aligned} \tag{5.31}$$

If we compare coefficients of z^{N-1} we infer

$$\begin{aligned} -\sum_{j=1}^{N}\lambda_j &= -\sum_{k=1}^{n-1}\mu_k^- - \sum_{l=1}^{N-n}\mu_l^+ - b_n \\ \Rightarrow \quad b_n &= \sum_{j=1}^{N}\lambda_j - \sum_{k=1}^{n-1}\mu_k^- - \sum_{l=1}^{N-n}\mu_l^+. \end{aligned} \tag{5.32}$$

This is a simple trace formula we knew all along. To determine the unknown residues α_l^+ and α_k^- we first set $z = \mu_i^-$, $1 \le i \le n-1$, in (5.31)

$$\prod_{j=1}^{N}(\mu_i^- - \lambda_j) = 0 - 0 - a_{n-1}^2 \alpha_i^- \prod_{l\neq i}(\mu_i^- - \mu_l^-) \prod_{l=1}^{N-n}(\mu_i^- - \mu_l^+). \tag{5.33}$$

Then

$$\beta_i^- := a_{n-1}^2 \alpha_i^- = -\frac{\prod_{j=1}^{N}(\mu_i^- - \lambda_j)}{\prod_{l\neq i}(\mu_i^- - \mu_l^-)\prod_{l=1}^{N-n}(\mu_i^- - \mu_l^+)} \tag{5.34}$$

is uniquely determined and since $\sum \alpha_i^- = 1$ (cf. (5.29)),

$$\sum_{i=1}^{n-1} \beta_i^- = a_{n-1}^2. \tag{5.35}$$

This uniquely determines α_i^- for $i = 1, \ldots, n-1$

$$\alpha_i^- = \frac{\beta_i^-}{a_{n-1}^2}. \tag{5.36}$$

In analogy, for $l = 1, \ldots, N-n$,

$$\alpha_l^+ = \frac{\beta_l^+}{a_n^2}, \tag{5.37}$$

where

$$\beta_l^+ = -\frac{\prod_{j=1}^{N}(\mu_l^+ - \lambda_j)}{\prod_{k=1}^{n-1}(\mu_l^+ - \mu_k^-)\prod_{p\neq l}(\mu_l^+ - \mu_p^+)}, \tag{5.38}$$

$$a_n^2 = \sum_{l=1}^{N-n} \beta_l^+. \tag{5.39}$$

It remains to consider the necessary conditions on the sets of eigenvalues to obtain $\alpha_l^+ > 0$ and $\alpha_k^- > 0$ for all l, k.

Lemma 5.11. *Set $\{\mu_j\}_j = \{\mu_k^-\}_k \cup \{\mu_l^+\}_l$. λ_j denote the eigenvalues of H_N, μ_k^- and μ_l^+ the eigenvalues of $H_{-,n}$ and $H_{+,n}$.*

(i) $\lambda_1 < \mu_1 \le \lambda_2 \le \mu_2 \le \ldots < \lambda_N$

(ii) $\mu_k^- = \mu_l^+ \quad \Rightarrow \quad \mu_k^- = \mu_l^+ = \lambda_j$

Remark 5.12. For the splitting points $n = 1$, $n = N$ the inequalities in (i) are strict, so (ii) cannot happen. If $\mu_k^- = \lambda_j$ or $\mu_l^+ = \lambda_j$, one obtains by the same proof that $\mu_k^- = \mu_l^+ = \lambda_j$.

