Contents

Preface

The name of the game

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 plays a fundamental role in the investigation of completely integrable nonlinear lattices, in particular the Toda lattice and its modified counterpart, the Kac-van Moerbeke lattice.

Why I have written this book

Whereas numerous books about Sturm-Liouville operators have been written, only few on Jacobi operators exist. In particular, there is currently no monograph available which covers all basic topics (like spectral and inverse spectral theory, scattering theory, oscillation theory and positive solutions, (quasi-)periodic operators, spectral deformations, etc.) typically found in textbooks on Sturm-Liouville operators.

In the case of the Toda lattice a textbook by M. Toda [**230**] exists, but none of the recent advances in the theory of nonlinear lattices are covered there.

Audience and prerequisites

As audience I had researchers in mind. This book can be used to get acquainted with selected topics as well as to look up specific results. Nevertheless, no previous knowledge on difference equations is assumed and all results are derived in a self-contained manner. Hence the present book is accessible to graduate students as well. Previous experience with Sturm-Liouville operators might be helpful but is not necessary. Still, a solid working knowledge from other branches of mathematics is needed. In particular, I have assumed that the reader is familiar with the theory of (linear) self-adjoint operators in Hilbert spaces which can be found in (e.g.)

[**192**] or [**241**]. This theory is heavily used in the first part. In addition, the reader might have to review material from complex analysis (see Appendix A and B) and differential equations on Banach manifolds (second part only) if (s)he feels (s)he does not have the necessary background. However, this knowledge is mainly needed for understanding proofs rather than the results themselves.

The style of this book

The style of this monograph is strongly influenced by my personal bias. I have striven to present an intuitive approach to each subject and to include the simplest possible proof for every result. Most proofs are rather sketchy in character, so that the main idea becomes clear instead of being drowned by technicalities. Nevertheless, I have always tried to include enough information for the reader to fill in the remaining details (her)himself if desired. To help researchers, using this monograph as a reference, to quickly spot the result they are looking for, most information is found in display style formulas.

The entire treatment is supposed to be mathematically rigorous. I have tried to prove *every* statement I make and, in particular, these little obvious things, which turn out less obvious once one tries to prove them. In this respect I had Marchenko's monograph on Sturm-Liouville operators [**167**] and the one by Weidmann [**241**] on functional analysis in mind.

Literature

The first two chapters are of an introductory nature and collect some well-known "folklore", the successive more advanced chapters are a synthesis of results from research papers. In most cases I have rearranged the material, streamlined proofs, and added further facts which are not published elsewhere. All results appear without special attribution to who first obtained them but there is a section entitled "Notes on literature" in each part which contains references to the literature plus hints for additional reading. The bibliography is selective and far from being complete. It contains mainly references I (am aware of and which I) have actually used in the process of writing this book.

Terminology and notation

For the most part, the terminology used agrees with generally accepted usage. Whenever possible, I have tried to preserve original notation. Unfortunately I had to break with this policy at various points, since I have given higher priority to a consistent (and self-explaining) notation throughout the entire monograph. A glossary of notation can be found towards the end.

Contents

For convenience of the reader, I have split the material into two parts; one on Jacobi operators and one on completely integrable lattices. In particular, the second part is to a wide extent independent of the first one and anybody interested only in completely integrable lattices can move directly to the second part (after browsing Chapter 1 to get acquainted with the notation).

Part I

Chapter 1 gives an introduction to the theory of second order difference equations and bounded Jacobi operators. All basic notations and properties are presented here. In addition, this chapter provides several easy but extremely helpful gadgets. We investigate the case of constant coefficients and, as a motivation for the reader, the infinite harmonic crystal in one dimension is discussed.

Chapter 2 establishes the pillars of spectral and inverse spectral theory for Jacobi operators. Here we develop what is known as discrete Weyl-Titchmarsh-Kodaira theory. Basic things like eigenfunction expansions, connections with the moment problem, and important properties of solutions of the Jacobi equation are shown in this chapter.

Chapter 3 considers qualitative theory of spectra. It is shown how the essential, absolutely continuous, and point spectrum of specific Jacobi operators can be located in some cases. The connection between existence of α-subordinate solutions and α-continuity of spectral measures is discussed. In addition, we investigate under which conditions the number of discrete eigenvalues is finite.

Chapter 4 covers discrete Sturm-Liouville theory. Both classical oscillation and renormalized oscillation theory are developed.

Chapter 5 gives an introduction to the theory of random Jacobi operators. Since there are monographs (e.g., [**40**]) devoted entirely to this topic, only basic results on the spectra and some applications to almost periodic operators are presented.

Chapter 6 deals with trace formulas and asymptotic expansions which play a fundamental role in inverse spectral theory. In some sense this can be viewed as an application of Krein's spectral shift theory to Jacobi operators. In particular, the tools developed here will lead to a powerful reconstruction procedure from spectral data for reflectionless (e.g., periodic) operators in Chapter 8.

Chapter 7 considers the special class of operators with periodic coefficients. This class is of particular interest in the one-dimensional crystal model and several profound results are obtained using Floquet theory. In addition, the case of impurities in one-dimensional crystals (i.e., perturbation of periodic operators) is studied.

Chapter 8 again considers a special class of Jacobi operators, namely reflectionless ones, which exhibit an algebraic structure similar to periodic operators. Moreover, this class will show up again in Chapter 10 as the stationary solutions of the Toda equations.

Chapter 9 shows how reflectionless operators with no eigenvalues (which turn out to be associated with quasi-periodic coefficients) can be expressed in terms of Riemann theta functions. These results will be used in Chapter 13 to compute explicit formulas for solutions of the Toda equations in terms of Riemann theta functions.

Chapter 10 provides a comprehensive treatment of (inverse) scattering theory for Jacobi operators with constant background. All important objects like reflection/transmission coefficients, Jost solutions and Gel'fand-Levitan-Marchenko equations are considered. Again this applies to impurities in one-dimensional crystals. Furthermore, this chapter forms the main ingredient of the inverse scattering transform for the Toda equations.

Chapter 11 tries to deform the spectra of Jacobi operators in certain ways. We compute transformations which are isospectral and such which insert a finite number of eigenvalues. The standard transformations like single, double, or Dirichlet commutation methods are developed. These transformations can be used as powerful tools in inverse spectral theory and they allow us to compute new solutions from old solutions of the Toda and Kac-van Moerbeke equations in Chapter 14.

Part II

Chapter 12 is the first chapter on integrable lattices and introduces the Toda system as hierarchy of evolution equations associated with the Jacobi operator via the standard Lax approach. Moreover, the basic (global) existence and uniqueness theorem for solutions of the initial value problem is proven. Finally, the stationary hierarchy is investigated and the Burchnall-Chaundy polynomial computed.

Chapter 13 studies various aspects of the initial value problem. Explicit formulas in case of reflectionless (e.g., (quasi-)periodic) initial conditions are given in terms of polynomials and Riemann theta functions. Moreover, the inverse scattering transform is established.

The final Chapter 14 introduces the Kac van-Moerbeke hierarchy as modified counterpart of the Toda hierarchy. Again the Lax approach is used to establish the basic (global) existence and uniqueness theorem for solutions of the initial value problem. Finally, its connection with the Toda hierarchy via a Miura-type transformation is studied and used to compute N-soliton solutions on arbitrary background.

Appendix

Appendix A reviews the theory of Riemann surfaces as needed in this monograph. While most of us will know Riemann surfaces from a basic course on complex analysis or algebraic geometry, this will be mainly from an abstract viewpoint like in [**86**] or [**129**], respectively. Here we will need a more "computational" approach and I hope that the reader can extract this knowledge from Appendix A.

Appendix B compiles some relevant results from the theory of Herglotz functions and Borel measures. Since not everybody is familiar with them, they are included for easy reference.

Appendix C shows how a program for symbolic computation, `Mathematica`®, can be used to do some of the computations encountered during the main bulk. While I don't believe that programs for symbolic computations are an indispensable tool for doing research on Jacobi operators (or completely integrable lattices), they are at least useful for checking formulas. Further information and `Mathematica`®notebooks can be found at

`http://www.mat.univie.ac.at/~gerald/ftp/book-jac/`

respectively

`ftp://ftp.mat.univie.ac.at/pub/teschl/book-jac/`

Acknowledgments

This book has greatly profited from collaborations and discussions with W. Bulla, F. Gesztesy, H. Holden, M. Krishna, and B. Simon. In addition, many people generously devoted considerable time and effort to reading earlier versions of the manuscript and making many corrections. In particular, I wish to thank D. Damanik, H. Hanßmann, A. von der Heyden, R. Killip, T. Sørensen, S. Timischl, K. Unterkofler, and H. Widom. Next, I am happy to express my gratitude to P. Deift, J. Geronimo, and E. Lieb for helpful suggestions and advise. I also like to thank the staff at the American Mathematical Society for the fast and professional production of this book.

Partly supported by the Austrian Science Fund (`http://www.fwf.ac.at/`) under Grant No. P12864-MAT.

Finally, no book is free of errors. So if you find one, or if you have comments or suggestions, please let me know. I will make all corrections and complements available at the URL above.

Gerald Teschl

Vienna, Austria
May, 1999

Gerald Teschl
Institut für Mathematik
Universität Wien
Strudlhofgasse 4
1090 Wien, Austria

E-mail address: `gerald@mat.univie.ac.at`
URL: `http://www.mat.univie.ac.at/~gerald/`

Chapter 1

Jacobi operators

This chapter introduces to the theory of second order difference equations and Jacobi operators. All the basic notation and properties are presented here. In addition, it provides several easy but extremely helpful gadgets. We investigate the case of constant coefficients and, as an application, discuss the infinite harmonic crystal in one dimension.

1.1. General properties

The issue of this section is mainly to fix notation and to establish all for us relevant properties of symmetric three-term recurrence relations in a self-contained manner.

We start with some preliminary notation. For $I \subseteq \mathbb{Z}$ and M a set we denote by $\ell(I, M)$ the set of M-valued sequences $(f(n))_{n\in I}$. Following common usage we will frequently identify the sequence $f = f(.) = (f(n))_{n\in I}$ with $f(n)$ whenever it is clear that n is the index (I being understood). We will only deal with the cases $M = \mathbb{R}$, $\mathbb{R}^2$, $\mathbb{C}$, and $\mathbb{C}^2$. Since most of the time we will have $M = \mathbb{C}$, we omit M in this case, that is, $\ell(I) = \ell(I, \mathbb{C})$. For $N_1, N_2 \in \mathbb{Z}$ we abbreviate $\ell(N_1, N_2) = \ell(\{n \in \mathbb{Z} | N_1 < n < N_2\})$, $\ell(N_1, \infty) = \ell(\{n \in \mathbb{Z} | N_1 < n\})$, and $\ell(-\infty, N_2) = \ell(\{n \in \mathbb{Z} | n < N_2\})$ (sometimes we will also write $\ell(N_2, -\infty)$ instead of $\ell(-\infty, N_2)$ for notational convenience). If M is a Banach space with norm $|.|$, we define

$$\begin{aligned} \ell^p(I, M) &= \{f \in \ell(I, M) | \sum_{n\in I} |f(n)|^p < \infty\}, \quad 1 \le p < \infty, \\ \ell^\infty(I, M) &= \{f \in \ell(I, M) | \sup_{n\in I} |f(n)| < \infty\}. \end{aligned} \tag{1.1}$$

Introducing the following norms

$$\|f\|_p = \left(\sum_{n\in I} |f(n)|^p \right)^{1/p}, \ 1 \le p < \infty, \qquad \|f\|_\infty = \sup_{n\in I} |f(n)|, \tag{1.2}$$

makes $\ell^p(I, M)$, $1 \le p \le \infty$, a Banach space as well.

Furthermore, $\ell_0(I,M)$ denotes the set of sequences with only finitely many values being nonzero and $\ell^p_\pm(\mathbb{Z},M)$ denotes the set of sequences in $\ell(\mathbb{Z},M)$ which are ℓ^p near $\pm\infty$, respectively (i.e., sequences whose restriction to $\ell(\pm\mathbb{N},M)$ belongs to $\ell^p(\pm\mathbb{N},M)$. Here $\mathbb{N}$ denotes the set of positive integers). Note that, according to our definition, we have

$$\ell_0(I,M) \subseteq \ell^p(I,M) \subseteq \ell^q(I,M) \subseteq \ell^\infty(I,M), \quad p < q, \tag{1.3}$$

with equality holding if and only if I is finite (assuming $\dim M > 0$).

In addition, if M is a (separable) Hilbert space with scalar product $\langle .,..\rangle_M$, then the same is true for $\ell^2(I,M)$ with scalar product and norm defined by

$$\langle f,g\rangle = \sum_{n\in I} \langle f(n), g(n)\rangle_M,$$
$$\|f\| = \|f\|_2 = \sqrt{\langle f,f\rangle}, \quad f,g \in \ell^2(I,M). \tag{1.4}$$

For what follows we will choose $I = \mathbb{Z}$ for simplicity. However, straightforward modifications can be made to accommodate the general case $I \subset \mathbb{Z}$.

During most of our investigations we will be concerned with difference expressions, that is, endomorphisms of $\ell(\mathbb{Z})$;

$$\begin{array}{rccc} R: & \ell(\mathbb{Z}) & \to & \ell(\mathbb{Z}) \\ & f & \mapsto & R\,f \end{array} \tag{1.5}$$

(we reserve the name difference operator for difference expressions defined on a subset of $\ell^2(\mathbb{Z})$). Any difference expression R is uniquely determined by its corresponding matrix representation

$$\big(R(m,n)\big)_{m,n\in\mathbb{Z}}, \quad R(m,n) = (R\delta_n)(m) = \langle \delta_m, R\,\delta_n\rangle, \tag{1.6}$$

where

$$\delta_n(m) = \delta_{m,n} = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases} \tag{1.7}$$

is the canonical basis of $\ell(\mathbb{Z})$. The **order** of R is the smallest nonnegative integer $N = N_+ + N_-$ such that $R(m,n) = 0$ for all m,n with $n-m > N_+$ and $m-n > N_-$. If no such number exists, the order is infinite.

We call R **symmetric** (resp. **skew-symmetric**) if $R(m,n) = R(n,m)$ (resp. $R(m,n) = -R(n,m)$).

Maybe the simplest examples for a difference expression are the **shift expressions**

$$(S^\pm f)(n) = f(n \pm 1). \tag{1.8}$$

They are of particular importance due to the fact that their powers form a basis for the space of all difference expressions (viewed as a module over the ring $\ell(\mathbb{Z})$). Indeed, we have

$$R = \sum_{k\in\mathbb{Z}} R(.,.+k)(S^+)^k, \qquad (S^\pm)^{-1} = S^\mp. \tag{1.9}$$

Here $R(.,.+k)$ denotes the multiplication expression with the sequence $(R(n,n+k))_{n\in\mathbb{Z}}$, that is, $R(.,.+k): f(n) \mapsto R(n,n+k)f(n)$. In order to simplify notation we agree to use the short cuts

$$f^\pm = S^\pm f, \quad f^{++} = S^+S^+f, \quad \text{etc.}, \tag{1.10}$$

whenever convenient. In connection with the difference expression (1.5) we also define the diagonal, upper, and lower triangular parts of R as follows

$$[R]_0 = R(.,.), \quad [R]_\pm = \sum_{k\in\mathbb{N}} R(.,.\pm k)(S^\pm)^k, \tag{1.11}$$

implying $R = [R]_+ + [R]_0 + [R]_-$.

Having these preparations out of the way, we are ready to start our investigation of second order symmetric difference expressions. To set the stage, let $a, b \in \ell(\mathbb{Z},\mathbb{R})$ be two real-valued sequences satisfying

$$a(n) \in \mathbb{R}\backslash\{0\}, \quad b(n) \in \mathbb{R}, \qquad n \in \mathbb{Z}, \tag{1.12}$$

and introduce the corresponding **second order, symmetric difference expression**

$$\begin{array}{rccl} \tau: & \ell(\mathbb{Z}) & \to & \ell(\mathbb{Z}) \\ & f(n) & \mapsto & a(n)f(n+1) + a(n-1)f(n-1) + b(n)f(n) \end{array}. \tag{1.13}$$

It is associated with the tridiagonal matrix

$$\begin{pmatrix} \ddots & \ddots & \ddots & & & \\ a(n-2) & b(n-1) & a(n-1) & & & \\ & a(n-1) & b(n) & a(n) & & \\ & & a(n) & b(n+1) & a(n+1) & \\ & & & \ddots & \ddots & \ddots \end{pmatrix} \tag{1.14}$$

and will be our main object for the rest of this section and the tools derived here – even though simple – will be indispensable for us.

Before going any further, I want to point out that there is a close connection between second order, symmetric difference expressions and second order, symmetric differential expressions. This connection becomes more apparent if we use the difference expressions

$$(\partial f)(n) = f(n+1) - f(n), \qquad (\partial^* f)(n) = f(n-1) - f(n), \tag{1.15}$$

(note that ∂, ∂^* are formally adjoint) to rewrite τ in the following way

$$\begin{aligned} (\tau f)(n) &= -(\partial^* a \partial f)(n) + (a(n-1) + a(n) + b(n))f(n) \\ &= -(\partial a^- \partial^* f)(n) + (a(n-1) + a(n) + b(n))f(n). \end{aligned} \tag{1.16}$$

This form resembles very much the Sturm-Liouville differential expression, well-known in the theory of ordinary differential equations.

In fact, the reader will soon realize that there are a whole lot more similarities between differentials, integrals and their discrete counterparts differences and sums. Two of these similarities are the product rules

$$\begin{aligned} (\partial fg)(n) &= f(n)(\partial g)(n) + g(n+1)(\partial f)(n), \\ (\partial^* fg)(n) &= f(n)(\partial^* g)(n) + g(n-1)(\partial^* f)(n) \end{aligned} \tag{1.17}$$

and the **summation by parts** formula (also known as **Abel transform**)

$$\sum_{j=m}^{n} g(j)(\partial f)(j) = g(n)f(n+1) - g(m-1)f(m) + \sum_{j=m}^{n} (\partial^* g)(j)f(j). \tag{1.18}$$

Both are readily verified. Nevertheless, let me remark that ∂, ∂^* are no derivations since they do not satisfy Leibnitz rule. This very often makes the discrete case different (and sometimes also harder) from the continuous one. In particular, many calculations become much messier and formulas longer.

There is much more to say about relations for the difference expressions (1.15) analogous to the ones for differentiation. We refer the reader to, for instance, [**4**], [**87**], or [**147**] and return to (1.13).

Associated with τ is the eigenvalue problem $\tau u = zu$. The appropriate setting for this eigenvalue problem is the Hilbert space $\ell^2(\mathbb{Z})$. However, before we can pursue the investigation of the eigenvalue problem in $\ell^2(\mathbb{Z})$, we need to consider the **Jacobi difference equation**

$$\tau u = z\, u, \qquad u \in \ell(\mathbb{Z}),\ z \in \mathbb{C}. \tag{1.19}$$

Using $a(n) \neq 0$ we see that a solution u is uniquely determined by the values $u(n_0)$ and $u(n_0+1)$ at two consecutive points n_0, n_0+1 (you have to work much harder to obtain the corresponding result for differential equations). It follows, that there are exactly two linearly independent solutions.

Combining (1.16) and the summation by parts formula yields **Green's formula**

$$\sum_{j=m}^{n} \Big(f(\tau g) - (\tau f) g \Big)(j) = W_n(f,g) - W_{m-1}(f,g) \tag{1.20}$$

for $f, g \in \ell(\mathbb{Z})$, where we have introduced the (modified) **Wronskian**

$$W_n(f,g) = a(n)\Big(f(n) g(n+1) - g(n) f(n+1) \Big). \tag{1.21}$$

Green's formula will be the key to self-adjointness of the operator associated with τ in the Hilbert space $\ell^2(\mathbb{Z})$ (cf. Theorem 1.5) and the Wronskian is much more than a suitable abbreviation as we will show next.

Evaluating (1.20) in the special case where f and g both solve (1.19) (with the same parameter z) shows that the Wronskian is constant (i.e., does not depend on n) in this case. (The index n will be omitted in this case.) Moreover, it is nonzero if and only if f and g are linearly independent.

Since the (linear) space of solutions is two dimensional (as observed above) we can pick two linearly independent solutions c, s of (1.19) and write any solution u of (1.19) as a linear combination of these two solutions

$$u(n) = \frac{W(u,s)}{W(c,s)} c(n) - \frac{W(u,c)}{W(c,s)} s(n). \tag{1.22}$$

For this purpose it is convenient to introduce the following **fundamental solutions** $c, s \in \ell(\mathbb{Z})$

$$\tau c(z,.,n_0) = z\, c(z,.,n_0), \qquad \tau s(z,.,n_0) = z\, s(z,.,n_0), \tag{1.23}$$

fulfilling the **initial conditions**

$$\begin{aligned} c(z,n_0,n_0) &= 1, \qquad & c(z,n_0+1,n_0) &= 0, \\ s(z,n_0,n_0) &= 0, \qquad & s(z,n_0+1,n_0) &= 1. \end{aligned} \tag{1.24}$$

Most of the time the base point n_0 will be unessential and we will choose $n_0 = 0$ for simplicity. In particular, we agree to omit n_0 whenever it is 0, that is,

$$c(z,n) = c(z,n,0), \qquad s(z,n) = s(z,n,0). \tag{1.25}$$

Since the Wronskian of $c(z,.,n_0)$ and $s(z,.,n_0)$ does not depend on n we can evaluate it at n_0

$$W(c(z,.,n_0),s(z,.,n_0)) = a(n_0) \tag{1.26}$$

and consequently equation (1.22) simplifies to

$$u(n) = u(n_0)c(z,n,n_0) + u(n_0+1)s(z,n,n_0). \tag{1.27}$$

Sometimes a lot of things get more transparent if (1.19) is regarded from the viewpoint of dynamical systems. If we introduce $\underline{u} = (u, u^+) \in \ell(\mathbb{Z}, \mathbb{C}^2)$, then (1.19) is equivalent to

$$\underline{u}(n+1) = U(z,n+1)\underline{u}(n), \qquad \underline{u}(n-1) = U(z,n)^{-1}\underline{u}(n), \tag{1.28}$$

where $U(z,.)$ is given by

$$\begin{aligned} U(z,n) &= \frac{1}{a(n)} \begin{pmatrix} 0 & a(n) \\ -a(n-1) & z-b(n) \end{pmatrix}, \\ U^{-1}(z,n) &= \frac{1}{a(n-1)} \begin{pmatrix} z-b(n) & -a(n) \\ a(n-1) & 0 \end{pmatrix}. \end{aligned} \tag{1.29}$$

The matrix $U(z,n)$ is often referred to as **transfer matrix**. The corresponding (non-autonomous) flow on $\ell(\mathbb{Z}, \mathbb{C}^2)$ is given by the **fundamental matrix**

$$\begin{aligned} \Phi(z,n,n_0) &= \begin{pmatrix} c(z,n,n_0) & s(z,n,n_0) \\ c(z,n+1,n_0) & s(z,n+1,n_0) \end{pmatrix} \\ &= \begin{cases} U(z,n)\cdots U(z,n_0+1) & n > n_0 \\ \mathbb{1} & n = n_0 \\ U^{-1}(z,n+1)\cdots U^{-1}(z,n_0) & n < n_0 \end{cases}. \end{aligned} \tag{1.30}$$

More explicitly, equation (1.27) is now equivalent to

$$\begin{pmatrix} u(n) \\ u(n+1) \end{pmatrix} = \Phi(z,n,n_0) \begin{pmatrix} u(n_0) \\ u(n_0+1) \end{pmatrix}. \tag{1.31}$$

Using (1.31) we learn that $\Phi(z,n,n_0)$ satisfies the usual group law

$$\Phi(z,n,n_0) = \Phi(z,n,n_1)\Phi(z,n_1,n_0), \qquad \Phi(z,n_0,n_0) = \mathbb{1} \tag{1.32}$$

and constancy of the Wronskian (1.26) implies

$$\det \Phi(z,n,n_0) = \frac{a(n_0)}{a(n)}. \tag{1.33}$$

Let us use $\Phi(z,n) = \Phi(z,n,0)$ and define the upper, lower **Lyapunov exponents**

$$\begin{aligned} \overline{\gamma}^{\pm}(z) &= \limsup_{n\to\pm\infty} \frac{1}{|n|} \ln \|\Phi(z,n,n_0)\| = \limsup_{n\to\pm\infty} \frac{1}{|n|} \ln \|\Phi(z,n)\|, \\ \underline{\gamma}^{\pm}(z) &= \liminf_{n\to\pm\infty} \frac{1}{|n|} \ln \|\Phi(z,n,n_0)\| = \liminf_{n\to\pm\infty} \frac{1}{|n|} \ln \|\Phi(z,n)\|. \end{aligned} \tag{1.34}$$

Here

$$\|\Phi\| = \sup_{u\in\mathbb{C}^2\backslash\{0\}} \frac{\|\Phi u\|_{\mathbb{C}^2}}{\|u\|_{\mathbb{C}^2}} \tag{1.35}$$

denotes the operator norm of Φ. By virtue of (use (1.32))

$$\|\Phi(z,n_0)\|^{-1}\|\Phi(z,n)\| \le \|\Phi(z,n,n_0)\| \le \|\Phi(z,n_0)^{-1}\|\|\Phi(z,n)\| \tag{1.36}$$

the definition of $\overline{\gamma}^{\pm}(z)$, $\underline{\gamma}^{\pm}(z)$ is indeed independent of n_0. Moreover, $\underline{\gamma}^{\pm}(z) \geq 0$ if $a(n)$ is bounded. In fact, since $\underline{\gamma}^{\pm}(z) < 0$ would imply $\lim_{j\to\pm\infty} \|\Phi(z, n_j, n_0)\| = 0$ for some subsequence n_j contradicting (1.33).