Proof. (i) The eigenvalues of a Jacobi operator are all real and simple, so we order them accordingly. Furthermore, it is well known that the poles and roots of a Herglotz function must be interlacing. $g(z, n)$ is Herglotz, so (i) follows from Proposition 5.10

$$g(z,n) = -\frac{\prod_{k=1}^{n-1}(z - \mu_k^-)\prod_{l=1}^{N-n}(z - \mu_l^+)}{\prod_{j=1}^{N}(z - \lambda_j)}.$$

(ii) By Theorem 5.1,

(1) $\lambda \in \sigma(H_{-,n_0}) \quad \Leftrightarrow \quad s(\lambda, n_0, 0) = 0$

(2) $\lambda \in \sigma(H_{+,n_0}) \quad \Leftrightarrow \quad s(\lambda, N, n_0) = 0$

(3) $\lambda \in \sigma(H_N) \quad \Leftrightarrow \quad s(\lambda, N, 0) = 0.$

Suppose (1) and (2) hold for λ,

$$s(\lambda, N, n_0) = 0 = s(\lambda, n_0, 0)$$

$$\Rightarrow \quad s(\lambda, N, n) = c\, s(\lambda, n, 0), \quad c \in \mathbb{R}\backslash\{0\}.$$

Since

$$0 = s(\lambda, N, N) = c\, s(\lambda, N, 0)$$

$$\Rightarrow \quad s(\lambda, N, 0) = 0 \qquad \Rightarrow \quad (3).$$

In the same manner (2) and (3) imply (1), as well as (3) and (1) imply (2). □

If we insert the assumption $\lambda_1 < \mu_1 < \lambda_2 < \mu_2 < \ldots < \lambda_N$, $\{\mu_j\}_j = \{\mu_k^-\}_k \cup \{\mu_l^+\}_l$, into

$$\beta_i^- = -\frac{\prod_{j=1}^{N}(\mu_i^- - \lambda_j)}{\prod_{l\neq i}(\mu_i^- - \mu_l^-)\prod_{l=1}^{N-n}(\mu_i^- - \mu_l^+)},$$

we obtain $\beta_i^- > 0$ and hence $\alpha_i^- > 0$ for $1 \leq i \leq n-1$ as desired. Analogously we infer $\alpha_l^+ > 0$ for $1 \leq l \leq N-n$. If we follow now the Weyl m-function reconstruction starting with $m_\pm(z, n)$, $H_{-,n}$ and $H_{+,n}$ are uniquely determined, as well as a_{n-1}^2, a_n^2, b_n.

It remains to show that $\lambda_1, \ldots, \lambda_N$ are indeed the eigenvalues of the Jacobi operator H_N we constructed above. But this is clear from Proposition 5.10, since the Green function $g(z, n)$ of H_N has poles exactly at the eigenvalues of H_N.

If $\mu_k^- = \mu_l^+ = \lambda_j$, the pole and one root cancel out and a root at $z = \lambda_j$ remains. Thus roots instead of poles in the set $\{\lambda_j\}$ indicate colliding eigenvalues. We will reconsider the proof for the case $\sigma(H_{-,n}) \cap \sigma(H_{+,n}) \neq \emptyset$ immediately, but before we have to introduce additional data σ_j.

Hypothesis 5.13. The spectral data of two submatrices of H_N are given by

$$\{\mu_j, \sigma_j\}_j,$$

where $\{\mu_j\}_j = \{\mu_k^-\}_k \cup \{\mu_l^+\}_l$. If $\mu_k^- = \mu_l^+ = \mu_j$, σ_j is determined by (5.42)

$$\sigma_j = \frac{a_n^2\alpha_l^+ - a_{n-1}^2\alpha_k^-}{a_n^2\alpha_l^+ + a_{n-1}^2\alpha_k^-} \in (-1, 1),$$

otherwise

$$\begin{aligned} \sigma_j &= -1 \quad \text{if} \quad \mu_j = \mu_k^-, \\ \sigma_j &= 1 \quad \text{if} \quad \mu_j = \mu_l^+. \end{aligned}$$

σ_j is either ± 1 (depending on whether μ_j is an eigenvalue of $H_{-,n}$ or $H_{+,n}$) or in $(-1, 1)$ (if μ_j is an eigenvalue of both submatrices and hence also of H_N).

Until now we have proven a special case of the following theorem.

Theorem 5.14. *Let $1 \leq n \leq N$ and denote $\sigma(H_N) = \{\lambda_j\}_{j=1}^N$, $\sigma(H_{-,n}) = \{\mu_k^-\}_{k=1}^{n-1}$ and $\sigma(H_{+,n}) = \{\mu_l^+\}_{l=1}^{N-n}$. Assume Hypothesis 5.13.*

The sets $\{\lambda_j\}_j$, $\{\mu_j, \sigma_j\}_j$ uniquely determine H_N. A corresponding H_N exists if and only if $\lambda_1 < \mu_1 \leq \lambda_2 \leq \ldots < \lambda_N$.

Proof. If $\lambda_1 < \mu_1 < \lambda_2 < \ldots < \lambda_N$, H_N can be reconstructed uniquely from (5.32), (5.34) - (5.39) by the proof above. It remains to consider the case $\mu_{j_0} = \mu_{k_0}^- = \mu_{l_0}^+ \, (= \lambda_{j_0})$, so $\sigma_{j_0} \in (-1, 1)$. The proof is the same in this case, except that some terms in (5.34) and (5.38) vanish. (5.30) becomes

$$\begin{aligned} \frac{\prod_{j \neq j_0}(z - \lambda_j)}{\prod_k (z - \mu_k^-) \prod_{l \neq l_0}(z - \mu_l^+)} &= z - b_n - a_n^2 \sum_{l \neq l_0} \frac{\alpha_l^+}{z - \mu_l^+} \\ &\quad - a_{n-1}^2 \sum_{k \neq k_0} \frac{\alpha_k^-}{z - \mu_k^-} - \frac{a_n^2 \alpha_{l_0}^+ + a_{n-1}^2 \alpha_{k_0}^-}{z - \mu_{j_0}}. \end{aligned}$$

Following the calculations thereafter, we obtain (insert $z = \mu_{j_0}$)

$$a_n^2 \alpha_{l_0}^+ + a_{n-1}^2 \alpha_{k_0}^- = - \frac{\prod_{j \neq j_0}(\mu_{j_0} - \lambda_j)}{\prod_{k \neq k_0}(\mu_{j_0} - \mu_k^-) \prod_{l \neq l_0}(\mu_{j_0} - \mu_l^+)} =: \delta_{j_0}. \tag{5.40}$$

Now the additional data σ_{j_0} distributes this sum among $\alpha_{k_0}^-$ and $\alpha_{l_0}^+$

$$\begin{aligned} \beta_{k_0}^- &= \frac{1 - \sigma_{j_0}}{2} \, \delta_{j_0} \qquad & \alpha_{k_0}^- &= \frac{\beta_{k_0}^-}{a_{n-1}^2} = \frac{1 - \sigma_{j_0}}{2} \frac{\delta_{j_0}}{a_{n-1}^2}, \\ \beta_{l_0}^+ &= \frac{1 + \sigma_{j_0}}{2} \, \delta_{j_0} \qquad & \alpha_{l_0}^+ &= \frac{\beta_{l_0}^+}{a_n^2} = \frac{1 + \sigma_{j_0}}{2} \frac{\delta_{j_0}}{a_n^2}. \end{aligned} \tag{5.41}$$

Positivity of the residues follows as before, since the terms which would be zero do not appear in (5.40). So H_N can be reconstructed uniquely from (5.32), (5.34) - (5.39), where (5.41) is to be used for α_{j_0} if $\sigma_{j_0} \in (-1, 1)$. □