If $\underline{\gamma}^{\pm}(z) = \overline{\gamma}^{\pm}(z)$ we will omit the bars. A number $\lambda \in \mathbb{R}$ is said to be hyperbolic at $\pm\infty$ if $\underline{\gamma}^{\pm}(\lambda) = \overline{\gamma}^{\pm}(\lambda) > 0$, respectively. The set of all hyperbolic numbers is denoted by $\mathrm{Hyp}_{\pm}(\Phi)$. For $\lambda \in \mathrm{Hyp}_{\pm}(\Phi)$ one has existence of corresponding **stable** and **unstable manifolds** $V^{\pm}(\lambda)$.

Lemma 1.1. *Suppose that $|a(n)|$ does not grow or decrease exponentially and that $|b(n)|$ does not grow exponentially, that is,*

$$\lim_{n\to\pm\infty} \frac{1}{|n|} \ln|a(n)| = 0, \qquad \lim_{n\to\pm\infty} \frac{1}{|n|} \ln(1+|b(n)|) = 0. \tag{1.37}$$

If $\lambda \in \mathrm{Hyp}_{\pm}(\Phi)$, then there exist one-dimensional linear subspaces $V^{\pm}(\lambda) \subseteq \mathbb{R}^2$ such that

$$\begin{aligned} \underline{v} \in V^{\pm}(\lambda) &\Leftrightarrow \lim_{n\to\pm\infty} \frac{1}{|n|} \ln\|\Phi(\lambda, n)\underline{v}\| = -\gamma^{\pm}(\lambda), \\ \underline{v} \notin V^{\pm}(\lambda) &\Leftrightarrow \lim_{n\to\pm\infty} \frac{1}{|n|} \ln\|\Phi(\lambda, n)\underline{v}\| = \gamma^{\pm}(\lambda), \end{aligned} \tag{1.38}$$

respectively.

Proof. Set

$$A(n) = \begin{pmatrix} 1 & 0 \\ 0 & a(n) \end{pmatrix} \tag{1.39}$$

and abbreviate

$$\begin{aligned} \tilde{U}(z,n) &= A(n)U(z,n)A(n-1)^{-1} = \frac{1}{a(n-1)} \begin{pmatrix} 0 & 1 \\ -a(n-1)^2 & z-b(n) \end{pmatrix}, \\ \tilde{\Phi}(z,n) &= A(n)\Phi(z,n)A(0)^{-1}. \end{aligned} \tag{1.40}$$

Then (1.28) translates into

$$\underline{\tilde{u}}(n+1) = \tilde{U}(z, n+1)\underline{\tilde{u}}(n), \qquad \underline{\tilde{u}}(n-1) = \tilde{U}(z,n)^{-1}\underline{\tilde{u}}(n), \tag{1.41}$$

where $\underline{\tilde{u}} = A\underline{u} = (u, au^+)$, and we have

$$\det \tilde{U}(z,n) = 1 \quad \text{and} \quad \lim_{n\to\infty} \frac{1}{|n|} \ln\|\tilde{U}(z,n)\| = 0 \tag{1.42}$$

due to our assumption (1.37). Moreover,

$$\frac{\min(1, a(n))}{\max(1, a(0))} \leq \frac{\|\tilde{\Phi}(z,n)\|}{\|\Phi(z,n)\|} \leq \frac{\max(1, a(n))}{\min(1, a(0))} \tag{1.43}$$

and hence $\lim_{n\to\pm\infty} |n|^{-1} \ln\|\tilde{\Phi}(z,n)\| = \lim_{n\to\pm\infty} |n|^{-1} \ln\|\Phi(z,n)\|$ whenever one of the limits exists. The same is true for the limits of $|n|^{-1}\ln\|\tilde{\Phi}(z,n)v\|$ and $|n|^{-1}\ln\|\Phi(z,n)v\|$. Hence it suffices to prove the result for matrices $\tilde{\Phi}$ satisfying (1.42). But this is precisely the (deterministic) multiplicative ergodic theorem of Osceledec (see [**201**]). □

Observe that by looking at the Wronskian of two solutions $u \in V^{\pm}(\lambda)$, $v \notin V^{\pm}(\lambda)$ it is not hard to see that the lemma becomes false if $a(n)$ is exponentially decreasing.

For later use observe that

$$\Phi(z,n,m)^{-1} = \frac{a(n)}{a(m)} J\,\Phi(z,n,m)^{\top} J^{-1}, \qquad J = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \tag{1.44}$$

(where $\Phi^{\top}$ denotes the transposed matrix of Φ) and hence

$$|a(m)| \|\Phi(z,n,m)^{-1}\| = |a(n)| \|\Phi(z,n,m)\|. \tag{1.45}$$

We will exploit this notation later in this monograph but for the moment we return to our original point of view.

The equation

$$(\tau - z) f = g \tag{1.46}$$

for fixed $z \in \mathbb{C}$, $g \in \ell(\mathbb{Z})$, is referred to as **inhomogeneous Jacobi equation**. Its solution can can be completely reduced to the solution of the corresponding **homogeneous Jacobi equation** (1.19) as follows. Introduce

$$K(z,n,m) = \frac{s(z,n,m)}{a(m)}. \tag{1.47}$$

Then the sequence

$$\begin{aligned} f(n) \;=\; & f_0\, c(z,n,n_0) + f_1 s(z,n,n_0) \\ & + \sum_{m=n_0+1}^{n}{}^{*}\; K(z,n,m) g(m), \end{aligned} \tag{1.48}$$

where

$$\sum_{j=n_0}^{n-1}{}^{*}\; f(j) = \begin{cases} \sum\limits_{j=n_0}^{n-1} f(j) & \text{for } n > n_0 \\ \quad 0 & \text{for } n = n_0 \\ -\sum\limits_{j=n}^{n_0-1} f(j) & \text{for } n < n_0 \end{cases}, \tag{1.49}$$

satisfies (1.46) and the initial conditions $f(n_0) = f_0$, $f(n_0+1) = f_1$ as can be checked directly. The summation kernel $K(z,n,m)$ has the following properties: $K(z,n,n) = 0$, $K(z,n+1,n) = a(n)^{-1}$, $K(z,n,m) = -K(z,m,n)$, and

$$K(z,n,m) = \frac{u(z,m)v(z,n) - u(z,n)v(z,m)}{W(u(z),v(z))} \tag{1.50}$$

for any pair $u(z)$, $v(z)$ of linearly independent solutions of $\tau u = zu$.

Another useful result is the **variation of constants** formula. It says that if one solution u of (1.19) with $u(n) \neq 0$ for all $n \in \mathbb{Z}$ is known, then a second (linearly independent, $W(u,v) = 1$) solution of (1.19) is given by

$$v(n) = u(n) \sum_{j=n_0}^{n-1}{}^{*}\; \frac{1}{a(j)u(j)u(j+1)}. \tag{1.51}$$

It can be verified directly as well.

Sometimes transformations can help to simplify a problem. The following two are of particular interest to us. If u fulfills (1.19) and $u(n) \neq 0$, then the sequence $\phi(n) = u(n+1)/u(n)$ satisfies the (discrete) **Riccati equation**

$$a(n)\phi(n) + \frac{a(n-1)}{\phi(n-1)} = z - b(n). \tag{1.52}$$

Conversely, if ϕ fulfills (1.52), then the sequence

$$u(n) = \prod_{j=n_0}^{n-1}{}^{*}\ \phi(j) = \begin{cases} \prod_{j=n_0}^{n-1} \phi(j) & \text{for } n > n_0 \\ 1 & \text{for } n = n_0 \\ \prod_{j=n}^{n_0-1} \phi(j)^{-1} & \text{for } n < n_0 \end{cases}, \tag{1.53}$$

fulfills (1.19) and is normalized such that $u(n_0) = 1$. In addition, we remark that the sequence $\phi(n)$ might be written as finite continued fraction,

$$a(n)\phi(n) = z - b(n) - \cfrac{a(n-1)^2}{z - b(n-1) - \ddots - \cfrac{a(n_0+1)^2}{z - b(n_0+1) - \cfrac{a(n_0)}{\phi(n_0)}}} \tag{1.54}$$

for $n > n_0$ and

$$a(n)\phi(n) = \cfrac{a(n)^2}{z - b(n+1) - \ddots - \cfrac{a(n_0-1)^2}{z - b(n_0) - a(n_0)\phi(n_0)}} \tag{1.55}$$

for $n < n_0$.

If $\tilde{a}$ is a sequence with $\tilde{a}(n) \neq 0$ and u fulfills (1.19), then the sequence

$$\tilde{u}(n) = u(n) \prod_{j=n_0}^{n-1}{}^{*}\ \tilde{a}(j), \tag{1.56}$$

fulfills

$$\frac{a(n)}{\tilde{a}(n)} \tilde{u}(n+1) + a(n-1)\tilde{a}(n-1)\tilde{u}(n-1) + b(n)\tilde{u}(n) = z\,\tilde{u}(n). \tag{1.57}$$

Especially, taking $\tilde{a}(n) = \mathrm{sgn}(a(n))$ (resp. $\tilde{a}(n) = -\mathrm{sgn}(a(n))$), we see that it is no restriction to assume $a(n) > 0$ (resp. $a(n) < 0$) (compare also Lemma 1.6 below).

We conclude this section with a detailed investigation of the fundamental solutions $c(z, n, n_0)$ and $s(z, n, n_0)$. To begin with, we note (use induction) that both $c(z, n \pm k, n)$ and $s(z, n \pm k, n)$, $k \geq 0$, are polynomials of degree at most k with respect to z. Hence we may set

$$s(z, n \pm k, n) = \sum_{j=0}^{k} s_{j,\pm k}(n) z^j, \quad c(z, n \pm k, n) = \sum_{j=0}^{k} c_{j,\pm k}(n) z^j. \tag{1.58}$$

Using the coefficients $s_{j,\pm k}(n)$ and $c_{j,\pm k}(n)$ we can derive a neat expansion for arbitrary difference expressions. By (1.9) it suffices to consider $(S^\pm)^k$.

Lemma 1.2. *Any difference expression R of order at most $2k+1$ can be expressed as*

$$R = \sum_{j=0}^{k} \Big(c_j + s_j S^+ \Big) \tau^j, \qquad c_j, s_j \in \ell(\mathbb{Z}),\ k \in \mathbb{N}_0, \tag{1.59}$$

with $c_j = s_j = 0$ if and only if $R = 0$. In other words, the set $\{\tau^j, S^+\tau^j\}_{j\in\mathbb{N}_0}$ forms a basis for the space of all difference expressions.

We have

$$(S^\pm)^k = \sum_{j=0}^{k} \Big(c_{j,\pm k} + s_{j,\pm k} S^+ \Big) \tau^j, \tag{1.60}$$

where $s_{j,\pm k}(n)$ and $c_{j,\pm k}(n)$ are defined in (1.58).

Proof. We first prove (1.59) by induction on k. The case $k = 0$ is trivial. Since the matrix element $\tau^k(n, n\pm k) = \prod_{j=0}^{k-1} a(n \pm j - {0 \atop 1}) \neq 0$ is nonzero we can choose $s_k(n) = R(n, n+k+1)/\tau^k(n-1, n+k-1)$, $c_k(n) = R(n, n-k)/\tau^k(n, n-k)$ and apply the induction hypothesis to $R - (c_k - s_k S^+)\tau^k$. This proves (1.59). The rest is immediate from

$$(R(s(z,.,n))(n) = \sum_{j=0}^{k} s_j(n) z^j, \quad (R(c(z,.,n))(n) = \sum_{j=0}^{k} c_j(n) z^j. \tag{1.61}$$

□

As a consequence of (1.61) we note

Corollary 1.3. *Suppose R is a difference expression of order k. Then $R = 0$ if and only if $R|_{\mathrm{Ker}(\tau - z)} = 0$ for $k+1$ values of $z \in \mathbb{C}$. (Here $R|_{\mathrm{Ker}(\tau - z)} = 0$ says that $Ru = 0$ for any solution u of $\tau u = zu$.)*

Next, $\Phi(z, n_0, n_1) = \Phi(z, n_1, n_0)^{-1}$ provides the useful relations

$$\begin{aligned} &\begin{pmatrix} c(z,n_0,n_1) & s(z,n_0,n_1) \\ c(z,n_0+1,n_1) & s(z,n_0+1,n_1) \end{pmatrix} \\ &\quad = \frac{a(n_1)}{a(n_0)} \begin{pmatrix} s(z,n_1+1,n_0) & -s(z,n_1,n_0) \\ -c(z,n_1+1,n_0) & c(z,n_1,n_0) \end{pmatrix} \end{aligned} \tag{1.62}$$

and a straightforward calculation (using (1.27)) yields

$$\begin{aligned} s(z,n,n_0+1) &= -\frac{a(n_0+1)}{a(n_0)} c(z,n,n_0), \\ s(z,n,n_0-1) &= c(z,n,n_0) + \frac{z-b(n_0)}{a(n_0)} s(z,n,n_0), \\ c(z,n,n_0+1) &= \frac{z-b(n_0+1)}{a(n_0)} c(z,n,n_0) + s(z,n,n_0), \\ c(z,n,n_0-1) &= -\frac{a(n_0-1)}{a(n_0)} s(z,n,n_0). \end{aligned} \tag{1.63}$$

Our next task will be expansions of $c(z,n,n_0)$, $s(z,n,n_0)$ for large z. Let J_{n_1,n_2} be the **Jacobi matrix**

$$J_{n_1,n_2} = \begin{pmatrix} b(n_1+1) & a(n_1+1) & & & \\ a(n_1+1) & b(n_1+2) & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & b(n_2-2) & a(n_2-2) \\ & & & a(n_2-2) & b(n_2-1) \end{pmatrix}. \tag{1.64}$$

Then we have the following expansion for $s(z,n,n_0)$, $n > n_0$,

$$s(z,n,n_0) = \frac{\det(z - J_{n_0,n})}{\prod_{j=n_0+1}^{n-1} a(j)} = \frac{z^k - \sum_{j=1}^k p_{n_0,n}(j) z^{k-j}}{\prod_{j=1}^k a(n_0+j)}, \tag{1.65}$$

where $k = n - n_0 - 1 \geq 0$ and

$$p_{n_0,n}(j) = \frac{\operatorname{tr}(J_{n_0,n}^j) - \sum_{\ell=1}^{j-1} p_{n_0,n}(\ell) \operatorname{tr}(J_{n_0,n}^{j-\ell})}{j}, \quad 1 \leq j \leq k. \tag{1.66}$$

To verify the first equation, use that if z is a zero of $s(.,n,n_0)$, then $(s(z,n_0+1,n_0),\dots,s(z,n-1,n_0))$ is an eigenvector of (1.64) corresponding to the eigenvalue z. Since the converse statement is also true, the polynomials (in z) $s(z,n,n_0)$ and $\det(z - J_{n_0,n})$ only differ by a constant which can be deduced from (1.30). The second is a well-known property of characteristic polynomials (cf., e.g., [**91**]).

The first few traces are given by

$$\begin{aligned} \operatorname{tr}(J_{n_0,n_0+k+1}) &= \sum_{j=n_0+1}^{n_0+k} b(j), \\ \operatorname{tr}(J_{n_0,n_0+k+1}^2) &= \sum_{j=n_0+1}^{n_0+k} b(j)^2 + 2 \sum_{j=n_0+1}^{n_0+k-1} a(j)^2, \\ \operatorname{tr}(J_{n_0,n_0+k+1}^3) &= \sum_{j=n_0+1}^{n_0+k} b(j)^3 + 3 \sum_{j=n_0+1}^{n_0+k-1} a(j)^2 (b(j) + b(j+1)), \\ \operatorname{tr}(J_{n_0,n_0+k+1}^4) &= \sum_{j=n_0+1}^{n_0+k} b(j)^4 - 4 \sum_{j=n_0+1}^{n_0+k-1} a(j)^2 \Big(b(j)^2 + b(j+1) b(j) \\ &\quad + b(j+1)^2 + \frac{a(j)^2}{2} \Big) + 4 \sum_{j=n_0+1}^{n_0+k-2} a(j+1)^2. \end{aligned} \tag{1.67}$$

An explicit calculation yields for $n > n_0 + 1$

$$
\begin{aligned}
c(z,n,n_0) &= \frac{-a(n_0) z^{n-n_0-2}}{\prod\limits_{j=n_0+1}^{n-1} a(j)} \left(1 - \frac{1}{z} \sum_{j=n_0+2}^{n-1} b(j) + O(\frac{1}{z^2}) \right), \\
s(z,n,n_0) &= \frac{z^{n-n_0-1}}{\prod\limits_{j=n_0+1}^{n-1} a(j)} \left(1 - \frac{1}{z} \sum_{j=n_0+1}^{n-1} b(j) + O(\frac{1}{z^2}) \right),
\end{aligned} \tag{1.68}
$$

and (using (1.63) and (1.62)) for $n < n_0$

$$
\begin{aligned}
c(z,n,n_0) &= \frac{z^{n_0-n}}{\prod\limits_{j=n}^{n_0-1} a(j)} \left(1 - \frac{1}{z} \sum_{j=n+1}^{n_0} b(j) + O(\frac{1}{z^2}) \right), \\
s(z,n,n_0) &= \frac{-a(n_0) z^{n_0-n-1}}{\prod\limits_{j=n}^{n_0-1} a(j)} \left(1 - \frac{1}{z} \sum_{j=n+1}^{n_0-1} b(j) + O(\frac{1}{z^2}) \right).
\end{aligned} \tag{1.69}
$$

1.2. Jacobi operators

In this section we scrutinize the eigenvalue problem associated with (1.19) in the Hilbert space $\ell^2(\mathbb{Z})$.

Recall that the scalar product and norm is given by

$$
\langle f, g\rangle = \sum_{n\in\mathbb{Z}} \overline{f(n)} g(n), \quad \|f\| = \sqrt{\langle f, f\rangle}, \quad f, g \in \ell^2(\mathbb{Z}), \tag{1.70}
$$

where the bar denotes complex conjugation.

For simplicity we assume from now on (and for the rest of this monograph) that a,b are bounded sequences.

Hypothesis H. 1.4. Suppose

$$
a, b \in \ell^\infty(\mathbb{Z}, \mathbb{R}), \qquad a(n) \neq 0. \tag{1.71}
$$

Associated with a, b is the **Jacobi operator**

$$
\begin{array}{rccc} H: & \ell^2(\mathbb{Z}) & \to & \ell^2(\mathbb{Z}) \\ & f & \mapsto & \tau f \end{array}, \tag{1.72}
$$

whose basic properties are summarized in our first theorem.

Theorem 1.5. *Assume (H.1.4). Then H is a bounded self-adjoint operator. Moreover, a,b bounded is equivalent to H bounded since we have $\|a\|_\infty \leq \|H\|$, $\|b\|_\infty \leq \|H\|$ and*

$$
\|H\| \leq 2\|a\|_\infty + \|b\|_\infty, \tag{1.73}
$$

where $\|H\|$ denotes the operator norm of H.

Proof. The fact that $\lim_{n\to\pm\infty} W_n(f,g) = 0$, $f,g \in \ell^2(\mathbb{Z})$, together with Green's formula (1.20) shows that H is self-adjoint, that is,

$$\langle f, Hg\rangle = \langle Hf, g\rangle, \qquad f,g \in \ell^2(\mathbb{Z}). \tag{1.74}$$

For the rest consider $a(n)^2 + a(n-1)^2 + b(n)^2 = \|H\delta_n\|^2 \le \|H\|^2$ and

$$|\langle f, Hf\rangle| \le (2\|a\|_\infty + \|b\|_\infty)\|f\|^2. \tag{1.75}$$

□

Before we pursue our investigation of Jacobi operators H, let us have a closer look at Hypothesis (H.1.4).

The previous theorem shows that the boundedness of H is due to the boundedness of a and b. This restriction on a, b is by no means necessary. However, it significantly simplifies the functional analysis involved and is satisfied in most cases of practical interest. You can find out how to avoid this restriction in Section 2.6.

The assumption $a(n) \neq 0$ is also not really necessary. In fact, we have not even used it in the proof of Theorem 1.5. If $a(n_0) = 0$, this implies that H can be decomposed into the direct sum $H_{n_0+1,-} \oplus H_{n_0,+}$ on $\ell^2(-\infty, n_0+1) \oplus \ell^2(n_0,\infty)$ (cf. (1.90) for notation). Nevertheless I want to emphasize that $a(n) \neq 0$ was crucial in the previous section and is connected with the existence of (precisely) two linearly independent solutions, which again is related to the fact that the spectrum of H has multiplicity at most two (cf. Section 2.5).

Hence the analysis of H in the case $a(n_0) = 0$ can be reduced to the analysis of restrictions of H which will be covered later in this section. In addition, the following lemma shows that the case $a(n) \neq 0$ can be reduced to the case $a(n) > 0$ or $a(n) < 0$.

Lemma 1.6. *Assume (H.1.4) and pick $\varepsilon \in \ell(\mathbb{Z}, \{-1,+1\})$. Introduce a_ε, b_ε by*

$$a_\varepsilon(n) = \varepsilon(n)a(n),\ b_\varepsilon(n) = b(n), \quad n \in \mathbb{Z}, \tag{1.76}$$

and the unitary involution U_ε by

$$U_\varepsilon = U_\varepsilon^{-1} = \Big(\prod_{j=0}^{n-1}{}^{*}\ \varepsilon(j)\,\delta_{m,n}\Big)_{m,n\in\mathbb{Z}}. \tag{1.77}$$

Let H be a Jacobi operator associated with the difference expression (1.13). Then H_ε defined as

$$H_\varepsilon = U_\varepsilon H U_\varepsilon^{-1} \tag{1.78}$$

is associated with the difference expression

$$(\tau_\varepsilon f)(n) = a_\varepsilon(n)f(n+1) + a_\varepsilon(n-1)f(n-1) + b_\varepsilon(n)f(n) \tag{1.79}$$

and is unitarily equivalent to H.

Proof. Straightforward. □

The next transformation is equally useful and will be referred to as **reflection** at n_0. It shows how information obtained near one endpoint, say $+\infty$, can be transformed into information near the other, $-\infty$.

Lemma 1.7. *Fix $n_0 \in \mathbb{Z}$ and consider the unitary involution*

$$(U_R f)(n) = (U_R^{-1} f)(n) = f(2n_0 - n) \tag{1.80}$$

or equivalently $(U_R f)(n_0 + k) = f(n_0 - k)$. Then the operator

$$H_R = U_R H U_R^{-1}, \tag{1.81}$$

is associated with the sequences

$$a_R(n_0 - k - 1) = a(n_0 + k), \quad b_R(n_0 - k) = b(n_0 + k), \quad k \in \mathbb{Z}, \tag{1.82}$$

or equivalently $a_R(n) = a(2n_0 - n - 1)$, $b_R(n) = b(2n_0 - n)$.

Proof. Again straightforward. □

Associated with U_R are the two orthogonal projections

$$P_R^{\pm} = \frac{1}{2}(\mathbb{1} \pm U_R), \qquad P_R^- + P_R^+ = \mathbb{1},\ P_R^- P_R^+ = P_R^+ P_R^- = 0 \tag{1.83}$$

and a corresponding splitting of H into two parts $H = H_R^+ \oplus H_R^-$, where

$$H_R^{\pm} = P_R^+ H P_R^{\pm} + P_R^- H P_R^{\mp} = \frac{1}{2}(H \pm H_R). \tag{1.84}$$

The symmetric part H_R^+ (resp. antisymmetric part H_R^-) commutes (resp. anticommutes) with U_R, that is, $[U_R, H_R^+] = U_R H_R^+ - H_R^+ U_R = 0$ (resp. $\{U_R, H_R^-\} = U_R H_R^- + H_R^- U_R = 0$). If $H = H_R^-$ we enter the realm of supersymmetric quantum mechanics (cf., e.g., [**225**] and Section 14.3).

After these two transformations we will say a little more about the spectrum $\sigma(H)$ of H. More precisely, we will estimate the location of $\sigma(H)$.

Lemma 1.8. *Let*

$$c_{\pm}(n) = b(n) \pm \big(|a(n)| + |a(n-1)|\big). \tag{1.85}$$

Then we have

$$\sigma(H) \subseteq [\inf_{n\in\mathbb{Z}} c_-(n), \sup_{n\in\mathbb{Z}} c_+(n)]. \tag{1.86}$$

Proof. We will first show that H is semi-bounded from above by $\sup c_+$. From (1.16) we infer

$$\begin{aligned}\langle f, Hf\rangle = \sum_{n\in\mathbb{Z}} \Big(&- a(n)|f(n+1) - f(n)|^2 \\ &+ \big(a(n-1) + a(n) + b(n)\big)|f(n)|^2\Big).\end{aligned} \tag{1.87}$$

By Lemma 1.6 we can first choose $a(n) > 0$ to obtain

$$\langle f, Hf\rangle \le \sup_{n\in\mathbb{Z}} c_+(n)\, \|f\|^2. \tag{1.88}$$

Similarly, choosing $a(n) < 0$ we see that H is semibounded from below by $\inf c_-$,

$$\langle f, Hf\rangle \ge \inf_{n\in\mathbb{Z}} c_-(n)\, \|f\|^2, \tag{1.89}$$

completing the proof. □

We remark that these bounds are optimal in the sense that equality is attained for (e.g.) $a(n) = 1/2, b(n) = 0$ (cf. Section 1.3).

We will not only consider H but also restrictions of H; partly because they are of interest on their own, partly because their investigation gives information about H.

To begin with, we define the following restrictions $H_{\pm,n_0}$ of H to the subspaces $\ell^2(n_0, \pm\infty)$,

$$H_{+,n_0} f(n) = \begin{cases} a(n_0+1) f(n_0+2) + b(n_0+1) f(n_0+1), \ n = n_0+1 \\ (\tau f)(n), \quad n > n_0+1 \end{cases},$$

$$H_{-,n_0} f(n) = \begin{cases} a(n_0-2) f(n_0-2) + b(n_0-1) f(n_0-1), \ n = n_0-1 \\ (\tau f)(n), \quad n < n_0-1 \end{cases}. \tag{1.90}$$

In addition, we also define for $\beta \in \mathbb{R} \cup \{\infty\}$

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

$$H^\infty_{-,n_0} = H_{-,n_0}, \quad H^\beta_{-,n_0} = H_{-,n_0+1} - a(n_0)\beta \langle \delta_{n_0}, .\rangle \delta_{n_0}, \quad \beta \neq \infty. \tag{1.91}$$

All operators $H^\beta_{\pm,n_0}$ are bounded and self-adjoint.

Last, we define the following finite restriction H_{n_1,n_2} to the subspaces $\ell^2(n_1, n_2)$

$$H_{n_1,n_2} f(n) = \begin{cases} a(n_1+1) f(n_1+2) + b(n_1+1) f(n_1+1), \ n = n_1+1 \\ (\tau f)(n), \quad n_1+1 < n < n_2-1 \\ a(n_2-2) f(n_2-2) + b(n_2-1) f(n_2-1), \ n = n_2-1 \end{cases}. \tag{1.92}$$

The operator H_{n_1,n_2} is clearly associated with the Jacobi matrix J_{n_1,n_2} (cf. (1.64)). Moreover, we set $H^{\infty,\infty}_{n_1,n_2} = H_{n_1,n_2}$, $H^{0,\beta_2}_{n_1,n_2} = H^{\infty,\beta_2}_{n_1+1,n_2}$, and

$$H^{\beta_1,\beta_2}_{n_1,n_2} = H^{\infty,\beta_2}_{n_1,n_2} - a(n_1)\beta_1^{-1} \langle \delta_{n_1+1}, .\rangle \delta_{n_1+1}, \quad \beta_1 \neq 0,$$

$$H^{\beta_1,\beta_2}_{n_1,n_2} = H^{\beta_1,\infty}_{n_1,n_2+1} - a(n_2)\beta_2 \langle \delta_{n_2}, .\rangle \delta_{n_2}, \quad \beta_2 \neq \infty. \tag{1.93}$$

Remark 1.9. H^β_{+,n_0} can be associated with the following domain

$$\mathfrak{D}(H^\beta_{+,n_0}) = \{ f \in \ell^2(n_0,\infty) | \cos(\alpha) f(n_0) + \sin(\alpha) f(n_0+1) = 0 \}, \tag{1.94}$$

$\beta = \cot(\alpha) \neq 0$, if one agrees that only points with $n > n_0$ are of significance and that the last point is only added as a dummy variable so that one does not have to specify an extra expression for $(\tau f)(n_0+1)$. In particular, the case $\beta = \infty$ (i.e., corresponding to the boundary condition $f(n_0) = 0$) will be referred to as **Dirichlet boundary condition** at n_0. Analogously for H^β_{-,n_0}, $H^{\beta_1,\beta_2}_{n_1,n_2}$.

One of the most important objects in spectral theory is the **resolvent** $(H-z)^{-1}$, $z \in \rho(H)$, of H. Here $\rho(H) = \mathbb{C} \backslash \sigma(H)$ denotes the resolvent set of H. The matrix elements of $(H-z)^{-1}$ are called **Green function**

$$G(z,n,m) = \langle \delta_n, (H-z)^{-1} \delta_m \rangle, \qquad z \in \rho(H). \tag{1.95}$$

Clearly,

$$(\tau - z) G(z,.,m) = \delta_m(.), \qquad G(z,m,n) = G(z,n,m) \tag{1.96}$$

and

$$((H-z)^{-1} f)(n) = \sum_{m \in \mathbb{Z}} G(z,n,m) f(m), \quad f \in \ell^2(\mathbb{Z}),\ z \in \rho(H). \tag{1.97}$$

We will derive an explicit formula for $G(z,n,m)$ in a moment. Before that we need to construct solutions $u_\pm(z)$ of (1.19) being square summable near $\pm\infty$.

Set

$$u(z,.) = (H-z)^{-1}\delta_0(.) = G(z,.,0), \qquad z \in \rho(H). \tag{1.98}$$

By construction u fulfills (1.19) only for $n > 0$ and $n < 0$. But if we take $u(z,-2)$, $u(z,-1)$ as initial condition we can obtain a solution $u_-(z,n)$ of $\tau u = zu$ on the whole of $\ell(\mathbb{Z})$ which coincides with $u(z,n)$ for $n < 0$. Hence $u_-(z)$ satisfies $u_-(z) \in \ell^2_-(\mathbb{Z})$ as desired. A solution $u_+(z) \in \ell^2_+(\mathbb{Z})$ is constructed similarly.

As anticipated, these solutions allow us to write down the Green function in a somewhat more explicit way

$$G(z,n,m) = \frac{1}{W(u_-(z),u_+(z))} \left\{ \begin{array}{ll} u_+(z,n)u_-(z,m) & \text{for } m \le n \\ u_+(z,m)u_-(z,n) & \text{for } n \le m \end{array} \right. , \tag{1.99}$$

$z \in \rho(H)$. Indeed, since the right hand side of (1.99) satisfies (1.96) and is square summable with respect to n, it must be the Green function of H.

For later use we also introduce the convenient abbreviations

$$\begin{aligned} g(z,n) &= G(z,n,n) = \frac{u_+(z,n)u_-(z,n)}{W(u_-(z),u_+(z))}, \\ h(z,n) &= 2a(n)G(z,n,n+1) - 1 \\ &= \frac{a(n)(u_+(z,n)u_-(z,n+1) + u_+(z,n)u_-(z,n+1))}{W(u_-(z),u_+(z))}. \end{aligned} \tag{1.100}$$

Note that for $n \le m$ we have

$$\begin{aligned} G(z,n,m) = {} & g(z,n_0)c(z,n,n_0)c(z,m,n_0) \\ & + g(z,n_0+1)s(z,n,n_0)s(z,m,n_0) \\ & + h(z,n_0)\frac{c(z,n,n_0)s(z,m,n_0) + c(z,m,n_0)s(z,n,n_0)}{2a(n_0)} \\ & - \frac{c(z,n,n_0)s(z,m,n_0) - c(z,m,n_0)s(z,n,n_0)}{2a(n_0)}. \end{aligned} \tag{1.101}$$

Similar results hold for the restrictions: Let

$$s_\beta(z,n,n_0) = \sin(\alpha)c(z,n,n_0) - \cos(\alpha)s(z,n,n_0) \tag{1.102}$$

with $\beta = \cot(\alpha)$ (i.e., the sequence $s_\beta(z,n,n_0)$ fulfills the boundary condition $\cos(\alpha)s_\beta(z,n_0,n_0) + \sin(\alpha)s_\beta(z,n_0+1,n_0) = 0$). Then we obtain for the resolvent of $H^\beta_{\pm,n_0}$

$$((H^\beta_{\pm,n_0} - z)^{-1}u)(n) = \sum_{m \gtrless n_0} G^\beta_{\pm,n_0}(z,m,n)u(m), \quad z \in \rho(H^\beta_{\pm,n_0}), \tag{1.103}$$

where

$$G^\beta_{\pm,n_0}(z,m,n) = \frac{\pm 1}{W(s_\beta(z),u_\pm(z))} \left\{ \begin{array}{ll} s_\beta(z,n,n_0)u_\pm(z,m) & \text{for } m \gtrless n \\ s_\beta(z,m,n_0)u_\pm(z,n) & \text{for } n \gtrless m \end{array} \right. \tag{1.104}$$

(use $(H^\beta_{\pm,n_0} - z)^{-1}$ to show the existence of $u_\pm(z,.)$ for $z \in \rho(H^\beta_{\pm,n_0})$).

Remark 1.10. The solutions being square summable near $\pm\infty$ (resp. satisfying the boundary condition $\cos(\alpha)f(n_0)+\sin(\alpha)f(n_0+1)=0$) are unique up to constant multiples since the Wronskian of two such solutions vanishes (evaluate it at $\pm\infty$ (resp. n_0)). This implies that the point spectrum of H, $H^\beta_{\pm,n_0}$ is always simple.

In addition to $H^\beta_{\pm,n_0}$ we will be interested in the following direct sums of these operators

$$H^\beta_{n_0} = H^\beta_{-,n_0} \oplus H^\beta_{+,n_0}, \tag{1.105}$$

in the Hilbert space $\{f\in\ell^2(\mathbb{Z}) | \cos(\alpha)f(n_0)+\sin(\alpha)f(n_0+1)=0\}$. The reason why $H^\beta_{n_0}$ is of interest to us follows from the close spectral relation to H as can be seen from their resolvents (resp. Green functions)

$$\begin{aligned} G^\infty_{n_0}(z,n,m) &= G(z,n,m) - \frac{G(z,n,n_0)G(z,n_0,m)}{G(z,n_0,n_0)},\\ G^\beta_{n_0}(z,n,m) &= G(z,n,m) - \gamma^\beta(z,n_0)^{-1}\big(G(z,n,n_0+1)+\beta G(z,n,n_0)\big)\\ &\quad \times\big(G(z,n_0+1,m)+\beta G(z,n_0,m)\big), \quad \beta\in\mathbb{R}, \end{aligned} \tag{1.106}$$

where

$$\begin{aligned} \gamma^\beta(z,n) &= \frac{(u_+(z,n+1)+\beta u_+(z,n))(u_-(z,n+1)+\beta u_-(z,n))}{W(u_-(z),u_+(z))}\\ &= g(z,n+1) + \frac{\beta}{a(n)}h(z,n) + \beta^2 g(z,n). \end{aligned} \tag{1.107}$$

Remark 1.11. The operator $H^\beta_{n_0}$ is equivalently given by

$$H^\beta_{n_0} = (\mathbb{1}-P^\beta_{n_0})H(\mathbb{1}-P^\beta_{n_0}) \tag{1.108}$$

in the Hilbert space $(\mathbb{1}-P^\beta_{n_0})\ell^2(\mathbb{Z}) = \{f\in\ell^2(\mathbb{Z}) | \langle\delta^\beta_{n_0}, f\rangle = 0\}$, where $P^\beta_{n_0}$ denotes the orthogonal projection onto the one-dimensional subspace spanned by $\delta^\beta_{n_0} = \cos(\alpha)\delta_{n_0}+\sin(\alpha)\delta_{n_0+1}$, $\beta=\cot(\alpha)$, $\alpha\in[0,\pi)$ in $\ell^2(\mathbb{Z})$.

Finally, we derive some interesting difference equations for $g(z,n)$ to be used in Section 6.1.

Lemma 1.12. *Let u,v be two solutions of (1.19). Then $g(n)=u(n)v(n)$ satisfies*

$$\frac{(a^+)^2 g^{++} - a^2 g}{z-b^+} + \frac{a^2 g^+ - (a^-)^2 g^-}{z-b} = (z-b^+)g^+ - (z-b)g, \tag{1.109}$$

and

$$\Big(a^2 g^+ - (a^-)^2 g^- + (z-b)^2 g\Big)^2 = (z-b)^2\Big(W(u,v)^2 + 4a^2 g g^+\Big). \tag{1.110}$$

Proof. First we calculate (using (1.19))

$$a^2 g^+ - (a^-)^2 g^- = -(z-b)^2 g + a(z-b)(uv^+ + u^+v). \tag{1.111}$$

Adding $(z-b)^2 g$ and taking squares yields the second equation. Dividing both sides by $z-b$ and adding the equations corresponding to n and $n+1$ yields the first. □

Remark 1.13. There exists a similar equation for $\gamma^\beta(z,n)$. Since it is quite complicated, it seems less useful. Set $\gamma^\beta(n) = (u(n+1) + \beta u(n))(v(n+1) + \beta v(n))$, then we have

$$\begin{aligned} &\Big((a^+A^-)^2(\gamma^\beta)^+ - (a^-A)^2(\gamma^\beta)^- + B^2\gamma^\beta\Big)^2 \\ &= (A^-B)^2\Big((\frac{A}{a}W(u,v))^2 + 4(a^+)^2\gamma^\beta(\gamma^\beta)^+\Big), \end{aligned} \tag{1.112}$$

with

$$\begin{aligned} A &= a + \beta(z-b^+) + \beta^2 a^+, \\ B &= a^-(z-b^+) + \beta((z-b^+)(z-b) + a^+a^- - a^2) \\ &\qquad + \beta^2 a^+(z-b). \end{aligned} \tag{1.113}$$

It can be verified by a long and tedious (but straightforward) calculation.

1.3. A simple example

We have been talking about Jacobi operators for quite some time now, but we have not seen a single example yet. Well, here is one, the free Jacobi operator H_0 associated with constant sequences $a(n) = a$, $b(n) = b$. The transformation $z \to 2az + b$ reduces this problem to the one with $a_0(n) = 1/2$, $b_0(n) = 0$. Thus we will consider the equation

$$\frac{1}{2}\Big(u(n+1) + u(n-1)\Big) = zu(n). \tag{1.114}$$

Without restriction we choose $n_0 = 0$ throughout this section (note that we have $s(z,n,n_0) = s(z,n-n_0)$, etc.) and omit n_0 in all formulas. By inspection (try the ansatz $u(n) = k^n$) $u_\pm(z,.)$ are given by

$$u_\pm(z,n) = (z \pm R_2^{1/2}(z))^n, \tag{1.115}$$

where $R_2^{1/2}(z) = -\sqrt{z-1}\sqrt{z+1}$. Here and in the sequel $\sqrt{.}$ always denotes the standard branch of the square root, that is,

$$\sqrt{z} = |\sqrt{z}| \exp(\mathrm{i}\arg(z)/2), \quad \arg(z) \in (-\pi,\pi], \quad z \in \mathbb{C}. \tag{1.116}$$

Since $W(u_-,u_+) = R_2^{1/2}(z)$ we need a second solution for $z^2 = 1$, which is given by $s(\pm 1, n) = (\pm 1)^{n+1} n$. For the fundamental solutions we obtain

$$\begin{aligned} s(z,n) &= \frac{(z + R_2^{1/2}(z))^n - (z - R_2^{1/2}(z))^n}{2R_2^{1/2}(z)}, \\ c(z,n) &= \frac{s(z,n-1)}{s(z,-1)} = -s(z,n-1). \end{aligned} \tag{1.117}$$

Notice that $s(-z,n) = (-1)^{n+1}s(z,n)$. For $n > 0$ we have the following expansion

$$\begin{aligned} s(z,n) &= \sum_{j=0}^{[\![n/2]\!]} \binom{n}{2j+1} (z^2-1)^j z^{n-2j-1} \\ &= \sum_{k=0}^{[\![n/2]\!]} \left((-1)^k \sum_{j=k}^{[\![n/2]\!]} \binom{n}{2j+1}\binom{j}{k} \right) z^{n-2k-1}, \end{aligned} \tag{1.118}$$

where $[\![x]\!] = \sup\{n \in \mathbb{Z} \,|\, n < x\}$. It is easily seen that we have $\|H_0\| = 1$ and further that

$$\sigma(H_0) = [-1, 1]. \tag{1.119}$$

For example, use unitarity of the Fourier transform

$$U: \begin{array}{ccc} \ell^2(\mathbb{Z}) & \to & L^2(-\pi,\pi) \\ u(n) & \mapsto & \sum_{n\in\mathbb{Z}} u(n)\mathrm{e}^{\mathrm{i}nx} \end{array}. \tag{1.120}$$

which maps H_0 to the multiplication operator by $\cos(x)$.

The Green function of H_0 explicitly reads ($z \in \mathbb{C}\backslash[-1,1]$)

$$G_0(z,m,n) = \frac{(z + R_2^{1/2}(z))^{|m-n|}}{R_2^{1/2}(z)}. \tag{1.121}$$

In particular, we have

$$\begin{aligned} g_0(z,n) &= \frac{1}{R_2^{1/2}(z)} = -2\sum_{j=0}^{\infty}\binom{2j}{j}\frac{1}{(2z)^{2j+1}} \\ h_0(z,n) &= \frac{z}{R_2^{1/2}(z)} = -\sum_{j=0}^{\infty}\binom{2j}{j}\frac{1}{(2z)^{2j}}. \end{aligned} \tag{1.122}$$

Note that it is sometimes convenient to set $k = z + R_2^{1/2}(z)$ (and conversely $z = \frac{1}{2}(k + k^{-1})$), or $k = \exp(\mathrm{i}\kappa)$ (and conversely $z = \cos(\kappa)$) implying

$$u_\pm(z,n) = k^{\pm n} = \mathrm{e}^{\pm\mathrm{i}\kappa n}. \tag{1.123}$$

The map $z \mapsto k = z + R_2^{1/2}(z)$ is a holomorphic mapping from the set $\Pi_+ \simeq (\mathbb{C}\cup\{\infty\})\backslash[-1,1]$ to the unit disk $\{z \in \mathbb{C} |\, |z| < 1\}$. In addition, viewed as a map on the Riemann surface of $R_2^{1/2}(z)$, it provides an explicit isomorphism between the Riemann surface of $R_2^{1/2}(z)$ and the Riemann sphere $\mathbb{C}\cup\{\infty\}$.

1.4. General second order difference expressions

We consider the difference expression

$$\hat\tau f(n) = \frac{1}{w(n)}\Big(f(n+1) + f(n-1) + d(n)f(n)\Big), \tag{1.124}$$

where $w(n) > 0$, $d(n) \in \mathbb{R}$, and $(w(n)w(n+1))^{-1}$, $w(n)^{-1}d(n)$ are bounded sequences. It gives rise to an operator $\hat H$, called **Helmholtz operator**, in the weighted Hilbert space $\ell^2(\mathbb{Z}; w)$ with scalar product

$$\langle f, g\rangle = \sum_{n\in\mathbb{Z}} w(n)\overline{f(n)}g(n), \qquad f, g \in \ell^2(\mathbb{Z}; w). \tag{1.125}$$

Green's formula (1.20) holds with little modifications and $\hat H$ is easily seen to be bounded and self-adjoint. There is an interesting connection between Jacobi and Helmholtz operators stated in the next theorem.