Given an arbitrary Jacobi operator H_N with $\mu_{j_0} = \mu_{k_0}^- = \mu_{l_0}^+$, one can evaluate σ_{j_0} by

$$\sigma_{j_0} = \frac{a_n^2 \alpha_{l_0}^+ - a_{n-1}^2 \alpha_{k_0}^-}{a_n^2 \alpha_{l_0}^+ + a_{n-1}^2 \alpha_{k_0}^-}, \tag{5.42}$$

since

$$a_n^2 \alpha_{l_0}^+ - a_{n-1}^2 \alpha_{k_0}^- = \frac{1 + \sigma_{j_0}}{2} \, \delta_{j_0} - \frac{1 - \sigma_{j_0}}{2} \, \delta_{j_0} = \sigma_{j_0} \delta_{j_0}.$$

Theorem 5.15. *Let $1 \leq n \leq N$ and $\{\mu_j\}_j = \{\mu_k^-\}_k \cup \{\mu_l^+\}_l$. The following parametrizations of a $N \times N$ Jacobi matrix H_N determine each other and the maps between these parameters are real bianalytic diffeomorphisms.*

(i) $\{a_n\}_{n=1}^{N-1} \cup \{b_n\}_{n=1}^N$ $(a_n > 0)$.

(ii) $\{\lambda_j\}_{j=1}^N \cup \{\mu_k^-\}_{k=1}^{n-1} \cup \{\mu_l^+\}_{l=1}^{N-n}$ $(\lambda_1 < \mu_1 < \lambda_2 < \ldots < \lambda_N)$.

(iii) $\{\mu_k^-\}_{k=1}^{n-1} \cup \{\mu_l^+\}_{l=1}^{N-n} \cup \{\beta_k^-\}_k \cup \{\beta_l^+\}_l \cup \{b_n\}$ $(\mu_1 < \ldots < \mu_{N-1}, \beta_j^\pm > 0)$.

There are $2N-1$ parameters. a_n, b_n are the coefficients of H_N and $\sigma(H_N) = \{\lambda_j\}_j$, $\sigma(H_{-,n}) = \{\mu_k^-\}_k$, $\sigma(H_{+,n}) = \{\mu_l^+\}_l$. $\beta_j^\pm$ are the residues of the poles in $m_\pm(z,n)$ up to a constant

$$m_\pm(z,n) = \sum_j \frac{\alpha_j^\pm}{\mu_j^\pm - z},$$

where

$$\alpha_j^+ = \frac{\beta_j^+}{a_n^2}, \quad \alpha_j^- = \frac{\beta_j^-}{a_{n-1}^2}.$$

Proof. It is known that the map from the N coefficients of a monic polynomial of degree N to the roots $\lambda_1, \ldots, \lambda_N$ of that polynomial is a bianalytic diffeomorphism in the region where the roots are all real and distinct. The determinant of the Jacobian matrix of this transformation map is $\pm \prod_{j<k}(\lambda_j - \lambda_k)^{-1}$ (cf. [9]). Since all eigenvalues are real and simple, the map from (i) to (ii) is real analytic.

The map from (ii) to (iii) is rational by (5.34), (5.38) and (5.32)

$$\begin{aligned}
\beta_i^- &= -\frac{\prod_{j=1}^N (\mu_i^- - \lambda_j)}{\prod_{l\neq i}(\mu_i^- - \mu_l^-)\prod_{l=1}^{N-n}(\mu_i^- - \mu_l^+)}, \\
\beta_l^+ &= -\frac{\prod_{j=1}^N (\mu_l^+ - \lambda_j)}{\prod_{k=1}^{n-1}(\mu_l^+ - \mu_k^-)\prod_{p\neq l}(\mu_l^+ - \mu_p^+)}, \\
b_n &= \sum_{j=1}^N \lambda_j - \sum_{k=1}^{n-1} \mu_k^- - \sum_{l=1}^{N-n} \mu_l^+.
\end{aligned}$$