Theorem 1.14. *Let H be the Jacobi operator associated with the sequences $a(n) > 0$, $b(n)$ and let $\hat{H}$ be the Helmholtz operator associated with the sequences $w(n) > 0$, $d(n)$. If we relate these sequences by*

$$\begin{array}{c} w(2m) = w(0) \prod_{j=0}^{m-1}{}^{*} \dfrac{a(2j)^2}{a(2j+1)^2} \\ w(2m+1) = \dfrac{1}{a(2m)^2 w(2m)} \end{array}, \qquad d(n) = w(n)b(n), \tag{1.126}$$

respectively

$$a(n) = \frac{1}{\sqrt{w(n)w(n+1)}}, \qquad b(n) = \frac{d(n)}{w(n)}, \tag{1.127}$$

then the operators H and $\hat{H}$ are unitarily equivalent, that is, $H = U\hat{H}U^{-1}$, where U is the unitary transformation

$$\begin{array}{cccc} U: & \ell^2(\mathbb{Z}; w) & \to & \ell^2(\mathbb{Z}) \\ & u(n) & \mapsto & \sqrt{w(n)}u(n) \end{array}. \tag{1.128}$$

Proof. Straightforward. □

Remark 1.15. (i). The most general three-term recurrence relation

$$\tilde{\tau} f(n) = \tilde{a}(n)f(n+1) + \tilde{b}(n)f(n) + \tilde{c}(n)f(n-1), \tag{1.129}$$

with $\tilde{a}(n)\tilde{c}(n+1) > 0$, can be transformed to a Jacobi recurrence relation as follows. First we render $\tilde{\tau}$ symmetric,

$$\tilde{\tau} f(n) = \frac{1}{w(n)}\Big(c(n)f(n+1) + c(n-1)f(n-1) + d(n)f(n)\Big), \tag{1.130}$$

where

$$\begin{aligned} w(n) &= \prod_{j=n_0}^{n-1}{}^{*} \frac{\tilde{a}(j)}{\tilde{c}(j+1)}, \\ c(n) &= w(n)\tilde{a}(n) = w(n+1)\tilde{c}(n+1), \quad d(n) = w(n)\tilde{b}(n). \end{aligned} \tag{1.131}$$

Let $\tilde{H}$ be the self-adjoint operator associated with $\tilde{\tau}$ in $\ell^2(\mathbb{Z}; w)$. Then the unitary operator

$$\begin{array}{cccc} U: & \ell^2(\mathbb{Z}; w) & \to & \ell^2(\mathbb{Z}) \\ & u(n) & \mapsto & \sqrt{w(n)}u(n) \end{array} \tag{1.132}$$

transforms $\tilde{H}$ into a Jacobi operator $H = U\tilde{H}U^{-1}$ in $\ell^2(\mathbb{Z})$ associated with the sequences

$$\begin{aligned} a(n) &= \frac{c(n)}{\sqrt{w(n)w(n+1)}} = \mathrm{sgn}(\tilde{a}(n))\sqrt{\tilde{a}(n)\tilde{c}(n+1)}, \\ b(n) &= \frac{d(n)}{w(n)} = \tilde{b}(n). \end{aligned} \tag{1.133}$$

In addition, the Wronskians are related by

$$c(n)\Big(f(n)g(n+1) - f(n+1)g(n)\Big) = \\ a(n)\Big((Uf)(n)(Ug)(n+1) - (Uf)(n+1)(Ug)(n)\Big). \tag{1.134}$$

(ii). Let $c(n) > 0$ be given. Defining

$$w(2m) = \prod_{j=0}^{m-1}{}^{*} \left(\frac{a(2j)c(2j+1)}{c(2j)a(2j+1)}\right)^2, \quad d(n) = w(n)b(n), \\ w(2m+1) = \frac{c(2m)^2}{a(2m)^2 w(2m)} \tag{1.135}$$

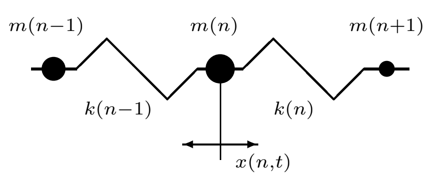
the transformation U maps H to an operator $\tilde{H} = UHU^{-1}$ associated with the difference expression (1.130).

1.5. The infinite harmonic crystal in one dimension

Finally, I want to say something about how Jacobi operators arise in applications. Despite the variety of possible applications of difference equations we will focus on only one model from solid state physics: the infinite harmonic crystal in one dimension. Hence we consider a linear chain of particles with harmonic nearest neighbor interaction. If $x(n,t)$ denotes the deviation of the n-th particle from its equilibrium position, the equations of motion read

$$\begin{aligned} m(n)\frac{d^2}{dt^2}x(n,t) &= -k(n)\big(x(n+1,t) - x(n,t)\big) - k(n-1)\big(x(n-1,t) - x(n,t)\big) \\ &= (\partial k \partial^* x)(n,t), \end{aligned} \tag{1.136}$$

where $m(n) > 0$ is the mass of the n-th particle and $k(n)$ is the force constant between the n-th and $(n+1)$-th particle.



This model is only valid as long as the relative displacement is not too large (i.e., at least smaller than the distance of the particles in the equilibrium position). Moreover, from a physical viewpoint it is natural to assume $k, m, m^{-1} \in \ell^\infty(\mathbb{Z}, \mathbb{R})$ and $k(n) \neq 0$. Introducing conjugate coordinates

$$p(n,t) = m(n)\frac{d}{dt}x(n,t), \quad q(n,t) = x(n,t), \tag{1.137}$$

the system (1.136) can be written as Hamiltonian system with Hamiltonian given by

$$\mathcal{H}(p,q) = \sum_{n\in\mathbb{Z}} \Big(\frac{p(n)^2}{2m(n)} + \frac{k(n)}{2}\big(q(n+1) - q(n)\big)^2\Big). \tag{1.138}$$

Since the total energy of the system is supposed to be finite, a natural phase space for this system is $(p, q) \in \ell^2(\mathbb{Z}, \mathbb{R}^2)$ with symplectic form

$$\omega\big((p_1, q_1), (p_2, q_2)\big) = \sum_{n\in\mathbb{Z}} \Big(p_1(n)q_2(n) - p_2(n)q_1(n)\Big). \tag{1.139}$$

Using the symplectic transform

$$(p, q) \to (v, u) = \big(\frac{p}{\sqrt{m}}, \sqrt{m}\, q\big) \tag{1.140}$$

we get a new Hamiltonian

$$\tilde{\mathcal{H}}(v, u) = \frac{1}{2}\sum_{n\in\mathbb{Z}} \Big(v(n)^2 + 2a(n)u(n)u(n+1) + b(n)u(n)^2\Big), \tag{1.141}$$

where

$$a(n) = \frac{-k(n)}{\sqrt{m(n)m(n+1)}}, \quad b(n) = \frac{k(n) + k(n-1)}{m(n)}. \tag{1.142}$$

The corresponding equations of evolution read

$$\begin{aligned} \frac{d}{dt}u(n,t) &= \frac{\partial\tilde{\mathcal{H}}(v,u)}{\partial v(n,t)} = v(n,t), \\ \frac{d}{dt}v(n,t) &= -\frac{\partial\tilde{\mathcal{H}}(v,u)}{\partial u(n,t)} = -Hu(n,t), \end{aligned} \tag{1.143}$$

where H is our usual Jacobi operator associated with the sequences (1.142). E-quivalently we have

$$\frac{d^2}{dt^2}u(n,t) = -Hu(n,t). \tag{1.144}$$

Since this system is linear, standard theory implies

$$\begin{aligned} u(n,t) &= \cos(t\sqrt{H})u(n,0) + \frac{\sin(t\sqrt{H})}{\sqrt{H}}v(n,0), \\ v(n,t) &= \cos(t\sqrt{H})v(n,0) - \frac{\sin(t\sqrt{H})}{\sqrt{H}}Hu(n,0), \end{aligned} \tag{1.145}$$

where

$$\cos(t\sqrt{H}) = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell t^{2\ell}}{(2\ell)!}H^\ell, \quad \frac{\sin(t\sqrt{H})}{\sqrt{H}} = \sum_{\ell=0}^{\infty} \frac{(-1)^\ell t^{2\ell+1}}{(2\ell+1)!}H^\ell. \tag{1.146}$$

In particular, introducing

$$\underline{S}(\lambda, n) = \big(c(\lambda, n), s(\lambda, n)\big) \tag{1.147}$$

and expanding the initial conditions in terms of eigenfunctions (cf. Section 2.5, equation (2.133))

$$\underline{u}(\lambda) = \sum_{n\in\mathbb{Z}} u(n,0)\underline{S}(\lambda,n), \quad \underline{v}(\lambda) = \sum_{n\in\mathbb{Z}} v(n,0)\underline{S}(\lambda,n) \tag{1.148}$$

we infer

$$u(n,t) = \int_{\sigma(H)} \big(\underline{u}(\lambda)\cos(t\sqrt{\lambda}) + \underline{v}(\lambda)\frac{\sin(t\sqrt{\lambda})}{\sqrt{\lambda}}\big)\underline{S}(\lambda,n)d\rho(\lambda),$$

$$v(n,t) = \int_{\sigma(H)} \big(\underline{v}(\lambda)\cos(t\sqrt{\lambda}) - \underline{u}(\lambda)\frac{\sin(t\sqrt{\lambda})}{\sqrt{\lambda}}\lambda\big)\underline{S}(\lambda,n)d\rho(\lambda), \tag{1.149}$$

where $\rho(\lambda)$ is the spectral matrix of H.

This shows that in order to understand the dynamics of (1.144) one needs to understand the spectrum of H.

For example, in the case where $H \geq 0$ (or if $\underline{u}(\lambda), \underline{u}(\lambda) = 0$ for $\lambda \leq 0$) we clearly infer

$$\|u(t)\| \leq \|u(0)\| + t\|v(0)\|,$$

$$\|v(t)\| \leq \|v(0)\| + \|\sqrt{H}v(0)\|, \tag{1.150}$$

since $|\cos(t\sqrt{\lambda})| \leq 1$, $|\frac{\sin(t\sqrt{\lambda})}{t\sqrt{\lambda}}| \leq 1$ for $t \in \mathbb{R}$, $\lambda \geq 0$.

Given this setting two questions naturally arise. Firstly, given $m(n)$, $k(n)$ what can be said about the characteristic frequencies of the crystal? Spectral theory for H deals with this problem. Secondly, given the set of characteristic frequencies (i.e., the spectrum of H), is it possible to reconstruct $m(n)$, $k(n)$? This question is equivalent to inverse spectral theory for H once we establish how to reconstruct k, m from a, b. This will be done next.

Note that $u(n) = \sqrt{m(n)} > 0$ solves $\tau u = 0$. Hence, if we assume $k > 0$, then $H \geq 0$ by Corollary 11.2. In particular,

$$\sigma(H) \subseteq [0, 2(\|k\|_\infty \|m^{-1}\|_\infty)] \tag{1.151}$$

and 0 is in the essential spectrum of H by Lemma 3.8. Moreover, since

$$\sum_{n\in\pm\mathbb{N}} \frac{1}{-a(n)u(n)u(n+1)} = \sum_{n\in\pm\mathbb{N}} \frac{1}{k(n)} = \infty \tag{1.152}$$

(recall $k \in \ell^\infty(\mathbb{Z})$), H is critical (cf. Section 2.3). Thus we can recover k, m via

$$k(n) = -m(0)a(n)u(n)u(n+1), \quad m(n) = m(0)u(n)^2, \tag{1.153}$$

where $u(n)$ is the unique positive solution of $\tau u = 0$ satisfying $u(0) = \sqrt{m(0)}$. That m, k can only be recovered up to a constant multiple (i.e., $m(0)$) is not surprising due to the corresponding scaling invariance of (1.136). If the positive solution of $\tau u = 0$ is not unique, we get a second free parameter. However, note that for each choice the corresponding Helmholtz operator $\hat{H} = m^{-1}\partial k \partial^*$ is unitary equivalent to H (and so are $\hat{H}_\pm$ and $H_\pm$).

From a physical viewpoint the case of a crystal with N atoms in the base cell is of particular interest, that is, k and m are assumed to be periodic with period N. In this case, the same is true for a, b and we are led to the study of periodic Jacobi operators. The next step is to consider impurities in this crystal. If such impurities appear only local, we are led to scattering theory with periodic background (to be dealt with in Chapter 7). If they are randomly distributed over the crystal we are led to random operators (to be dealt with in Chapter 5).

But for the moment let us say a little more about the simplest case where m and k are both constants (i.e., $N = 1$). After the transformation $t \mapsto \sqrt{\frac{m}{2k}}$ we can even assume $m = k = 1$, that is,

$$\frac{d^2}{dt^2} x(n,t) = -\frac{1}{2}\big(x(n+1,t) + x(n-1,t)\big) + x(n,t). \tag{1.154}$$

The so-called plane wave solutions are given by

$$u^{\pm}(n,t) = \mathrm{e}^{\mathrm{i}(\kappa n \pm \nu(\kappa) t)}, \tag{1.155}$$

where the wavelength κ^{-1} and the frequency ν are connected by the **dispersion relation**

$$\nu(\kappa) = \sqrt{1 - \cos(\kappa)} = \sqrt{2}\sin(\frac{\kappa}{2}). \tag{1.156}$$

Since $u^{\pm}(n,t)$ is only meaningful for $n \in \mathbb{Z}$, we can restrict κ to values in the first Brillouin zone, that is, $\kappa \in (-\pi, \pi]$.

These solutions correspond to infinite total energy of the crystal. However, one can remedy this problem by taking (continuous) superpositions of these plane waves. Introducing

$$u(\kappa) = \sum_{n \in \mathbb{Z}} u(n,0)\mathrm{e}^{\mathrm{i}\kappa n}, \quad v(\kappa) = \sum_{n \in \mathbb{Z}} v(n,0)\mathrm{e}^{\mathrm{i}\kappa n} \tag{1.157}$$

we obtain

$$u(n,t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \Big(u(\kappa)\cos(\nu(\kappa)t) + v(\kappa)\frac{\sin(\nu(\kappa)t)}{\nu(\kappa)}\Big)\mathrm{e}^{-\mathrm{i}\kappa n} d\kappa. \tag{1.158}$$

Or, equivalently,

$$u(n,t) = \sum_{m \in \mathbb{Z}} c_{n-m}(t) u(m,0) + s_{n-m}(t) v(m,0), \tag{1.159}$$

where

$$\begin{aligned} c_n(t) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \cos(\nu(\kappa)t)\mathrm{e}^{\mathrm{i}\kappa n} d\kappa = J_{2|n|}(\sqrt{2}t), \\ s_n(t) &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\sin(\nu(\kappa)t)}{\nu(\kappa)}\mathrm{e}^{\mathrm{i}\kappa n} d\kappa = \int_0^t c_n(s) ds \\ &= \frac{t^{2|n|+1}}{2^{|n|}(|n|+1)!}\, {}_1F_2\Big(\frac{2|n|+1}{2}; (\frac{2|n|+3}{2}, 2|n|+1); -\frac{t^2}{2}\Big). \end{aligned} \tag{1.160}$$

Here $J_n(x)$, ${}_pF_q(\underline{u}; \underline{v}; x)$ denote the Bessel and generalized hypergeometric functions, respectively. From this form one can deduce that a localized wave (say compactly supported at $t = 0$) will spread as t increases (cf. [**194**], Corollary to Theorem XI.14). This phenomenon is due to the fact that different plane waves travel with different speed and is called dispersion.

You might want to observe the following fact: if the coupling constant $k(n_0)$ between the n_0-th and $(n_0 + 1)$-th particle is zero (i.e., no interaction between these particles), then the chain separates into two parts (cf. the discussion after Theorem 1.5 and note that $k(n_0) = 0$ implies $a(n_0) = 0$ for the corresponding Jacobi operator).

We will encounter chains of particles again in Section 12.1. However, there we will consider a certain nonlinear interaction.

Chapter 2

Foundations of spectral theory for Jacobi operators

The theory presented in this chapter is the discrete analog of what is known as Weyl-Titchmarsh-Kodaira theory for Sturm-Liouville operators. The discrete version has the advantage of being less technical and more transparent.

Again, the present chapter is of fundamental importance and the tools developed here are the pillars of spectral theory for Jacobi operators.

2.1. Weyl m-functions

In this section we will introduce and investigate Weyl m-functions. Rather than the classical approach of Weyl (cf. Section 2.4) we advocate a different one which is more natural in the discrete case.

As in the previous chapter, $u_\pm(z,.)$ denote the solutions of (1.19) in $\ell(\mathbb{Z})$ which are square summable near $\pm\infty$, respectively.

We start by defining the **Weyl m-functions**

$$m_\pm(z,n_0) = \langle \delta_{n_0\pm 1}, (H_{\pm,n_0} - z)^{-1}\delta_{n_0\pm 1}\rangle = G_{\pm,n_0}(z, n_0 \pm 1, n_0 \pm 1). \tag{2.1}$$

By virtue of (1.104) we also have the more explicit form

$$m_+(z,n_0) = -\frac{u_+(z,n_0+1)}{a(n_0)u_+(z,n_0)}, \qquad m_-(z,n_0) = -\frac{u_-(z,n_0-1)}{a(n_0-1)u_-(z,n_0)}. \tag{2.2}$$

The base point n_0 is of no importance in what follows and we will only consider $m_\pm(z) = m_\pm(z,0)$ most of the time. Moreover, all results for $m_-(z)$ can be obtained from the corresponding results for $m_+(z)$ using reflection (cf. Lemma 1.7).

The definition (2.1) implies that the function $m_\pm(z)$ is holomorphic in $\mathbb{C}\backslash\sigma(H_\pm)$ and that it satisfies

$$m_\pm(\overline{z}) = \overline{m_\pm(z)}, \qquad |m_\pm(z)| \le \|(H_\pm - z)^{-1}\| \le \frac{1}{|\mathrm{Im}(z)|}. \tag{2.3}$$

Moreover, $m_\pm(z)$ is a Herglotz function (i.e., it maps the upper half plane into itself, cf. Appendix B). In fact, this is a simple consequence of the first resolvent identity

$$\begin{aligned}\mathrm{Im}(m_\pm(z)) &= \mathrm{Im}(z)\langle\delta_{\pm1}, (H_\pm - \overline{z})^{-1}(H_\pm - z)^{-1}\delta_{\pm1}\rangle \\ &= \mathrm{Im}(z)\|(H_\pm - z)^{-1}\delta_{\pm1}\|^2. \end{aligned} \tag{2.4}$$

Hence by Theorem B.2, $m_\pm(z)$ has the following representation

$$m_\pm(z) = \int_{\mathbb{R}} \frac{d\rho_\pm(\lambda)}{\lambda - z}, \qquad z \in \mathbb{C}\backslash\mathbb{R}, \tag{2.5}$$

where $\rho_\pm = \int_{(-\infty,\lambda]} d\rho_\pm$ is a nondecreasing bounded function which is given by Stieltjes inversion formula (cf. Theorem B.2)

$$\rho_\pm(\lambda) = \frac{1}{\pi}\lim_{\delta\downarrow 0}\lim_{\varepsilon\downarrow 0}\int_{-\infty}^{\lambda+\delta} \mathrm{Im}(m_\pm(x + \mathrm{i}\varepsilon))dx. \tag{2.6}$$

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

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

$$m_\pm(z) = \langle\delta_{\pm1}, (H_\pm - z)^{-1}\delta_{\pm1}\rangle = \int_{\mathbb{R}} \frac{d\langle\delta_{\pm1}, P_{(-\infty,\lambda]}(H_\pm)\delta_{\pm1}\rangle}{\lambda - z}. \tag{2.7}$$

Thus we see that $d\rho_\pm = d\langle\delta_{\pm1}, P_{(-\infty,\lambda]}(H_\pm)\delta_{\pm1}\rangle$ is the spectral measure of $H_\pm$ associated to the sequence $\delta_{\pm1}$.

Remark 2.1. (i). Clearly, similar considerations hold for arbitrary expectations of resolvents of self-adjoint operators (cf. Lemma 6.1).
(ii). Let me note at this point that the fact which makes discrete life so much easier than continuous life is, that δ_1 is an element of our Hilbert space. In contradistinction, the continuous analog of δ_n, the delta distribution δ_x, is not a square integrable function. (However, if one considers non-negative Sturm-Liouville operators H, then δ_x lies in the scale of spaces associated to H. See [**206**] for further details.)

It follows in addition that all moments $m_{\pm,\ell}$ of $d\rho_\pm$ are finite and given by

$$m_{\pm,\ell} = \int_{\mathbb{R}} \lambda^\ell d\rho_\pm(\lambda) = \langle\delta_{\pm1}, (H_+)^\ell\delta_{\pm1}\rangle. \tag{2.8}$$

Moreover, there is a close connection between the so-called moment problem (i.e., determining $d\rho_\pm$ from all its moments $m_{\pm,\ell}$) and the reconstruction of $H_\pm$ from $d\rho_\pm$. Indeed, since $m_{\pm,0} = 1$, $m_{\pm,1} = b(\pm1)$, $m_{\pm,2} = a(\pm1 - {}^0_1)^2 + b(\pm1)^2$, etc., we infer

$$b(\pm1) = m_{\pm,1}, \quad a(\pm1 - {}^0_1)^2 = m_{\pm,2} - (m_{\pm,1})^2, \quad \text{etc. }. \tag{2.9}$$

We will consider this topic in Section 2.5.

You might have noticed, that $m_\pm(z,n)$ has (up to the factor $-a(n - {}^0_1)$) the same structure as the function $\phi(n)$ used when deriving the Riccati equation (1.52).

Comparison with the formulas for $\phi(n)$ shows that

$$u_\pm(z,n) = u_\pm(z,n_0) \prod_{j=n_0}^{n-1}{}^{*} \; (-a(j - {}^{0}_{1}) m_\pm(z,j))^{\pm 1} \tag{2.10}$$

and that $m_+(z,n)$ satisfies the following recurrence relation

$$a(n - {}^{0}_{1})^2 m_\pm(z,n) + \frac{1}{m_\pm(z, n \mp 1)} + z - b(n) = 0. \tag{2.11}$$

The functions $m_\pm(z,n)$ are the correct objects from the viewpoint of spectral theory. However, when it comes to calculations, the following pair of Weyl m-functions

$$\tilde{m}_\pm(z,n) = \mp \frac{u_\pm(z,n+1)}{a(n) u_\pm(z,n)}, \quad \tilde{m}_\pm(z) = \tilde{m}_\pm(z,0) \tag{2.12}$$

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

$$m_+(z,n) = \tilde{m}_+(z,n), \qquad m_-(z,n) = \frac{a(n)^2 \tilde{m}_-(z,n) - z + b(n)}{a(n-1)^2} \tag{2.13}$$

(note also $m_-(z,n+1)^{-1} = -a(n)^2 \tilde{m}_-(z,n)$) and the corresponding spectral measures (for $n = 0$) are related by

$$d\rho_+ = d\tilde{\rho}_+, \qquad d\rho_- = \frac{a(0)^2}{a(-1)^2} d\tilde{\rho}_-. \tag{2.14}$$

You might want to note that $\tilde{m}_-(z)$ does not tend to 0 as $\mathrm{Im}(z) \to \infty$ since the linear part is present in its Herglotz representation

$$\tilde{m}_-(z) = \frac{z - b(n)}{a(0)^2} + \int_{\mathbb{R}} \frac{d\tilde{\rho}_-(\lambda)}{\lambda - z}. \tag{2.15}$$

Finally, we introduce the Weyl m-functions $m_\pm^\beta(z,n)$ associated with $H_{\pm,n}^\beta$. They are defined analogously to $m_\pm(z,n)$. Moreover, the definition of $H_{+,n}^\beta$ in terms of $H_{+,n}$ suggests that $m_+^\beta(z,n)$, $\beta \neq 0$, can be expressed in terms of $m_+(z,n)$. Using (1.91) and the second resolvent identity we obtain

$$m_+^\beta(z,n) = \langle \delta_{n+1}, (H_{+,n}^\beta - z)^{-1} \delta_{n+1} \rangle = \frac{\beta m_+(z,n)}{\beta - a(n) m_+(z,n)}. \tag{2.16}$$

Similarly, the Weyl m-functions $m_-^\beta(z,n)$ associated with $H_{-,n}^\beta$, $\beta \neq \infty$, can be expressed in terms of $m_-(z,n+1)$,

$$m_-^\beta(z,n) = \langle \delta_n, (H_{-,n}^\beta - z)^{-1} \delta_n \rangle = \frac{m_-(z,n+1)}{1 - \beta a(n) m_-(z,n+1)}. \tag{2.17}$$

2.2. Properties of solutions

The aim of the present section is to establish some fundamental properties of special solutions of (1.19) which will be indispensable later on.

As an application of Weyl m-functions we first derive some additional properties of the solutions $u_\pm(z,.)$. By (1.27) we have

$$u_\pm(z,n) = a(0) u_\pm(z,0) \Big(a(0)^{-1} c(z,n) \mp \tilde{m}_\pm(z) s(z,n) \Big), \tag{2.18}$$

where the constant (with respect to n) $a(0)u_\pm(z,0)$ is at our disposal. If we choose $a(0)u_\pm(z,0) = 1$ (bearing in mind that $c(z,n)$, $s(z,n)$ are polynomials with respect to z), we infer for instance (using (2.4))

$$\overline{u_\pm(z,n)} = u_\pm(\overline{z},n). \tag{2.19}$$

Moreover, $u_\pm(z,n)$ are holomorphic with respect to $z \in \mathbb{C}\backslash\sigma(H_\pm)$. But we can do even better. If μ is an isolated eigenvalue of $H_\pm$, then $\tilde{m}_\pm(z)$ has a simple pole at $z = \mu$ (since it is Herglotz; see also (2.36)). By choosing $a(0)u_\pm(z,0) = (z-\mu)$ we can remove the singularity at $z = \mu$. In summary,

Lemma 2.2. *The solution $u_\pm(z,n)$ of (1.19) which is square summable near $\pm\infty$ exist for $z \in \mathbb{C}\backslash\sigma_{ess}(H_\pm)$, respectively. If we choose*

$$u_\pm(z,n) = \frac{c(z,n)}{a(0)} \mp \tilde{m}_\pm(z)s(z,n), \tag{2.20}$$

then $u_\pm(z,n)$ is holomorphic for $z \in \mathbb{C}\backslash\sigma(H_\pm)$, $u_\pm(z,.) \not\equiv 0$, and $\overline{u_\pm(z,.)} = u_\pm(\overline{z},.)$. In addition, we can include a finite number of isolated eigenvalues in the domain of holomorphy of $u_\pm(z,n)$.

Moreover, the sums

$$\sum_{j=n}^{\infty} u_+(z_1,j)u_+(z_2,j), \qquad \sum_{j=-\infty}^{n} u_-(z_1,j)u_-(z_2,j) \tag{2.21}$$

are holomorphic with respect to z_1 (resp. z_2) provided $u_\pm(z_1,.)$ (resp. $u_\pm(z_2,.)$) are.

Proof. Only the last assertion has not been shown yet. It suffices to prove the claim for one n, say $n = 1$. Without restriction we suppose $u_+(z,0) = -a(0)^{-1}$ (if $u_+(z,0) = 0$, shift everything by one). Then $u_+(z,n) = (H_+ - z)^{-1}\delta_1(n)$, $n \ge 1$, and hence

$$\sum_{j=1}^{\infty} u_+(z_1,j)u_+(z_2,j) = \langle\delta_1, (H_+ - z_1)^{-1}(H_+ - z_2)^{-1}\delta_1\rangle_{\ell^2(\mathbb{N})}. \tag{2.22}$$

The remaining case is similar. □

Remark 2.3. If $(\lambda_0,\lambda_1) \subset \rho(H)$, we can define $u_\pm(\lambda,n)$, $\lambda \in [\lambda_0,\lambda_1]$. Indeed, by (2.20) it suffices to prove that $m_\pm(\lambda)$ tends to a limit (in $\mathbb{R} \cup \{\infty\}$) as $\lambda \downarrow \lambda_0$ or $\lambda \uparrow \lambda_1$. This follows from monotonicity of $m_\pm(\lambda)$,

$$m_\pm'(\lambda) = -\langle\delta_{\pm1}, (H_\pm - \lambda)^{-2}\delta_{\pm1}\rangle < 0, \quad \lambda \in (\lambda_0,\lambda_1) \tag{2.23}$$

(compare also equation (B.18)). Here the prime denotes the derivative with respect to λ. However, $u_\pm(\lambda_{0,1},n)$ might not be square summable near $\pm\infty$ in general.

In addition, the discrete eigenvalues of H_+^β are the zeros of $\frac{\beta}{a(0)} - m_+(\lambda)$ (see (2.16)) and hence decreasing as a function of β. Similarly, the discrete eigenvalues of H_-^β are the zeros of $\frac{1}{a(0)\beta} - m_-(\lambda)$ (see (2.17)) and hence increasing as a function of β.

Let $u(z)$ be a solution of (1.19) with $z \in \mathbb{C}\backslash\mathbb{R}$. If we choose $f = u(z)$, $g = \overline{u(z)}$ in (1.20), we obtain

$$[u(z)]_n = [u(z)]_{m-1} - \sum_{j=m}^{n}{}^{*} \; |u(z,j)|^2, \tag{2.24}$$

where $[.]_n$ denotes the **Weyl bracket**,

$$[u(z)]_n = \frac{W_n(u(z), \overline{u(z)})}{2\mathrm{i}\mathrm{Im}(z)} = a(n) \frac{\mathrm{Im}(u(z,n)\overline{u(z,n+1)})}{\mathrm{Im}(z)}. \tag{2.25}$$

Especially for $u_\pm(z,n)$ as in Lemma 2.2 we get

$$[u_\pm(z)]_n = \begin{cases} \sum\limits_{j=n+1}^{\infty} |u_+(z,j)|^2 \\ -\sum\limits_{j=-\infty}^{n} |u_-(z,j)|^2 \end{cases} \tag{2.26}$$

and for $s(z,n)$

$$[s(z)]_n = \begin{cases} -\sum\limits_{j=0}^{n} |s(z,j)|^2, & n \geq 0 \\ \sum\limits_{j=n+1}^{0} |s(z,j)|^2, & n < 0 \end{cases}. \tag{2.27}$$

Moreover, let $u(z,n), v(z,n)$ be solutions of (1.19). If $u(z,n)$ is differentiable with respect to z, we obtain

$$(\tau - z)u'(z,n) = u(z,n) \tag{2.28}$$

(here the prime denotes the derivative with respect to z) and using Green's formula (1.20) we infer

$$\sum_{j=m}^{n} v(z,j)u(z,j) = W_n(v(z), u'(z)) - W_{m-1}(v(z), u'(z)). \tag{2.29}$$

Even more interesting is the following result.

Lemma 2.4. *Let $u_\pm(z,n)$ be solutions of (1.19) as in Lemma 2.2. Then we have*

$$W_n(u_\pm(z), \frac{d}{dz} u_\pm(z)) = \begin{cases} -\sum\limits_{j=n+1}^{\infty} u_+(z,j)^2 \\ \sum\limits_{j=-\infty}^{n} u_-(z,j)^2 \end{cases}. \tag{2.30}$$

Proof. Green's formula (1.20) implies

$$W_n(u_+(z), u_+(\tilde{z})) = (z - \tilde{z}) \sum_{j=n+1}^{\infty} u_+(z,j)u_+(\tilde{z},j) \tag{2.31}$$

and furthermore,

$$\begin{aligned} W_n(u_+(z), u'_+(z)) &= \lim_{\tilde{z} \to z} W_n\big(u_+(z), \frac{u_+(z) - u_+(\tilde{z})}{z - \tilde{z}}\big) \\ &= \sum_{j=n+1}^{\infty} u_+(z,j)^2. \end{aligned} \tag{2.32}$$

□

As a first application of this lemma, let us investigate the isolated poles of $G(z,n,m)$. If $z=\lambda_0$ is such an isolated pole (i.e., an isolated eigenvalue of H), then $W(u_-(\lambda_0),u_+(\lambda_0))=0$ and hence $u_\pm(\lambda_0,n)$ differ only by a (nonzero) constant multiple. Moreover,

$$\begin{aligned}\frac{d}{dz}W(u_-(z),u_+(z))\Big|_{z=\lambda_0} &= W_n(u_-(\lambda_0),u_+'(\lambda_0))+W_n(u_-'(\lambda_0),u_+(\lambda_0))\\ &= -\sum_{j\in\mathbb{Z}} u_-(\lambda_0,j)u_+(\lambda_0,j) \qquad (2.33)\end{aligned}$$

by the lemma and hence

$$G(z,n,m)=-\frac{P(\lambda_0,n,m)}{z-\lambda_0}+O(z-\lambda_0)^0, \qquad (2.34)$$

where

$$P(\lambda_0,n,m)=\frac{u_\pm(\lambda_0,n)u_\pm(\lambda_0,m)}{\sum\limits_{j\in\mathbb{Z}} u_\pm(\lambda_0,j)^2}. \qquad (2.35)$$

Similarly, for $H_\pm$ we obtain

$$\lim_{z\to\mu}(z-\mu)G_\pm(z,n,m)=-\frac{s(\mu,n)s(\mu,m)}{\sum\limits_{j\in\pm\mathbb{N}} s(\mu,j)^2}. \qquad (2.36)$$

Thus the poles of the kernel of the resolvent at isolated eigenvalues are simple. Moreover, the negative residue equals the kernel of the projector onto the corresponding eigenspace.

As a second application we show monotonicity of $G(z,n,n)$ with respect to z in a spectral gap. Differentiating (1.99), a straightforward calculation shows

$$G'(z,n,n)=\frac{u_+(z,n)^2W_n(u_-(z),\dot u_-(z))-u_-(z,n)^2W_n(u_+(z),\dot u_+(z))}{W(u_-(z),u_+(z))^2}, \qquad (2.37)$$

which is positive for $z\in\mathbb{R}\backslash\sigma(H)$ by Lemma 2.4. The same result also follows from

$$\begin{aligned}G'(z,n,m) &= \frac{d}{dz}\langle\delta_n,(H-z)^{-1}\delta_m\rangle=\langle\delta_n,(H-z)^{-2}\delta_m\rangle\\ &= \sum_{j\in\mathbb{Z}} G(z,n,j)G(z,j,m). \qquad (2.38)\end{aligned}$$

Finally, let us investigate the qualitative behavior of the solutions $u_\pm(z)$ more closely.

Lemma 2.5. *Suppose $z\in\mathbb{C}\backslash\sigma_{ess}(H_\pm)$. Then we can find $C_\pm$, $\gamma^\pm>0$ such that*

$$|u_\pm(z,n)|\le C_\pm\exp(-\gamma^\pm n),\quad \pm n\in\mathbb{N}. \qquad (2.39)$$

For $\gamma^\pm$ we can choose

$$\gamma^\pm=\ln\Big(1+(1-\varepsilon)\frac{\sup_{\beta\in\mathbb{R}\cup\{\infty\}}\mathrm{dist}(\sigma(H_\pm^\beta),z)}{2\sup_{n\in\mathbb{N}}|a(\pm n)|}\Big),\quad \varepsilon>0 \qquad (2.40)$$

(the corresponding constant $C_\pm$ will depend on ε).

Proof. By the definition of $H_\pm^\beta$ it suffices to consider the case $\beta = \infty$, $\delta = \mathrm{dist}(\sigma(H_+), z) > 0$ (otherwise alter $b(1)$ or shift the interval). Recall $G_+(z,1,n) = u_+(z,n)/(-a(0)u_+(z,0))$ and consider $(\gamma > 0)$

$$\begin{aligned} \mathrm{e}^{\gamma(n-1)} G_+(z,1,n) &= \langle \delta_1, P_{-\gamma}(H_+ - z)^{-1} P_\gamma \delta_n\rangle = \langle \delta_1, (P_{-\gamma} H_+ P_\gamma - z)^{-1}\delta_n\rangle \\ &= \langle \delta_1, (H_+ - z + Q_\gamma)^{-1}\delta_n\rangle, \end{aligned} \tag{2.41}$$

where

$$(P_\gamma u)(n) = \mathrm{e}^{\gamma n} u(n) \tag{2.42}$$

and

$$(Q_\gamma u)(n) = a(n)(\mathrm{e}^{\gamma} - 1)u(n+1) + a(n-1)(\mathrm{e}^{-\gamma} - 1)u(n-1). \tag{2.43}$$

Moreover, choosing $\gamma = \ln(1 + (1-\varepsilon)\delta/(2\sup_{n\in\mathbb{N}} |a(\pm n)|))$ we have

$$\|Q_\gamma\| \le 2 \sup_{n\in\mathbb{N}} |a(\pm n)|(\mathrm{e}^{\gamma} - 1) = (1-\varepsilon)\delta. \tag{2.44}$$

Using the first resolvent equation

$$\begin{aligned} \|(H_+ - z + Q_\gamma)^{-1}\| \;&\le\; \|(H_+ - z)^{-1}\| + \|(H_+ - z)^{-1}\| \\ &\quad \times \|Q_\gamma\| \|(H_+ - z + Q_\gamma)^{-1}\| \end{aligned} \tag{2.45}$$

and $\|(H_+ - z)^{-1}\| = \delta^{-1}$ implies the desired result

$$|\mathrm{e}^{\gamma(n-1)} G_+(z,1,n)| \le \|(H_+ - z + Q_\gamma)^{-1}\| \le \frac{1}{\delta\varepsilon}. \tag{2.46}$$

□

This result also shows that for any solution $u(z,n)$ which is not a multiple of $u_\pm(z,.)$, we have

$$\sqrt{|u(z,n)|^2 + |u(z,n+1)|^2} \ge \frac{const}{|a(n)|} \mathrm{e}^{\gamma^\pm n} \tag{2.47}$$

since otherwise the Wronskian of u and $u_\pm(z)$ would vanish as $n \to \pm\infty$. Hence, (cf. (1.34))

$$\{\lambda \in \mathbb{R} | \underline{\gamma}^\pm(\lambda) = 0\} \subseteq \sigma_{ess}(H_\pm) \tag{2.48}$$

since $\underline{\gamma}^\pm(\lambda) > \gamma^\pm$, $\lambda \notin \sigma_{ess}(H_\pm)$.

2.3. Positive solutions

In this section we want to investigate solutions of $\tau u = \lambda u$ with $\lambda \le \sigma(H)$. We will assume

$$a(n) < 0 \tag{2.49}$$

throughout this section. As a warm-up we consider the case $\lambda < \sigma(H)$.

Lemma 2.6. *Suppose $a(n) < 0$ and let $\lambda < \sigma(H)$. Then we can assume*

$$u_\pm(\lambda, n) > 0, \quad n \in \mathbb{Z}, \tag{2.50}$$

and we have

$$(n - n_0) s(\lambda, n, n_0) > 0, \quad n \in \mathbb{Z}\backslash\{n_0\}. \tag{2.51}$$

Proof. From $(H-\lambda)>0$ one infers $(H_{+,n}-\lambda)>0$ and hence

$$0 < \langle \delta_{n+1}, (H_{+,n}-\lambda)^{-1}\delta_{n+1}\rangle = \frac{u_+(\lambda,n+1)}{-a(n)u_+(\lambda,n)}, \tag{2.52}$$

showing that $u_+(\lambda)$ can be chosen to be positive. Furthermore, for $n > n_0$ we obtain

$$0 < \langle \delta_n, (H_{+,n_0}-\lambda)^{-1}\delta_n\rangle = \frac{u_+(\lambda,n)s(\lambda,n,n_0)}{-a(n_0)u_+(\lambda,n_0)}, \tag{2.53}$$

implying $s(\lambda,n,n_0)>0$ for $n>n_0$. The remaining case is similar. □

The general case $\lambda \le \sigma(H)$ requires an additional investigation. We first prove that (2.51) also holds for $\lambda \le \sigma(H)$ with the aid of the following lemma.

Lemma 2.7. *Suppose $a(n)<0$ and let $u \not\equiv 0$ solve $\tau u = u$. Then $u(n)\ge 0$, $n \ge n_0$ (resp. $n \le n_0$), implies $u(n)>0$, $n>n_0$ (resp. $n<n_0$). Similarly, $u(n)\ge 0$, $n\in\mathbb{Z}$, implies $u>0$, $n\in\mathbb{Z}$.*

Proof. Fix $n>n_0$ (resp. $n<n_0$). Then, $u(n)=0$ implies $u(n\pm 1)>0$ (since u cannot vanish at two consecutive points) contradicting $0=(b(n)-\lambda)u(n) = -a(n)u(n+1)-a(n-1)u(n-1)>0$. □

The desired result now follows from

$$s(\lambda,n,n_0) = \lim_{\varepsilon\downarrow 0} s(\lambda-\varepsilon,n,n_0)\ge 0, \quad n>n_0, \tag{2.54}$$

and the lemma. In addition, we note

$$b(n)-\lambda = -a(n)s(\lambda,n+1,n-1)>0, \quad \lambda\le\sigma(H). \tag{2.55}$$

The following corollary is simple but powerful.

Corollary 2.8. *Suppose $u_j(\lambda,n)$, $j=1,2$, are two solutions of $\tau u=\lambda u$, $\lambda\le\sigma(H)$, with $u_1(\lambda,n_0)=u_2(\lambda,n_0)$ for some $n_0\in\mathbb{Z}$. Then if*

$$(n-n_0)\big(u_1(\lambda,n)-u_2(\lambda,n)\big)>0 \quad (\textit{resp.} <0) \tag{2.56}$$

holds for one $n\in\mathbb{Z}\backslash\{n_0\}$, then it holds for all. If $u_1(\lambda,n)=u_2(\lambda,n)$ for one $n\in\mathbb{Z}\backslash\{n_0\}$, then u_1 and u_2 are equal.

Proof. Use $u_1(\lambda,n)-u_2(\lambda,n) = c\, s(\lambda,n,n_0)$ for some $c\in\mathbb{R}$. □

In particular, this says that for $\lambda\le\sigma(H)$ solutions $u(\lambda,n)$ can change sign (resp. vanish) at most once (since $s(z,n,n_0)$ does).

For the sequence

$$u_m(\lambda,n) = \frac{s(\lambda,n,m)}{s(\lambda,0,m)}, \quad m\in\mathbb{N}, \tag{2.57}$$

this corollary implies that

$$\phi_m(\lambda) = u_m(\lambda,1) = \frac{s(\lambda,1,m)}{s(\lambda,0,m)} \tag{2.58}$$

is increasing with m since we have $u_{m+1}(\lambda,m)>0=u_m(\lambda,m)$. Next, since $a(0)s(\lambda,1,m)+a(-1)s(\lambda,-1,m) = (\lambda-b(0))s(\lambda,0,m)$ implies

$$\phi_m(\lambda) < \frac{\lambda-b(0)}{a(0)}, \tag{2.59}$$

we can define

(2.60)
$$\phi_+(\lambda) = \lim_{m\to\infty} \phi_m(\lambda), \quad u_+(\lambda, n) = \lim_{m\to\infty} u_m(\lambda, n) = c(\lambda, n) + \phi_+(\lambda)s(\lambda, n).$$

By construction we have $u_+(\lambda, n) > u_m(\lambda, n)$, $n \in \mathbb{N}$, implying $u_+(\lambda, n) > 0$, $n \in \mathbb{N}$. For $n < 0$ we have at least $u_+(\lambda, n) \geq 0$ since $u_m(\lambda, n) > 0$ and thus $u_+(\lambda, n) > 0$, $n \in \mathbb{Z}$, by Lemma 2.7.

Let $u(\lambda, n)$ be a solution with $u(\lambda, 0) = 1$, $u(\lambda, 1) = \phi(\lambda)$. Then, by the above analysis, we infer that $u(\lambda, n) > 0$, $n \in \mathbb{N}$, is equivalent to $\phi(\lambda) \geq \phi_+(\lambda)$ and hence $u(\lambda, n) \geq u_+(\lambda, n)$, $n \in \mathbb{N}$ (with equality holding if and only if $u(\lambda) = u_+(\lambda)$). In this sense $u_+(\lambda)$ is the **minimal positive solution** (also **principal** or **recessive** solution) near $+\infty$. In particular, since every solution can change sign at most once, we infer that if there is a square summable solution near $+\infty$, then it must be equal to $u_+(\lambda, n)$ (up to a constant multiple), justifying our notation.

Moreover, if $u(\lambda)$ is different from $u_+(\lambda)$, then constancy of the Wronskian

$$\frac{u_+(\lambda, n)}{u(\lambda, n)} - \frac{u_+(\lambda, n+1)}{u(\lambda, n+1)} = \frac{W(u(\lambda), u_+(\lambda))}{-a(n)u(\lambda, n)u(\lambda, n+1)} \tag{2.61}$$

together with $W(u(\lambda), u_+(\lambda)) = a(0)(\phi_+(\lambda) - \phi(\lambda)) > 0$ shows that the sequence $u_+(\lambda, n)/u(\lambda, n)$ is decreasing for all $u(\lambda) \neq u_+(\lambda)$ if and only if $u_+(\lambda)$ is minimal. Moreover, we claim

$$\lim_{n\to\infty} \frac{u_+(\lambda, n)}{u(\lambda, n)} = 0. \tag{2.62}$$

In fact, suppose $\lim_{n\to\infty} u_+(\lambda, n)/u(\lambda, n) = \varepsilon > 0$. Then $u_+(\lambda, n) > \varepsilon u(\lambda, n)$, $n \in \mathbb{N}$, and hence $u_\varepsilon = (u_+(\lambda, n) - \varepsilon u(\lambda, n))/(1-\varepsilon) > 0$, $n \in \mathbb{N}$. But $u_+(\lambda, n) < u_\varepsilon(\lambda, n)$ implies $u(\lambda, n) < u_+(\lambda, n)$, a contradiction.