$\sum \beta_i^- = a_{n-1}^2$, $\sum \beta_l^+ = a_n^2$ and the Weyl m-function reconstruction of $H_{-,n}$ and $H_{+,n}$ from

$$m_\pm(z,n) = \sum_j \frac{\alpha_j^\pm}{\mu_j^\pm - z}$$

shows that the coefficients a, b are real analytic functions of (iii). □

Theorem 5.16. *$\{\lambda_j\}_{j=1}^N \cup \{\mu_k^-\}_{k=1}^{n-1} \cup \{\mu_l^+\}_{l=1}^{N-n}$ uniquely determine H_N. Any set of real λ and μ is allowed as long as*

$$\lambda_1 < \mu_1 < \lambda_2 < \mu_2 < \ldots < \lambda_N,$$

where $\{\mu_j\}_j = \{\mu_k^-\}_k \cup \{\mu_l^+\}_l$.

Corollary 5.17. ([3]). *The following parametrizations of H_N determine each other and the maps between these parameters are real bianalytic diffeomorphisms.*

(i) $\{a_n\}_{n=1}^{N-1} \cup \{b_n\}_{n=1}^N$ $(a_n > 0)$.

(ii) $\{\lambda_j\}_{j=1}^N \cup \{\nu_l\}_{l=1}^{N-1}$ $(\lambda_1 < \nu_1 < \lambda_2 < \ldots < \nu_{N-1} < \lambda_N)$.

(iii) $\{\lambda_j\}_{j=1}^N \cup \{\alpha_j\}_{j=1}^N$ $(\lambda_1 < \ldots < \lambda_N,\ \alpha_j > 0,\ \sum_{k=1}^N \alpha_k = 1)$.

λ_j are the eigenvalues of H_N, ν_l the eigenvalues of $H_{1,N+1}$ and α_j the residues of the poles in $m_+(z)$

$$m_+(z) = \sum_{j=1}^{N} \frac{\alpha_j}{\lambda_j - z} \quad or \quad d\rho_+(\lambda) = \sum \alpha_j \, \delta(\lambda - \lambda_j) d\lambda.$$

At last we give an incomplete survey of spectral information which is sufficient to reconstruct a finite Jacobi operator uniquely. Unlike our case, the following theorems do not assert the existence of such an operator, but uniqueness, if it exists.

Denote the coefficients $b_1, a_1, b_2, a_2 \ldots$ by a single sequence $c_1, c_2, \ldots$, so

$$c_{2n-1} = b_n, \qquad c_{2n} = a_n.$$

Theorem 5.18. ([7]). *Let $N \in \mathbb{N}$. Suppose that $c_{N+1}, \ldots, c_{2N-1}$ are known, as well as the eigenvalues $\lambda_1, \ldots, \lambda_N$ of H_{N+1}. Then $c_1, \ldots, c_N$ are uniquely determined.*

Proof. A proof can be found in [7], but it is modeled on that given in [6]. □

This result is sharpened in [3].

Theorem 5.19. ([3]). *Suppose that $1 \leq j \leq N$ and $c_{j+1}, \ldots, c_{2N-1}$ are known, as well as j of the eigenvalues. Then $c_1, \ldots, c_j$ are uniquely determined.*

Proof. A proof is given in [3]. Notice that one need not know which of the j eigenvalues one has. □

Define $H(b)_N$ to be the Jacobi operator where b_1 is replaced by $b_1 + b$

$$H(b)_N = H_N + b\langle \delta_1, . \rangle \delta_1.$$

Theorem 5.20. ([3]). *The eigenvalues $\lambda_1, \ldots, \lambda_N$ of H_N together with b and $N-1$ eigenvalues $\lambda(b)_1, \ldots, \lambda(b)_{N-1}$ of $H(b)_N$ uniquely determine H_N.*

$\lambda_1, \ldots, \lambda_N$ together with the N eigenvalues $\lambda(b)_1, \ldots, \lambda(b)_N$ of $H(b)_{N+1}$ (with b unknown) determine H_N and b.

Proof. A proof can be found in [3]. □

Appendix A

Herglotz Functions

[12], Appendix B, gives an extensive survey of Herglotz functions. We present the theorems we cited above and follow the notation of [12].