Conversely, (2.62) for one $u(\lambda)$ uniquely characterizes $u_+(\lambda, n)$ since (2.62) remains valid if we replace $u(\lambda)$ by any positive linear combination of $u(\lambda)$ and $u_+(\lambda)$.

Summing up (2.61) shows that

$$\sum_{j=0}^{\infty} \frac{1}{-a(j)u(\lambda, j)u(\lambda, j+1)} = \frac{1}{a(0)(\phi_+(\lambda) - \phi(\lambda))} < \infty. \tag{2.63}$$

Moreover, the sequence

$$v(\lambda, n) = u(\lambda, n) \sum_{j=n}^{\infty} \frac{1}{-a(j)u(\lambda, j)u(\lambda, j+1)} > 0 \tag{2.64}$$

solves $\tau u = \lambda u$ (cf. (1.51)) and equals $u_+(\lambda, n)$ up to a constant multiple since $\lim_{n\to\infty} v(\lambda, n)/u(\lambda, n) = 0$.

By reflection we obtain a corresponding minimal positive solution $u_-(\lambda, n)$ near $-\infty$. Let us summarize some of the results obtained thus far.

Lemma 2.9. *Suppose $a(n) < 0$, $\lambda \leq \sigma(H)$ and let $u(\lambda, n)$ be a solution with $u(\lambda, n) > 0$, $\pm n \geq 0$. Then the following conditions are equivalent.*

(i). *$u(\lambda, n)$ is minimal near $\pm\infty$.*

(ii). *We have*

$$\frac{u(\lambda,n)}{v(\lambda,n)} \le \frac{v(\lambda,0)}{u(\lambda,0)}, \quad \pm n \ge 0, \tag{2.65}$$

for any solution $v(\lambda,n)$ *with* $v(\lambda,n) > 0$, $\pm n \ge 0$.

(iii). *We have*

$$\lim_{n\to\pm\infty} \frac{u(\lambda,n)}{v(\lambda,n)} = 0. \tag{2.66}$$

for one solution $v(\lambda,n)$ *with* $v(\lambda,n) > 0$, $\pm n \ge 0$.

(iv). *We have*

$$\sum_{j\in\pm\mathbb{N}} \frac{1}{-a(j)u(j)u(j+1)} = \infty. \tag{2.67}$$

Recall that minimality says that for a solution $u(\lambda,n)$ with $u(\lambda,0)=1$, $u(\lambda,1)=\phi(\lambda)$ to be positive on $\mathbb{N}$, we need $\phi(\lambda)\ge\phi_+(\lambda)$. Similarly, for $u(\lambda,n)$ to be positive on $-\mathbb{N}$ we need $\phi(\lambda)\le\phi_-(\lambda)$. In summary, $u(n)>0$, $n\in\mathbb{Z}$, if and only if $\phi_+(\lambda)\le\phi(\lambda)\le\phi_-(\lambda)$ and thus any positive solution can (up to constant multiples) be written as

$$u(\lambda,n) = \frac{1-\sigma}{2}u_-(\lambda,n) + \frac{1+\sigma}{2}u_+(\lambda,n), \quad \sigma\in[-1,1]. \tag{2.68}$$

Two cases may occur

(i). $u_-(\lambda,n)$, $u_+(\lambda,n)$ are linearly dependent (i.e., $\phi_+(\lambda)=\phi_-(\lambda)$) and there is only one (up to constant multiples) positive solution. In this case $H-\lambda$ is called **critical**.

(ii). $u_-(\lambda,n)$, $u_+(\lambda,n)$ are linearly independent and

$$u_\sigma(\lambda,n) = \frac{1+\sigma}{2}u_+(\lambda,n) + \frac{1-\sigma}{2}u_-(\lambda,n), \tag{2.69}$$

is positive if and only if $\sigma\in[-1,1]$. In this case $H-\lambda$ is called **subcritical** .

If $H-\lambda>\sigma(H)$, then $H-\lambda$ is always subcritical by Lemma 2.6. To emphasize this situation one sometimes calls $H-\lambda$ **supercritical** if $H-\lambda>\sigma(H)$.

In case (ii) it is not hard to show using (2.62) that for two positive solutions $u_j(\lambda,n)$, $j=1,2$, we have

$$u_\sigma(\lambda,n) = \frac{1+\sigma}{2}u_1(\lambda,n) + \frac{1-\sigma}{2}u_2(\lambda,n) > 0 \quad\Leftrightarrow\quad \sigma\in[-1,1], \tag{2.70}$$

if and only if the solutions $u_{1,2}$ equal $u_\pm$ up to constant multiples.

Remark 2.10. Assuming $a(n)<0$, the requirement $H-\lambda\ge 0$ is also necessary for a positive solution to exist. In fact, any positive solution can be used to factor $H-\lambda = A^*A\ge 0$ (cf. Corollary 11.2).

Similarly, if $a(n)>0$, the requirement $H-\lambda\le 0$ is sufficient and necessary for a positive solution to exist (consider $-(H-\lambda)\ge 0$). If $a(n)$ is not of a fixed sign, no general statement is possible.

2.4. Weyl circles

In this section we will advocate a different approach for Weyl m-functions. There are two main reasons for doing this. First of all this approach is similar to Weyl's original one for differential equations and second it will provide an alternative characterization of Weyl m-functions as limits needed later.

Let $s_\beta(z,.), c_\beta(z,.)$ be the fundamental system of (1.19) corresponding to the initial conditions

$$\begin{aligned} s_\beta(z,0) &= -\sin(\alpha), & s_\beta(z,1) &= \cos(\alpha), \\ c_\beta(z,0) &= \cos(\alpha), & c_\beta(z,1) &= \sin(\alpha), \end{aligned} \tag{2.71}$$

where $\beta = \cot(\alpha)$. Clearly,

$$W(c_\beta(z), s_\beta(z)) = a(0). \tag{2.72}$$

The general idea is to approximate $H_\pm^\beta$ by finite matrices. We will choose the boundary conditions associated with β, β_N at $n = 0$, N, respectively. The corresponding matrix $H_{0,N}^{\beta,\beta_N}$ will have eigenvalues $\lambda_j(N)$, $1 \le j \le \tilde{N}$, and corresponding eigenvectors $s_\beta(\lambda_j(N), n)$ (since $s_\beta(z,n)$ fulfills the boundary condition at 0). We note that $\lambda_j(N)$, $1 \le j \le \tilde{N}$, depend also on β.

If we set

$$\tilde{m}_N^\beta(z) = \mathrm{sgn}(N) \frac{W_N(s_\beta(\lambda_j(N)), c_\beta(z))}{a(0) W_N(s_\beta(\lambda_j(N)), s_\beta(z))}, \qquad N \in \mathbb{Z}\backslash\{0\} \tag{2.73}$$

(independent of the eigenvalue chosen), then the solution

$$u_N(z,n) = a(0)^{-1} c_\beta(z,n) - \mathrm{sgn}(N) \tilde{m}_N^\beta(z) s_\beta(z,n) \tag{2.74}$$

satisfies the boundary condition at N, that is, $W_N(s_\beta(\lambda_1), u_N(z)) = 0$. The function $\tilde{m}_N^\beta(z)$ is rational (w.r.t. z) and has poles at the eigenvalues $\lambda_j(N)$. In particular, they are the analogs of the Weyl $\tilde{m}$-functions for finite Jacobi operators. Hence it suggests itself to consider the limit $N \to \pm\infty$, where our hope is to obtain the Weyl $\tilde{m}$-functions for the Jacobi operators $H_\pm^\beta$.

We fix $\lambda_0 \in \mathbb{R}$ and set

$$\beta_N = -\frac{s_\beta(\lambda_0, N+1)}{s_\beta(\lambda_0, N)} \tag{2.75}$$

implying $\lambda_0 = \lambda_j(N)$ for one j. It will turn out that the above choice for β_N is not really necessary since $\tilde{m}_N^\beta(z)$ will, as a consequence of boundedness of H, converge for arbitrary sequences β_N. However, the above choice also works in the case of unbounded operators.

Before we turn to the limit, let us derive some additional properties for finite N. The limits

$$\begin{aligned} \lim_{z\to\lambda_j(N)} W_N(s_\beta(\lambda_j(N)), c_\beta(z)) &= -a(0), \\ \lim_{z\to\lambda_j(N)} \frac{W_N(s_\beta(\lambda_j(N)), s_\beta(z))}{z - \lambda_j(N)} &= W_N(s_\beta(\lambda_j(N)), s'_\beta(\lambda_j(N))) \end{aligned} \tag{2.76}$$

imply that all poles of $m_N(z,\beta)$ are simple. Using (2.29) to evaluate (2.76) one infers that the negative residue at $\lambda_j(N)$ is given by

$$\gamma_N^\beta(\lambda_j(N)) = \Big(\sum_{n=\substack{1\\N+1}}^{\substack{N\\0}} s_\beta(\lambda_j(N),n)^2\Big)^{-1}, \quad N \gtrless 0. \tag{2.77}$$

The numbers $\gamma_N^\beta(\lambda_j(N))$ are called norming constants. Hence one gets

$$\tilde{m}_N^\beta(z) = -\sum_{j=1}^{\tilde{N}} \frac{\gamma_N^\beta(\lambda_j(N))}{z-\lambda_j(N)} + \begin{cases} \frac{\beta^{\mp 1}}{a(0)}, & \beta^{\mp 1} \neq \infty \\ \frac{z-b(\substack{1\\0})}{a(0)^2}, & \beta^{\mp 1} = \infty \end{cases}, \quad N \gtrless 0, \tag{2.78}$$

and with the help of (2.24) we obtain

$$\sum_{n=\substack{1\\N+1}}^{\substack{N\\0}} |u_N(z,n)|^2 = \frac{\mathrm{Im}(\tilde{m}_N^\beta(z))}{\mathrm{Im}(z)}, \quad N \gtrless 0, \tag{2.79}$$

that is, $m_N^\beta(z)$ are Herglotz functions.

Now we turn to the limits $N \to \pm\infty$. Fix $z \in \mathbb{C}\backslash\mathbb{R}$. Observe that if λ_1 varies in $\mathbb{R}$, then β_N takes all values in $\mathbb{R}\cup\{\infty\}$ $\tilde{N}$ times. Rewriting (2.73) shows that

$$\tilde{m}_N^\beta(z) = \frac{\mathrm{sgn}(N)}{a(0)} \frac{c_\beta(z,N)\beta_N + c_\beta(z,N+1)}{s_\beta(z,N)\beta_N + s_\beta(z,N+1)} \tag{2.80}$$

is a Möbius transformation and hence the values of $\tilde{m}_N^\beta(z)$ for different $\beta_N \in \mathbb{R}\cup\{\infty\}$ lie on a circle (also called Weyl circle) in the complex plane (note that $z \in \mathbb{R}$ would correspond to the degenerate circle $\mathbb{R}\cup\{\infty\}$). The center of this circle is

$$c_N = \mathrm{sgn}(N) \frac{W_N(c_\beta(z), \overline{s_\beta(z)})}{2a(0)\mathrm{Im}(z)[s_\beta(z)]_N} \tag{2.81}$$

and the radius is

$$r_N = \left|\frac{W(c_\beta(z), s_\beta(z))}{2a(0)\mathrm{Im}(z)[s_\beta(z)]_N}\right| = \frac{1}{2|\mathrm{Im}(z)[s_\beta(z)]_N|}. \tag{2.82}$$

Using

$$[a(0)^{-1}c_\beta(z) - \mathrm{sgn}(N)\tilde{m}s_\beta(z)]_N = [s_\beta(z)]_N\big(|\tilde{m}-c_N|^2 - r_N^2\big) \tag{2.83}$$

we see that this circle is equivalently characterized by the equation

$$\{\tilde{m} \in \mathbb{C} | [a(0)^{-1}c_\beta(z) + \mathrm{sgn}(N)\tilde{m}s_\beta(z)]_N = 0\}. \tag{2.84}$$

Since $[.]_N$, $N > 0$, is decreasing with respect to N, the circle corresponding to $N+1$ lies inside the circle corresponding to N. Hence these circles tend to a limit point for any sequence $(\beta_N \in \mathbb{R}\cup\{\infty\})_{N\in\mathbb{N}}$ since

$$\lim_{N\to\infty} -[s_\beta(z)]_N = \sum_{n=0}^{\infty} |s_\beta(z,n)|^2 = \infty \tag{2.85}$$

(otherwise H_+^β would have a non-real eigenvalue). Similarly for $N < 0$. Thus the pointwise convergence of $\tilde{m}_N^\beta(z)$ is clear and we may define

$$\tilde{m}_\pm^\beta(z) = \lim_{N\to\pm\infty} \tilde{m}_N^\beta(z). \tag{2.86}$$

Moreover, the above sequences are locally bounded in z (fix N and take all circles corresponding to a (sufficiently small) neighborhood of any point z and note that all following circles lie inside the ones corresponding to N) and by Vitali's theorem ([**229**], p. 168) they converge uniformly on every compact set in $\mathbb{C}_\pm = \{z \in \mathbb{C} | \pm \mathrm{Im}(z) > 0\}$, implying that $\tilde{m}_\pm^\beta(z)$ are again holomorphic on $\mathbb{C}_\pm$.

Remark 2.11. (i). Since $\tilde{m}_N^\beta(z)$ converges for arbitrary choice of the sequence β_N we even have

$$\tilde{m}_\pm^\beta(z) = \lim_{N\to\pm\infty} \frac{c_\beta(z,N)}{a(0)s_\beta(z,N)}. \tag{2.87}$$

Moreover, this approach is related to (2.60). Using (1.62), (1.63) shows $\phi_m(\lambda) = -c(\lambda,m)/s(\lambda,m)$ and establishes the equivalence.
(ii). That the Weyl circles converge to a point is a consequence of the boundedness of $a(n), b(n)$. In the general case the limit could be a circle or a point (independent of $z \in \mathbb{C}\backslash\mathbb{R}$). Accordingly one says that τ is limit circle or limit point at $\pm\infty$. (See Section 2.6 for further information on unbounded operators.)

As anticipated by our notation, $\tilde{m}_\pm^\beta(z)$ are closely related to $m_\pm^\beta(z)$. This will be shown next. We claim that

$$u_\pm(z,n) = a(0)^{-1} c_\beta(z,n) \mp \tilde{m}_\pm^\beta(z) s_\beta(z,n) \tag{2.88}$$

is square summable near $\pm\infty$. Since $\tilde{m}_+^\beta$ lies in the interior of all Weyl circles the limit $\lim_{N\to\infty}[u_+(z)]_N \geq 0$ must exist and hence $u_+ \in \ell_+^2(\mathbb{Z})$ by (2.24). Moreover, $u_+ \in \ell_+^2(\mathbb{Z})$ implies $[u_+]_\infty = 0$. Similarly for $u_-(z)$. In addition, (cf. (2.4))

$$\sum_{n=\substack{1\\ -\infty}}^{\substack{\infty\\ 0}} |u_\pm(z,n)|^2 = \frac{\mathrm{Im}(\tilde{m}_\pm^\beta(z))}{\mathrm{Im}(z)}, \tag{2.89}$$

implies that $\tilde{m}_\pm^\beta(z)$ are Herglotz functions (note that $u_\pm(z,n)$ depends on β because of the normalization $u_\pm(z,0) = a(0)^{-1}\cos(\alpha) \pm \tilde{m}_\pm^\beta(z)\sin(\alpha)$). In particular, their Herglotz representation reads

$$\tilde{m}_\pm^\beta(z) = \frac{\beta^{\mp 1}}{a(0)} + \int_{\mathbb{R}} \frac{d\tilde{\rho}_\pm^\beta(\lambda)}{\lambda - z}, \qquad \beta \neq \begin{matrix} 0 \\ \infty \end{matrix}. \tag{2.90}$$

This finally establishes the connection

$$\tilde{m}_\pm^\infty(z) = \tilde{m}_\pm(z) = \frac{\mp u_\pm(z,1)}{a(0)u_\pm(z,0)} \tag{2.91}$$

as expected. Furthermore, $\tilde{m}_\pm^{\beta_1}(z)$ can be expressed in terms of $\tilde{m}_\pm^{\beta_2}(z)$ (use that $u_\pm$ is unique up to a constant) by

$$\tilde{m}_\pm^{\beta_1}(z) = \pm\frac{1}{a(0)} \frac{a(0)\cos(\alpha_2-\alpha_1)\tilde{m}_\pm^{\beta_2}(z) \mp \sin(\alpha_2-\alpha_1)}{a(0)\sin(\alpha_2-\alpha_1)\tilde{m}_\pm^{\beta_2}(z) \pm \cos(\alpha_2-\alpha_1)}, \tag{2.92}$$

where $\beta_{1,2} = \cot(\alpha_{1,2})$. Specializing to the case $\beta_1 = \beta$, $\beta_2 = \infty$ we infer

$$\tilde{m}_+^{\beta}(z,n) = \frac{\beta m_+(z) + a(0)^{-1}}{\beta - a(0) m_+(z)}, \quad \tilde{m}_-^{\beta}(z,n) = \frac{m_-(z,1) + a(0)^{-1}\beta}{1 - \beta a(0) m_-(z,1)} \tag{2.93}$$

which should be compared with (2.16), (2.17), respectively.

2.5. Canonical forms of Jacobi operators and the moment problem

The aim of this section is to derive canonical forms for H, $H_\pm$ and to relate the spectra of these operators to the corresponding measures encountered in the previous sections.

Since $s(z,n)$ is a polynomial in z we infer by induction (cf. Lemma 1.2)

$$s(H_+,n)\delta_1 = \sum_{j=0}^{n} s_{j,n}(0) H_+^j \delta_1 = \delta_n, \tag{2.94}$$

implying that δ_1 is a cyclic vector for H_+. We recall the measure

$$d\rho_+(\lambda) = d\langle \delta_1, P_{(-\infty,\lambda]}(H_+)\delta_1\rangle \tag{2.95}$$

and consider the Hilbert space $L^2(\mathbb{R}, d\rho_+)$. Since $d\rho_+$ is supported on $\sigma(H_+)$ this space is the same as the space $L^2(\sigma(H_+), d\rho_+)$. The scalar product is given by

$$\langle f, g\rangle_{L^2} = \int_{\mathbb{R}} \overline{f(\lambda)} g(\lambda)\, d\rho_+(\lambda). \tag{2.96}$$

If f, g are polynomials we can evaluate their scalar product without even knowing $d\rho_+(\lambda)$ since

$$\langle f, g\rangle_{L^2} = \langle f(H_+)\delta_1, g(H_+)\delta_1\rangle. \tag{2.97}$$

Applying this relation in the special case $f(\lambda) = s(\lambda, m)$, $g(\lambda) = s(\lambda,n)$, we obtain from equation (2.94) that the polynomials $s(z,n)$, $n \in \mathbb{N}$, are orthogonal with respect to this scalar product, that is,

$$\langle s(\lambda,m), s(\lambda,n)\rangle_{L^2} = \int_{\mathbb{R}} s(\lambda,m) s(\lambda,n)\, d\rho_+(\lambda) = \delta_{m,n}. \tag{2.98}$$

We will see in Theorem 4.5 that $s(\lambda,n)$ has $n-1$ distinct real roots which interlace the roots of $s(\lambda, n+1)$.

Now consider the following transformation U from the set $\ell_0(\mathbb{N})$ onto the set of all polynomials (**eigenfunction expansion**)

$$\begin{aligned} (Uf)(\lambda) &= \sum_{n=1}^{\infty} f(n) s(\lambda,n), \\ (U^{-1}F)(n) &= \int_{\mathbb{R}} s(\lambda,n) F(\lambda) d\rho_+(\lambda). \end{aligned} \tag{2.99}$$

A simple calculation for $F(\lambda) = (Uf)(\lambda)$ shows that U is unitary,

$$\sum_{n=1}^{\infty} |f(n)|^2 = \int_{\mathbb{R}} |F(\lambda)|^2 d\rho_+(\lambda). \tag{2.100}$$

This leads us to the following result.

Theorem 2.12. *The unitary transformation*

$$\begin{array}{rccl} \tilde{U}: & \ell^2(\mathbb{N}) & \to & L^2(\mathbb{R}, d\rho_+) \\ & f(n) & \mapsto & \sum_{n=1}^{\infty} f(n) s(\lambda, n) \end{array} \tag{2.101}$$

(where the sum is to be understood as norm limit) maps the operator H_+ to the multiplication operator by λ. More explicitly,

$$H_+ = \tilde{U}^{-1} \tilde{H} \tilde{U}, \tag{2.102}$$

where

$$\begin{array}{rccl} \tilde{H}: & L^2(\mathbb{R}, d\rho_+) & \to & L^2(\mathbb{R}, d\rho_+) \\ & F(\lambda) & \mapsto & \lambda F(\lambda) \end{array}. \tag{2.103}$$

Proof. Since $d\rho_+$ is compactly supported the set of all polynomials is dense in $L^2(\mathbb{R}, d\rho_+)$ (Lemma B.1) and U extends to the unitary transformation $\tilde{U}$. The rest follows from

$$\begin{aligned} \tilde{H}F(\lambda) &= \tilde{U} H_+ \tilde{U}^{-1} F(\lambda) = \tilde{U} H_+ \int_{\mathbb{R}} s(\lambda, n) F(\lambda) d\rho_+(\lambda) \\ &= \tilde{U} \int_{\mathbb{R}} \lambda s(\lambda, n) F(\lambda) d\rho_+(\lambda) = \lambda F(\lambda). \end{aligned} \tag{2.104}$$

□

This implies that the spectrum of H_+ can be characterized as follows (see Lemma B.5). Let the Lebesgue decomposition of $d\rho_+$ be given by

$$d\rho_+ = d\rho_{+,pp} + d\rho_{+,ac} + d\rho_{+,sc}, \tag{2.105}$$

where *pp*, *ac*, and *sc* refer to the pure point, absolutely continuous, and singularly continuous part of the measure ρ_+ (with respect to Lebesgue measure), respectively.

Then the **pure point**, **absolutely continuous**, and **singular continuous spectra** of H_+ are given by (see Lemma B.5)

$$\begin{aligned} \sigma(H_+) &= \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho_+\}, \\ \sigma_{pp}(H_+) &= \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho_{+,pp}\}, \\ \sigma_{ac}(H_+) &= \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho_{+,ac}\}, \\ \sigma_{sc}(H_+) &= \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho_{+,sc}\}. \end{aligned} \tag{2.106}$$

Recall that $\sigma_{pp}(H_+)$ is in general not equal to the **point spectrum** $\sigma_p(H_+)$ (i.e., the set of eigenvalues of H_+). However, we have at least

$$\sigma_{pp}(H_+) = \overline{\sigma_p(H_+)}, \tag{2.107}$$

where the bar denotes closure.

An additional decomposition in continuous and singular part with respect to the Hausdorff measure dh^α (see Appendix B) will be of importance as well,

$$d\rho_+ = d\rho_{+,\alpha c} + d\rho_{+,\alpha s}. \tag{2.108}$$

The corresponding spectra are defined analogously

$$\begin{aligned} \sigma_{\alpha c}(H_+) &= \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho_{+,\alpha c}\}, \\ \sigma_{\alpha s}(H_+) &= \{\lambda \in \mathbb{R} | \lambda \text{ is a growth point of } \rho_{+,\alpha s}\}. \end{aligned}$$

They will be used in Section 3.3.

Finally, we show how a^2, b can be reconstructed from the measure ρ_+. In fact, even 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

$$C(k) = \det \begin{pmatrix} m_0 & m_1 & \cdots & m_{k-1} \\ m_1 & m_2 & \cdots & m_k \\ \vdots & \vdots & \ddots & \vdots \\ m_{k-1} & m_k & \cdots & m_{2k-2} \end{pmatrix} > 0, \quad k \in \mathbb{N}. \tag{2.109}$$

Without restriction we will assume $m_0 = 1$. Using this we can define a sesquilinear form on the set of polynomials as follows

$$\langle P(\lambda), Q(\lambda) \rangle_{L^2} = \sum_{j,k=0}^{\infty} m_{j+k} \overline{p_j} q_k, \tag{2.110}$$

where $P(z) = \sum_{j=0}^{\infty} p_j z^j$, $Q(z) = \sum_{j=0}^{\infty} q_j z^j$ (note that all sums are finite). The polynomials

$$s(z,k) = \frac{1}{\sqrt{C(k-1)C(k)}} \det \begin{pmatrix} m_0 & m_1 & \cdots & m_{k-1} \\ m_1 & m_2 & \cdots & m_k \\ \vdots & \vdots & \ddots & \vdots \\ m_{k-2} & m_{k-1} & \cdots & m_{2k-3} \\ 1 & z & \cdots & z^{k-1} \end{pmatrix}, \ k \in \mathbb{N} \tag{2.111}$$

(set $C(0) = 1$), form a basis for the set of polynomials which is immediate from

$$s(z,k) = \sqrt{\frac{C(k-1)}{C(k)}} \left(z^{k-1} + \frac{D(k-1)}{C(k-1)} z^{k-2} + O(z^{k-3}) \right), \tag{2.112}$$

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

$$D(k) = \det \begin{pmatrix} m_0 & m_1 & \cdots & m_{k-2} & m_k \\ m_1 & m_2 & \cdots & m_{k-1} & m_{k+1} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ m_{k-1} & m_k & \cdots & m_{2k-3} & m_{2k-1} \end{pmatrix}, \ k \in \mathbb{N}. \tag{2.113}$$

Moreover, this basis is orthonormal, that is,

$$\langle s(\lambda, j), s(\lambda, k) \rangle_{L^2} = \delta_{j,k}, \tag{2.114}$$

since

$$\begin{aligned} \langle s(\lambda,k), \lambda^j \rangle &= \frac{1}{\sqrt{C(k-1)C(k)}} \det \begin{pmatrix} m_0 & m_1 & \cdots & m_{k-1} \\ m_1 & m_2 & \cdots & m_k \\ \vdots & \vdots & \ddots & \vdots \\ m_{k-2} & m_{k-1} & \cdots & m_{2k-3} \\ m_j & m_{j+1} & \cdots & m_{j+k-1} \end{pmatrix} \\ &= \begin{cases} 0, & 0 \le j \le k-2 \\ \sqrt{\frac{C(k)}{C(k-1)}}, & j = k-1 \end{cases}. \end{aligned} \tag{2.115}$$

In particular, the sesquilinear form (2.110) is positive definite and hence an inner product (note that $C(k) > 0$ is also necessary for this).

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

$$\begin{aligned} zs(z,k) &= \sum_{j=0}^{k+1} \langle s(\lambda,j), \lambda s(\lambda,k)\rangle_{L^2} s(z,j) \\ &= a(k)s(z,k+1) + b(k)s(z,k) + a(k-1)s(z,k-1) \end{aligned} \tag{2.116}$$

(set $s(z,0)=0$) with

$$a(k) = \langle s(\lambda,k+1), \lambda s(\lambda,k)\rangle_{L^2}, \quad b(k) = \langle s(\lambda,k), \lambda s(\lambda,k)\rangle_{L^2}, \quad k \in \mathbb{N}. \tag{2.117}$$

In addition, comparing powers of z in (2.116) shows

$$a(k) = \frac{\sqrt{C(k-1)C(k+1)}}{C(k)}, \quad b(k) = \frac{D(k)}{C(k)} - \frac{D(k-1)}{C(k-1)}. \tag{2.118}$$

In terms of our original setting 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 λ^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 $s(\lambda,n)$). Summarizing, $d\rho_+$ uniquely determines $a(n)^2$ and $b(n)$. Since knowing $d\rho_+(\lambda)$ is equivalent to knowing $m_+(z)$, the same is true for $m_+(z)$ (compare also the proof of Theorem 2.29). In fact, we have an even stronger result.

Theorem 2.13. *Suppose that the bounded measure $d\rho_+$ is* not *supported on a finite set. Then there exists a unique bounded Jacobi operator H_+ having $d\rho_+$ as spectral measure.*

Proof. We have already seen that the necessary and sufficient condition for our reconstruction procedure to work is that the sesquilinear form generated by the moments m_j of $d\rho_+$ is positive definite. Pick any nonzero polynomial $P(\lambda)$. Due to our assumption we can find $\varepsilon > 0$ and an interval I such that $\rho_+(I) \neq 0$ and $P(\lambda)^2 \geq \varepsilon$, $\lambda \in I$. Hence $\langle P(\lambda), P(\lambda)\rangle \geq \varepsilon\rho_+(I)$.

As a consequence we can define $a(n)$, $b(n)$, $s(\lambda,n)$, and the unitary transform $\tilde{U}$ as before. By construction $H_+ = \tilde{U}^{-1}\tilde{H}\tilde{U}$ is a bounded Jacobi operator associated with $a(n)$, $b(n)$. That ρ_+ is the spectral measure of H_+ follows from (using $(\tilde{U}\delta_1)(\lambda) = 1$)

$$\langle \delta_1, P_\Lambda(H_+)\delta_1\rangle = \langle \tilde{U}\delta_1, P_\Lambda(\tilde{H})\tilde{U}\delta_1\rangle = \int_{\mathbb{R}} \chi_\Lambda(\lambda) d\rho_+(\lambda) \tag{2.119}$$

for any Borel set $\Lambda \subseteq \mathbb{R}$. □

If $d\rho_+$ is supported on N points, the reconstruction procedure will break down after N steps (i.e., $C(N+1)=0$) and we get a finite Jacobi matrix with $d\rho_+$ as spectral measure.

We also remark

$$c(z,n) = -a(0)\int_{\mathbb{R}} \frac{s(z,n) - s(\lambda,n)}{z-\lambda}\, d\rho_+(\lambda), \quad n \in \mathbb{N}, \tag{2.120}$$

since one easily verifies $\tau_+ c(z,n) = zc(z,n) - a(0)\delta_0(n)$, $n \in \mathbb{N}$ (use (2.98) with $m = 1$). Moreover, this implies

$$u_+(z,n) = \frac{c(z,n)}{a(0)} - m_+(z)s(z,n) = \int_{\mathbb{R}} \frac{s(\lambda,n)}{z-\lambda}\, d\rho_+(\lambda) \tag{2.121}$$

and it is not hard to verify

$$G_+(z,n,m) = \int_{\mathbb{R}} \frac{s(\lambda,n)s(\lambda,m)}{\lambda - z} d\rho_+(\lambda). \tag{2.122}$$

The Jacobi operator H can be treated along the same lines. Since we essentially repeat the analysis of H_+ we will be more sketchy.

Consider the vector valued polynomials

$$\underline{S}(z,n) = \Big(c(z,n), s(z,n)\Big). \tag{2.123}$$

The analog of (2.94) reads

$$s(H,n)\delta_1 + c(H,n)\delta_0 = \delta_n. \tag{2.124}$$

This is obvious for $n = 0,1$ and the rest follows from induction upon applying H to (2.124). We introduce the spectral measures

$$d\rho_{i,j}(.) = d\langle \delta_i, P_{(-\infty,\lambda]}(H)\delta_j\rangle, \tag{2.125}$$

and the (hermitian) matrix valued measure

$$d\rho = \left(\begin{array}{cc} d\rho_{0,0} & d\rho_{0,1} \\ d\rho_{1,0} & d\rho_{1,1} \end{array} \right). \tag{2.126}$$

The diagonal part consists of positive measures and the off-diagonal part can be written as the difference of two positive measures

$$d\rho_{0,1}(\lambda) = d\rho_{1,0}(\lambda) = d\rho_{0,1,+}(\lambda) - d\rho_{0,1,-}(\lambda), \tag{2.127}$$

where

$$\begin{aligned} d\rho_{0,1,+}(\lambda) &= \frac{1}{2} d\langle(\delta_0 + \delta_1), P_{(-\infty,\lambda]}(H)(\delta_0 + \delta_1)\rangle, \\ d\rho_{0,1,-}(\lambda) &= \frac{1}{2}(d\langle\delta_0, P_{(-\infty,\lambda]}(H)\delta_0\rangle + d\langle\delta_1, P_{(-\infty,\lambda]}(H)\delta_1\rangle). \end{aligned} \tag{2.128}$$

Moreover, $d\rho$ is a positive matrix measure and we have a corresponding Hilbert space $L^2(\mathbb{R}, \mathbb{C}^2, d\rho)$ with scalar product given by

$$\langle \underline{F}, \underline{G}\rangle_{L^2} = \sum_{i,j=0}^{1} \int_{\mathbb{R}} \overline{F_i(\lambda)} G_j(\lambda) d\rho_{i,j}(\lambda) \equiv \int_{\mathbb{R}} \overline{\underline{F}(\lambda)} \underline{G}(\lambda) d\rho(\lambda) \tag{2.129}$$

and if $\underline{F}, \underline{G}$ are vector valued polynomials, then

$$\langle \underline{F}, \underline{G}\rangle_{L^2} = \langle F_0(H)\delta_0 + F_1(H)\delta_1, G_0(H)\delta_0 + G_1(H)\delta_1\rangle. \tag{2.130}$$

By (2.124) the vector valued polynomials $\underline{S}(\lambda,n)$ are orthogonal with respect to $d\rho$,

$$\langle \underline{S}(.,m), \underline{S}(.,n)\rangle_{L^2} = \delta_{m,n}. \tag{2.131}$$

The formulas analogous to (2.117) then read

$$a(n) = \langle \underline{S}(\lambda,n+1), \lambda\underline{S}(\lambda,n)\rangle_{L^2}, \quad b(n) = \langle \underline{S}(\lambda,n), \lambda\underline{S}(\lambda,n)\rangle_{L^2}, \quad n \in \mathbb{Z}. \tag{2.132}$$

Next, we consider the following transformation U from the set $\ell_0(\mathbb{Z})$ onto the set of vector-valued polynomials (**eigenfunction expansion**)

$$\begin{aligned} (Uf)(\lambda) &= \sum_{n\in\mathbb{Z}} f(n)\underline{S}(\lambda,n), \\ (U^{-1}\underline{F})(n) &= \int_{\mathbb{R}} \underline{S}(\lambda,n)\underline{F}(\lambda)d\rho(\lambda). \end{aligned} \tag{2.133}$$

Again a simple calculation for $\underline{F}(\lambda) = (Uf)(\lambda)$ shows that U is unitary,

$$\sum_{n\in\mathbb{Z}} |f(n)|^2 = \int_{\mathbb{R}} \overline{\underline{F}(\lambda)}\underline{F}(\lambda)d\rho(\lambda). \tag{2.134}$$

Extending U to a unitary transformation $\tilde{U}$ we obtain as in the case of H_+ the following

Theorem 2.14. *The unitary transformation*

$$\begin{array}{rccl} \tilde{U}: & \ell^2(\mathbb{Z}) & \to & L^2(\mathbb{R},\mathbb{C}^2,d\rho) \\ & f(n) & \mapsto & \sum_{n=-\infty}^{\infty} f(n)\underline{S}(\lambda,n) \end{array} \tag{2.135}$$

(where the sum is to be understood as norm limit) maps the operator H to the multiplication operator by λ, that is,

$$\tilde{H} = \tilde{U}H\tilde{U}^{-1}, \tag{2.136}$$

where

$$\begin{array}{rccl} \tilde{H}: & L^2(\mathbb{R},\mathbb{C}^2,d\rho) & \to & L^2(\mathbb{R},\mathbb{C}^2,d\rho) \\ & \underline{F}(\lambda) & \mapsto & \lambda\underline{F}(\lambda) \end{array}. \tag{2.137}$$

For the Green function of H we obtain

$$G(z,n,m) = \int_{\mathbb{R}} \frac{\underline{S}(\lambda,n)\underline{S}(\lambda,m)}{\lambda - z} d\rho(\lambda). \tag{2.138}$$

By Lemma B.13, in order to characterize the spectrum of H one only needs to consider the trace $d\rho^{tr}$ of $d\rho$ given by

$$d\rho^{tr} = d\rho_{0,0} + d\rho_{1,1}. \tag{2.139}$$

Let the Lebesgue decomposition (cf. (2.105)) of $d\rho^{tr}$ be given by

$$d\rho^{tr} = d\rho^{tr}_{pp} + d\rho^{tr}_{ac} + d\rho^{tr}_{sc}, \tag{2.140}$$

then the **pure point**, **absolutely continuous**, and **singular continuous spectra** of H are given by

$$\begin{aligned} \sigma(H) &= \{\lambda\in\mathbb{R} | \lambda \text{ is a growth point of } \rho^{tr}\}, \\ \sigma_{pp}(H) &= \{\lambda\in\mathbb{R} | \lambda \text{ is a growth point of } \rho^{tr}_{pp}\}, \\ \sigma_{ac}(H) &= \{\lambda\in\mathbb{R} | \lambda \text{ is a growth point of } \rho^{tr}_{ac}\}, \\ \sigma_{sc}(H) &= \{\lambda\in\mathbb{R} | \lambda \text{ is a growth point of } \rho^{tr}_{sc}\}. \end{aligned} \tag{2.141}$$

The **Weyl matrix** $M(z)$ is defined as

$$M(z) = \int_{-\infty}^{\infty} \frac{d\rho(\lambda)}{\lambda - z} - \frac{1}{2a(0)} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$(2.142) \qquad = \begin{pmatrix} g(z,0) & \frac{h(z,0)}{2a(0)} \\ \frac{h(z,0)}{2a(0)} & g(z,1) \end{pmatrix}, \qquad z \in \mathbb{C}\backslash\sigma(H).$$

Explicit evaluation yields

$$(2.143) \qquad M(z) = \frac{1}{\tilde{m}_+(z) + \tilde{m}_-(z)} \begin{pmatrix} -\frac{1}{a(0)^2} & \frac{\tilde{m}_+(z) - \tilde{m}_-(z)}{2a(0)} \\ \frac{\tilde{m}_+(z) - \tilde{m}_-(z)}{2a(0)} & \tilde{m}_+(z)\tilde{m}_-(z) \end{pmatrix},$$

and the determinant reads

$$(2.144) \qquad \det M(z) = -\frac{1}{4a(0)^2}.$$

In terms of the original Weyl m-functions we obtain

$$g(z,0) = \frac{-1}{z - b(0) - a(0)^2 m_+(z) - a(-1)^2 m_-(z)},$$

$$(2.145) \qquad h(z,0) = \big(z - b(0) + a(0)^2 m_+(z) - a(-1)^2 m_-(z)\big) g(z,0).$$

Finally, notice that we can replace $c(z,n)$, $s(z,n)$ by any other pair of linearly independent solutions. For example, we could use $c_\beta(z,n)$, $s_\beta(z,n)$. As in (2.123) we define

$$(2.146) \qquad \underline{S}_\beta(z,n) = \big(c_\beta(z,n), s_\beta(z,n)\big) = U_\alpha \underline{S}(z,n),$$

where U_α is rotation by the angle α ($\beta = \cot\alpha$), that is,

$$(2.147) \qquad U_\alpha = \begin{pmatrix} \cos\alpha & \sin\alpha \\ -\sin\alpha & \cos\alpha \end{pmatrix}.$$

Hence all objects need to be rotated by the angle α. For instance, introducing $M^\beta(z) = U_\alpha M(z) U_\alpha^{-1}$ we infer

$$(2.148) \qquad M^\beta(z) = \frac{1}{\tilde{m}_+^\beta(z) + \tilde{m}_-^\beta(z)} \begin{pmatrix} -\frac{1}{a(0)^2} & \frac{\tilde{m}_+^\beta(z) - \tilde{m}_-^\beta(z)}{2a(0)} \\ \frac{\tilde{m}_+^\beta(z) - \tilde{m}_-^\beta(z)}{2a(0)} & \tilde{m}_+^\beta(z)\tilde{m}_-^\beta(z) \end{pmatrix}.$$

Note also

$$(2.149) \qquad \frac{-1}{a(0)^2(\tilde{m}_+^\beta(z) + \tilde{m}_-^\beta(z))} = \sin^2(\alpha)\, \gamma^\beta(z,0).$$

If we restrict ourselves to the absolutely continuous part of the spectrum, we can do even more. We abbreviate $\tilde{m}_\pm(\lambda) = \lim_{\varepsilon\downarrow 0} \tilde{m}_\pm(\lambda + \mathrm{i}\varepsilon)$, $\lambda \in \mathbb{R}$, implying (cf. Appendix B)

$$d\rho_{0,0,ac}(\lambda) = \frac{\mathrm{Im}(\tilde{m}_+(\lambda) + \tilde{m}_-(\lambda))}{\pi a(0)^2 |\tilde{m}_+(\lambda) + \tilde{m}_-(\lambda)|^2} d\lambda,$$

$$d\rho_{0,1,ac}(\lambda) = \frac{\mathrm{Im}(\tilde{m}_+(\lambda))\mathrm{Re}(\tilde{m}_-(\lambda)) - \mathrm{Re}(\tilde{m}_+(\lambda))\mathrm{Im}(\tilde{m}_-(\lambda))}{\pi a(0) |\tilde{m}_+(\lambda) + \tilde{m}_-(\lambda)|^2} d\lambda,$$

$$(2.150) \qquad d\rho_{1,1,ac}(\lambda) = \frac{\mathrm{Im}(|\tilde{m}_-(\lambda)|^2 \tilde{m}_+(\lambda) + |\tilde{m}_-(\lambda)|^2 \tilde{m}_+(\lambda))}{\pi |\tilde{m}_+(\lambda) + \tilde{m}_-(\lambda)|^2} d\lambda.$$

Choosing the new basis

$$\begin{pmatrix} u_+(\lambda, n) \\ u_-(\lambda, n) \end{pmatrix} = V(\lambda) \begin{pmatrix} c(\lambda, n) \\ s(\lambda, n) \end{pmatrix} \tag{2.151}$$

with

$$V(\lambda) = \frac{1}{\tilde{m}_+(\lambda) + \tilde{m}_-(\lambda)} \begin{pmatrix} \frac{1}{a(0)} & -\tilde{m}_+(\lambda) \\ \frac{1}{a(0)} & \tilde{m}_-(\lambda) \end{pmatrix} \tag{2.152}$$

we get

$$(V^{-1}(\lambda))^* \, d\rho_{ac}(\lambda) \, V^{-1}(\lambda) = \begin{pmatrix} \mathrm{Im}(\tilde{m}_-(\lambda)) & 0 \\ 0 & \mathrm{Im}(\tilde{m}_+(\lambda)) \end{pmatrix} d\lambda. \tag{2.153}$$

Note that $V(\lambda)$ is not unitary. We will show how to diagonalize all of $d\rho$ in Section 3.1.

2.6. Some remarks on unbounded operators

In this section we temporarily drop the boundedness assumption on the coefficients a, b. This renders H unbounded and implies that we are no longer able to define H on all of $\ell^2(\mathbb{Z})$. Nevertheless we can define the **minimal and maximal operator** allied with τ as follows

$$\begin{array}{llll} H_{min}: & \mathfrak{D}(H_{min}) & \to & \ell^2(\mathbb{Z}) \\ & f & \mapsto & \tau f \end{array}, \quad \begin{array}{llll} H_{max}: & \mathfrak{D}(H_{max}) & \to & \ell^2(\mathbb{Z}) \\ & f & \mapsto & \tau f \end{array}, \tag{2.154}$$

with

$$\mathfrak{D}(H_{min}) = \ell_0(\mathbb{Z}), \qquad \mathfrak{D}(H_{max}) = \{f \in \ell^2(\mathbb{Z}) | \tau f \in \ell^2(\mathbb{Z})\}. \tag{2.155}$$

By Green's formula (1.20) we have $H_{min}^* = H_{max}$ and

$$\begin{array}{llll} H_{max}^* = \overline{H_{min}}: & \mathfrak{D}(H_{max}^*) & \to & \ell^2(\mathbb{Z}) \\ & f & \mapsto & \tau f \end{array}, \tag{2.156}$$

with

$$\mathfrak{D}(H_{max}^*) = \{f \in \mathfrak{D}(H_{max}) | \lim_{n \to \pm\infty} W_n(\overline{f}, g) = 0, \; g \in \mathfrak{D}(H_{max})\}. \tag{2.157}$$

Here $H^*, \overline{H}$ denote the adjoint, closure of an operator H, respectively. We also remark that $\lim_{n\to\pm\infty} W_n(\overline{f}, g)$ exists for $f, g \in \mathfrak{D}(H_{max})$ as can be easily shown using (1.20). Similar definitions apply to $H_\pm$.

Since we might have $H_{max}^* \neq H_{max}$, H_{max} might not be self-adjoint in general. The key to this problem will be the **limit point** (*l.p.*), **limit circle** (*l.c.*) classification alluded to in Remark 2.11 (ii). To make things precise, we call τ *l.p.* at $\pm\infty$ if $s(z_0, .) \notin \ell^2(\pm\mathbb{N})$ for some $z_0 \in \mathbb{C}\backslash\mathbb{R}$. Otherwise τ is called *l.c.* at $\pm\infty$.

In order to draw some first consequences from this definition we note that all considerations of Section 2.4 do not use boundedness of a, b except for (2.85). However, if $\sum_{n\in\mathbb{N}} s(z_0, n) < \infty$ (considering only $\beta = \infty$ for simplicity), then the circle corresponding to $\tilde{m}_N(z_0)$ converges to a circle instead of a point as $N \to \infty$. If $\tilde{m}_\pm(z_0)$ is defined to be any point on this limiting circle, everything else remains unchanged. In particular, $u_+(z_0, .) \in \ell^2(\mathbb{N})$ and $s(z_0, .) \in \ell^2(\mathbb{N})$ shows that every solution of $\tau u = z_0 u$ is in $\ell^2(\mathbb{N})$ if τ is *l.c.* at $+\infty$.

This enables us to reveal the connections between the *l.p.* / *l.c.* characterization and the self-adjointness of unbounded Jacobi operators. We first consider $H_\pm$.