Set $\mathbb{C}_\pm = \{z \in \mathbb{C} \,|\, \pm \operatorname{Im}(z) > 0\}$. A function $F : \mathbb{C}_+ \to \mathbb{C}_+$ is called a Herglotz function (sometimes also Pick or Nevanlinna-Pick function), if F is analytic in $\mathbb{C}_+$. One usually defines F on $\mathbb{C}_-$ by $F(\overline{z}) = \overline{F(z)}$.

Herglotz functions can be characterized by

Theorem A.1. *F is a Herglotz function if and only if*

$$F(z) = a + b\,z + \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) d\rho(\lambda), \quad z \in \mathbb{C}, \tag{A.1}$$

where ρ is a measure on $\mathbb{R}$ which satisfies

$$\int_{\mathbb{R}} \frac{1}{1+\lambda^2} d\rho(\lambda) < \infty.$$

a, b, and ρ are determined by F using

$$\begin{aligned} a &= \operatorname{Re}\big(F(i)\big) \in \mathbb{R}, \\ b &= \lim_{\substack{z \to \infty \\ \operatorname{Im}(z) \geq \epsilon > 0}} \frac{F(z)}{z} \geq 0, \end{aligned}$$

and **Stieltjes inversion formula**

$$\rho\big((\lambda_0, \lambda_1]\big) = \lim_{\delta \downarrow 0} \lim_{\epsilon \downarrow 0} \frac{1}{\pi} \int_{\lambda_0 + \delta}^{\lambda_1 + \delta} \operatorname{Im}\big(F(\lambda + i\,\epsilon)\big) d\lambda. \tag{A.2}$$

We will use an alternate integral representation of Herglotz functions which we obtain by considering the logarithm $\ln(z)$. Let $\ln(z)$ be defined such that

$$\ln(z) = \ln|z| + i \arg(z), \quad -\pi < \arg(z) \leq \pi. \tag{A.3}$$

$\ln(z)$ is holomorphic and $\operatorname{Im}\big(\ln(z)\big) > 0$ for $z \in \mathbb{C}_+$, so $\ln(z)$ is a Herglotz function. The representation of $\ln(z)$ according to Theorem A.1 reads

$$\ln(z) = \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2} \right) \chi_{(-\infty,0)}(\lambda) d\lambda, \quad z \in \mathbb{C}_\pm.$$

The sum and the composition of two Herglotz functions are again Herglotz functions, so in particular, $\ln(F(z))$ is Herglotz. Thus, using the representation in Theorem A.1 for $\ln(F(z))$ we get another representation for $F(z)$.

Theorem A.2. *F is a Herglotz function if and only if it has the representation*

$$F(z) = \exp\left(c + \int_{\mathbb{R}} \left(\frac{1}{\lambda - z} - \frac{\lambda}{1+\lambda^2}\right) \xi(\lambda) d\lambda\right), \quad z \in \mathbb{C}_{\pm}, \tag{A.4}$$

where $c = \ln|F(i)| \in \mathbb{R}$ and $\xi \in L^1(\mathbb{R}, (1+\lambda^2)^{-1} d\lambda)$ is the ξ function (cf. [4])

$$\xi(\lambda) = \frac{1}{\pi} \lim_{\epsilon \downarrow 0} \operatorname{Im}\big(\ln\big(F(\lambda + i\epsilon)\big)\big) = \frac{1}{\pi} \lim_{\epsilon \downarrow 0} \arg\big(F(\lambda + i\epsilon)\big) \tag{A.5}$$

for a.e. $\lambda \in \mathbb{R}$ and $0 \le \xi(\lambda) \le 1$ for a.e. $\lambda \in \mathbb{R}$. Here $-\pi < \arg\big(F(\lambda + i\epsilon)\big) \le \pi$ according to the definition of $\ln(z)$.

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Curriculum Vitae

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