We recall that $H_{min,+}$ is symmetric and that $(H_{min,+})^* = H_{max,+}$. We need to investigate the deficiency indices $d_\pm = \dim \mathrm{Ker}(H_{max,+} - z_\pm)$, $z_\pm \in \mathbb{C}_\pm$, of $H_{min,+}$. They are independent of $z_\pm \in \mathbb{C}_\pm$ and equal (i.e., $d_- = d_+$) since $H_{min,+}$ is real (cf. [**192**], [**241**], Chapter 8). Thus, to compute $d_\pm$ it suffices to consider $\mathrm{Ker}(H_{max,+} - z_0)$. Since any element of $\mathrm{Ker}(H_{max,+} - z_0)$ is a multiple of $s(z_0)$ we infer $d_- = d_+ = 0$ if $s(z_0) \notin \ell^2(\mathbb{N})$ and $d_- = d_+ = 1$ if $s(z_0) \in \ell^2(\mathbb{N})$. This shows that $H_{max,+}$ is self-adjoint if and only if τ is *l.p.* at $+\infty$. Moreover, $s(z_0) \in \ell^2(\mathbb{N})$ implies $s(z) \in \ell^2(\mathbb{N})$ for all $z \in \mathbb{C}\backslash\mathbb{R}$ since $d_\pm = 1$ independent of $z \in \mathbb{C}\backslash\mathbb{R}$. Or, put differently, the *l.p.* / *l.c.* definition is independent of $z \in \mathbb{C}\backslash\mathbb{R}$.

If τ is *l.c.* at $\pm\infty$, then our considerations imply that all solutions of (1.19) for all $z \in \mathbb{C}\backslash\mathbb{R}$ are square summable near $\pm\infty$, respectively. This is even true for all $z \in \mathbb{C}$.

Lemma 2.15. *Suppose that all solutions of $\tau u = zu$ are square summable near $\pm\infty$ for one value $z = z_0 \in \mathbb{C}$. Then this is true for all $z \in \mathbb{C}$.*

Proof. If u fulfills (1.19), we may apply (1.48) to $(\tau - z_0)u = (z - z_0)u$,

$$\begin{aligned} u(n) &= u(n_0)c(z_0,n,n_0) + u(n_0+1)s(z_0,n,n_0) \\ &\quad - \frac{z-z_0}{a(0)} \sum_{j=n_0+1}^{n}{}^{*} \big(c(z_0,n)s(z_0,j) - c(z_0,j)s(z_0,n)\big)u(j). \end{aligned} \tag{2.158}$$

By assumption, there exists a constant $M \geq 0$ such that

$$\sum_{j=n_0+1}^{\infty} |c(z_0,j)|^2 \leq M, \qquad \sum_{j=n_0+1}^{\infty} |s(z_0,j)|^2 \leq M. \tag{2.159}$$

Invoking the Cauchy-Schwarz inequality we obtain the estimate $(n > n_0)$

$$\begin{aligned} \Big| \sum_{j=n_0+1}^{n} &\big(c(z_0,n)s(z_0,j) - c(z_0,j)s(z_0,n)\big)u(j)\Big|^2 \\ &\leq \sum_{j=n_0+1}^{n} |c(z_0,n)s(z_0,j) - c(z_0,j)s(z_0,n)|^2 \sum_{j=n_0+1}^{n} |u(j)|^2 \\ &\leq M\Big(|c(z_0,n)|^2 + |s(z_0,n)|^2\Big) \sum_{j=n_0+1}^{n} |u(j)|^2. \end{aligned} \tag{2.160}$$

Since n_0 is arbitrary we may choose n_0 in (2.159) so large, that we have $4a(0)^{-1}|z - z_0|M^2 \leq 1$. Again using Cauchy-Schwarz

$$\begin{aligned} \sum_{j=n_0+1}^{n} |u(j)|^2 &\leq (|u(n_0)|^2 + |u(n_0+1)|^2)\tilde{M} + \frac{2|z-z_0|}{a(0)} M^2 \sum_{j=n_0+1}^{n} |u(j)|^2 \\ &\leq (|u(n_0)|^2 + |u(n_0+1)|^2)\tilde{M} + \frac{1}{2} \sum_{j=n_0+1}^{n} |u(j)|^2, \end{aligned} \tag{2.161}$$

where $\tilde{M}$ is chosen such that $\sum_{j=n_0+1}^{\infty} |c(z_0,j,n_0)|^2 \le \tilde{M}$, $\sum_{j=n_0+1}^{\infty} |s(z_0,j,n_0)|^2 \le \tilde{M}$ holds. Solving for the left hand side finishes the proof,

$$\sum_{j=n_0+1}^{n} |u(j)|^2 \le 2(|u(n_0)|^2 + |u(n_0+1)|^2)\tilde{M}. \tag{2.162}$$

□

In summary, we have the following lemma.

Lemma 2.16. *The operator $H_{max,\pm}$ is self-adjoint if and only if one of the following statements holds.*

(i) *τ is l.p. at $\pm\infty$.*
(ii) *There is a solution of (1.19) for some $z \in \mathbb{C}$ (and hence for all) which is not square summable near $\pm\infty$.*
(iii) *$W_{\pm\infty}(f,g) = 0$, for all $f, g \in \mathfrak{D}(H_{max,\pm})$.*

To simplify notation, we will only consider the endpoint $+\infty$ in the following. The necessary modifications for $-\infty$ are straightforward.

Next, let us show a simple but useful criterion for τ being *l.p.* at $+\infty$. If τ is *l.c.* at $+\infty$, we can use the Wronskian

$$\frac{a(0)}{a(n)} = c(z,n)s(z,n+1) - c(z,n+1)s(z,n), \tag{2.163}$$

to get (using the Cauchy-Schwarz inequality)

$$\sum_{n\in\mathbb{N}} \frac{1}{|a(n)|} \le \frac{2}{|a(0)|}\sqrt{\sum_{n\in\mathbb{N}} |c(z,n)|^2 \sum_{n\in\mathbb{N}} |s(z,n)|^2}. \tag{2.164}$$

This shows that a sufficient condition for τ to be *l.p.* at $+\infty$ is

$$\sum_{n\in\mathbb{N}} \frac{1}{|a(n)|} = \infty. \tag{2.165}$$

The remaining question is: What happens in the *l.c.* case? Obviously we need some suitable boundary conditions. The boundary condition

$$BC_{n_0,\alpha}(f) = \cos(\alpha) f(n_0) + \sin(\alpha) f(n_0+1) = 0 \tag{2.166}$$

of Remark 1.9 makes no sense if $n_0 = \pm\infty$. However, (2.166) can be written as $W_{n_0}(v,f) = 0$, where v is any sequence satisfying $BC_{n_0,\alpha}(v) = 0$ and $|v(n_0)| + |v(n_0+1)| \ne 0$. Moreover, all different boundary conditions can be obtained by picking v such that $W_{n_0}(\overline{v},v) = 0$ and $W_{n_0}(v,f) \ne 0$ for some f. This latter characterization of the boundary condition may be generalized.

We define the set of boundary conditions for τ at $+\infty$ by

$$BC_+(\tau) = \{v \in \mathfrak{D}(H_{max,+}) |\; W_{+\infty}(\overline{v},v) = 0,\ W_{+\infty}(\overline{v},f) \ne 0 \text{ for some } f \in \mathfrak{D}(H_{max,+}) \text{ if } \tau \text{ is } l.c. \text{ at } \pm\infty\}. \tag{2.167}$$

Observe that the first requirement holds if v is real. The second is void if τ is *l.p.* (at $+\infty$). Otherwise, if τ is *l.c.*, there is at least one *real* v for which it holds (if not, (iii) of Lemma 2.16 implies that τ is *l.p.*). Two sequences $v_{1,2} \in BC_+(\tau)$ are called equivalent if $W_{+\infty}(v_1,v_2) = 0$.

Lemma 2.17. *Let $v \in BC_+(\tau)$ and set*

$$\mathfrak{D}_+(v) = \{f \in \mathfrak{D}(H_{max,+}) | W_{+\infty}(v, f) = 0\}. \tag{2.168}$$

Then

(i) $W_{+\infty}(v, f) = 0 \quad \Leftrightarrow \quad W_{+\infty}(v, \overline{f}) = 0$,
(ii) $W_{+\infty}(g, f) = 0$ *for* $f, g \in \mathfrak{D}_+(v)$.

Moreover, $W_{+\infty}(v_1, v_2) = 0$ *is equivalent to* $\mathfrak{D}_+(v_1) = \mathfrak{D}_+(v_2)$.

Proof. For all $f_1, \dots, f_4 \in \mathfrak{D}(H_{max})$ we can take the limits $n \to +\infty$ in the Plücker identity

$$W_n(f_1, f_2)W_n(f_3, f_4) + W_n(f_1, f_3)W_n(f_4, f_2) + W_n(f_1, f_4)W_n(f_2, f_3) = 0. \tag{2.169}$$

Now choose $f_1 = v$, $f_2 = \hat{f}$, $f_3 = \overline{v}$, $f_4 = f$ to conclude $W_{+\infty}(v, f) = 0$ implies $W_{+\infty}(\overline{v}, f) = 0$. Then choose $f_1 = v$, $f_2 = \hat{f}$, $f_3 = f$, $f_4 = \overline{g}$ to show (ii). The last assertion follows from (ii) upon choosing $v = v_1$, $g = v_2$. □

Combining this lemma with Green's formula (1.20) shows

Theorem 2.18. *Choose $v \in BC_+(\tau)$, then*

$$\begin{array}{rlcl} H_+ : & \mathfrak{D}_+(v) & \to & \ell^2(\mathbb{N}) \\ & f & \mapsto & \tau f \end{array} \tag{2.170}$$

is a self-adjoint extension of $H_{min,+}$.

In the *l.p.* case the boundary condition $W_{+\infty}(v, f) = 0$ is of course always fulfilled and thus $\mathfrak{D}_+(v) = \mathfrak{D}(H_{max,+})$ for any $v \in BC_+(\tau)$.

Clearly, we can also define self-adjoint operators $H_{n_0,+}$ and $H^{\beta}_{n_0,+}$ corresponding to H_+ as we did in Section 1.2 for the bounded case.

Now, that we have found self-adjoint extensions, let us come back to the Weyl m-functions. We fix $v(n) = s_\beta(\lambda, n)$, $\lambda \in \mathbb{R}$, for the boundary condition at $+\infty$. Observe that

$$\tilde{m}^{\beta}_+(z) = \frac{1}{a(0)} \lim_{n \to +\infty} \frac{W_n(s_\beta(\lambda), c_\beta(z))}{W_n(s_\beta(\lambda), s_\beta(z))} \tag{2.171}$$

lies on the limiting circle. This is clear if τ is *l.p.* at $+\infty$. Otherwise, τ *l.c.* at $+\infty$ implies $c_\beta(z)$, $s_\beta(z) \in \mathfrak{D}(H_{max,+})$ and both Wronskians converge to a limit as pointed out earlier in this section. Moreover, if $W_n(s_\beta(\lambda), s_\beta(z)) = 0$, then $s_\beta(z) \in \mathfrak{D}(H^{\beta}_+)$ and hence $z \in \sigma(H^{\beta}_+)$. In particular, $W_n(s_\beta(\lambda), s_\beta(z)) \neq 0$ for $z \in \mathbb{C}\backslash\mathbb{R}$ and we can call $\tilde{m}^{\beta}_+(z)$ the Weyl $\tilde{m}$-function of H^{β}_+.

In addition, the function

$$u_+(z, n) = \frac{c_\beta(z, n)}{a(0)} \mp \tilde{m}^{\beta}_+(z) s_\beta(z, n) \tag{2.172}$$

is in $\ell^2_+(\mathbb{Z})$ and satisfies the boundary condition

$$W_{+\infty}(s_\beta(\lambda), u_\pm(z)) = 0. \tag{2.173}$$

The boundary condition uniquely characterizes $u_+(z, n)$ up to a constant in the *l.c.* case.

We have seen that the question of self-adjointness is simple if τ is *l.p.*. One the other hand, the spectrum gets simple if τ is *l.c.*.

Lemma 2.19. *If τ is l.c. at $+\infty$, then the resolvent of H_+ is a Hilbert-Schmidt operator. In particular, this implies that H_+ has purely discrete spectrum, $\sigma(H_+) = \sigma_d(H_+)$, and*

$$\sum_{\lambda\in\sigma_d(H_+)} \frac{1}{1+\lambda^2} < \infty. \tag{2.174}$$

Proof. The result is a consequence of the following estimate

$$\sum_{(n,m)\in\mathbb{Z}^2} |G_+(z,m,n)|^2 = \frac{1}{|W|^2} \sum_{n\in\mathbb{Z}} \Big(|u_+(z,n)|^2 \sum_{m<n} |s(z,m)|^2 + |s(z,n)|^2 \sum_{m\geq n} |u_+(z,m)|^2 \Big) \leq \frac{2}{|W|^2} \|u_+(z)\|^2 \, \|s(z)\|^2,$$

where $W = W(s(z), u_+(z))$. □

Our next goal is to find a good parameterization of all self-adjoint extensions if τ is *l.c.* at $+\infty$.

First of all note that any real solution of $\tau u = \lambda u$, $\lambda\in\mathbb{R}$, is in $BC_+(\tau)$ (since $W(u,\tilde{u}) \neq 0$ for any linearly independent solution of $\tau u = \lambda u$). Now fix

$$v_\alpha(n) = \cos(\alpha) c(0,n) + \sin(\alpha) s(0,n), \qquad \alpha\in[0,\pi), \tag{2.175}$$

and note that different α's imply different extensions since $W(v_{\alpha_1}, v_{\alpha_2}) = \sin(\alpha_2 - \alpha_1)/a(0)$.

Lemma 2.20. *All self-adjoint extensions of $H_{min,+}$ correspond to some v_α with unique $\alpha\in[0,\pi)$.*

Proof. Let H_+ be a self-adjoint extension of $H_{min,+}$ and $\lambda_0 \in \sigma(H_+)$ be an eigenvalue with corresponding eigenfunction $s(\lambda_0, n)$. Using Green's formula (1.20) with $f = s(\lambda_0)$, $g\in\mathfrak{D}(H_+)$ we see $\mathfrak{D}(H_+) \subseteq \mathfrak{D}_+(s(\lambda_0))$ and hence $\mathfrak{D}(H_+) = \mathfrak{D}_+(s(\lambda_0))$ by maximality of self-adjoint operators. Let $\alpha\in[0,\pi)$ be the unique value for which

$$W_{+\infty}(v_\alpha, s(\lambda_0)) = \cos(\alpha) W_{+\infty}(c(0), s(\lambda_0)) + \sin(\alpha) W_{+\infty}(s(0), s(\lambda_0)) = 0. \tag{2.176}$$

Then $\mathfrak{D}_+(s(\lambda_0)) = \mathfrak{D}_+(v_\alpha)$. □

Now we turn back again to operators on $\ell^2(\mathbb{Z})$. We use that corresponding definitions and results hold for the other endpoint $-\infty$ as well. With this in mind we have

Theorem 2.21. *Choose $v_\pm \in BC_\pm(\tau)$ as above, then the operator H with domain*

$$\mathfrak{D}(H) = \{f\in\mathfrak{D}(H_{max}) | W_{+\infty}(v_+, f) = W_{-\infty}(v_-, f) = 0\} \tag{2.177}$$

is self-adjoint.

Again, if τ is *l.p.* at $\pm\infty$, the corresponding boundary condition is void and can be omitted. We also note that if τ is *l.c.* at both $\pm\infty$, then we have not found all self-adjoint extensions since we only consider separated boundary conditions (i.e., one for each endpoint) and not coupled ones which connect the behavior of functions at $-\infty$ and $+\infty$.

As before we have

Lemma 2.22. *If τ is l.c. at both $\pm\infty$, then the resolvent of H is a Hilbert-Schmidt operator. In particular, the spectrum of H is purely discrete.*

Most results found for bounded Jacobi operators still hold with minor modifications. One result that requires some changes is Theorem 2.13.

Theorem 2.23. *A measure $d\rho_+$ which is* not *supported on a finite set is the spectral measure of a unique Jacobi operator H_+ if and only if the set of polynomials is dense in $L^2(\mathbb{R}, d\rho_+)$.*

Proof. If the set of polynomials is dense in $L^2(\mathbb{R}, d\rho_+)$ we can use the same proof as in Theorem 2.13 to show existence of a unique Jacobi operator with $d\rho_+$ as spectral measure.

Conversely, let H_+ be given, and let U be a unitary transform mapping H_+ to multiplication by λ in $L^2(\mathbb{R}, d\rho_+)$ (which exists by the spectral theorem). Then $|(U\delta_1)(\lambda)|^2 = 1$ since

$$\int_\Lambda d\rho_+ = \langle \delta_1, P_\Lambda(H_+)\delta_1\rangle = \langle U\delta_1, P_\Lambda(\lambda)U\delta_1\rangle = \int_\Lambda |(U\delta_1)(\lambda)|^2 d\rho_+(\lambda) \tag{2.178}$$

for any Borel set $\Lambda \subseteq \mathbb{R}$. So, by another unitary transformation, we can assume $(U\delta_1)(\lambda) = 1$. And since the span of $(H_+)^j\delta_1$, $j \in \mathbb{N}_0$, is dense in $\ell^2(\mathbb{Z})$, so is the span of $(U(H_+)^j\delta_1)(\lambda) = \lambda^j$ in $L^2(\mathbb{R}, d\rho_+)$. □

A measure $d\rho_+$ which is not supported on a finite set and for which the set of polynomials is dense in $L^2(\mathbb{R}, d\rho_+)$ will be called **Jacobi measure**.

There are some interesting consequences for the moment problem.

Lemma 2.24. *A set $\{m_{+,j}\}_{j\in\mathbb{N}}$ forms the moments of a Jacobi measure if and only if (2.109) holds.*

Moreover,

$$\operatorname{supp}(\rho_+) \subseteq [-R, R] \quad \Leftrightarrow \quad |m_{+,j}| \le R^j, \quad j \in \mathbb{N}. \tag{2.179}$$

Proof. If (2.109) holds we get sequences $a(n)$, $b(n)$ by (2.118). The spectral measure of any self-adjoint extension has $m_{+,j}$ as moments.

If $\operatorname{supp}(\rho_+) \subseteq [-R, R]$, then $|m_{+,j}| \le \int |\lambda|^j d\rho_+(\lambda) \le R^j \int d\rho_+(\lambda) = R^j$. Conversely, if $\operatorname{supp}(\rho_+) \not\subseteq [-R, R]$, then there is an $\varepsilon > 0$ such that $C_\varepsilon = \rho_+(\{\lambda| |\lambda| > R + \varepsilon\}) > 0$ and hence $|m_{+,2j}| \ge \int_{|\lambda|>R+\varepsilon} \lambda^{2j} d\rho_+(\lambda) \ge C_\varepsilon (R+\varepsilon)^{2j}$. □

Finally, let us look at uniqueness.

Theorem 2.25. *A measure is uniquely determined by its moments if and only if the associated Jacobi difference expression τ (defined via (2.118)) is l.p. at $+\infty$.*

Proof. Our assumption implies that $H_{min,+}$ is essentially self-adjoint and hence $(H_{min,+} - z)\mathfrak{D}(H_{min,+})$ is dense in $\ell^2(\mathbb{N})$ for any $z \in \mathbb{C}_\pm$. Denote by $\mathfrak{H}_0$ the set of polynomials on $\mathbb{R}$ and by $\mathfrak{H}$ the closure of $\mathfrak{H}_0$ with respect to the scalar product (2.110). Then $(\lambda - z)\mathfrak{H}_0$ is dense in $\mathfrak{H}$ and hence there is a sequence of polynomials $P_{z,n}(\lambda)$, $z \in \mathbb{C}_\pm$, such that $(\lambda - z)P_{z,n}(\lambda)$ converges to 1 in $\mathfrak{H}$. Let ρ be a measure with correct moments. Then

$$\int_\mathbb{R} |P_{z,n}(\lambda) - \frac{1}{\lambda - z}|^2 d\rho(\lambda) \le \int_\mathbb{R} \frac{|\lambda - z|^2}{\operatorname{Im}(z)^2} |P_{z,n}(\lambda) - \frac{1}{\lambda - z}|^2 d\rho(\lambda) \tag{2.180}$$

shows that $P_{z,n}(\lambda)$ converges to $(\lambda - z)^{-1}$ in $L^2(\mathbb{R}, d\rho)$ and consequently the Borel transform

$$\int \frac{d\rho(\lambda)}{\lambda - z} = \langle 1, \frac{1}{\lambda - z}\rangle_{L^2} = \lim_{n\to\infty} \langle 1, P_{z,n}\rangle \tag{2.181}$$

is uniquely determined by the moments. Since ρ is uniquely determined by its Borel transform we are done. □

We know that τ is *l.p.* at $+\infty$ if the moments are polynomially bounded by (2.179). However, a weaker bound on the growth of the moments also suffices to ensure the *l.p.* case.

Lemma 2.26. *Suppose*

$$|m_{+,j}| \le C R^j j!, \quad j \in \mathbb{N}, \tag{2.182}$$

then τ associated with $\{m_{+,j}\}_{j\in\mathbb{N}}$ is l.p. at $+\infty$.

Proof. Our estimate implies that $\mathrm{e}^{\mathrm{i}z\lambda} \in L^1(\mathbb{R}, d\rho)$ for $|\mathrm{Im}(z)| < 1/R$. Hence the Fourier transform

$$\int_{\mathbb{R}} \mathrm{e}^{\mathrm{i}z\lambda} d\rho(\lambda) = \sum_{j=0}^{\infty} m_{+,j} \frac{(\mathrm{i}z)^j}{j!} \tag{2.183}$$

is holomorphic in the strip $|\mathrm{Im}(z)| < 1/R$. This shows that the Fourier transform is uniquely determined by the moments and so is the Borel transform and hence the measure (see (B.9)). □

2.7. Inverse spectral theory

In this section we present a simple recursive method of reconstructing the sequences a^2, b when the Weyl matrix (cf. (2.142))

$$M(z,n) = \begin{pmatrix} g(z,n) & \frac{h(z,n)}{2a(n)} \\ \frac{h(z,n)}{2a(n)} & g(z,n+1) \end{pmatrix}, \qquad z \in \mathbb{C}\backslash\sigma(H), \tag{2.184}$$

is known for one fixed $n \in \mathbb{Z}$. As a consequence, we are led to several uniqueness results.

By virtue of the Neumann series for the resolvent of H we infer (cf. (6.2) below and Section 6.1 for more details)

$$\begin{aligned} g(z,n) &= -\frac{1}{z} - \frac{b(n)}{z^2} + O(\frac{1}{z^3}), \\ h(z,n) &= -1 - \frac{2a(n)^2}{z^2} + O(\frac{1}{z^3}). \end{aligned} \tag{2.185}$$

Hence $a(n)^2$, $b(n)$ can be easily recovered as follows

$$\begin{aligned} b(n) &= -\lim_{z\to\infty} z(1 + z g(z,n)), \\ a(n)^2 &= -\frac{1}{2} \lim_{z\to\infty} z^2(1 + h(z,n)). \end{aligned} \tag{2.186}$$

Furthermore, we have the useful identities (use (1.100))

$$4a(n)^2 g(z,n) g(z,n+1) = h(z,n)^2 - 1 \tag{2.187}$$

and

$$h(z,n+1)+h(z,n)=2(z-b(n+1))g(z,n+1), \tag{2.188}$$

which 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.

In addition, we infer that $a(n)^2$, $g(z,n)$, $g(z,n+1)$ determine $h(z,n)$ up to one sign,

$$h(z,n)=\Big(1+4a(n)^2 g(z,n)g(z,n+1)\Big)^{1/2}, \tag{2.189}$$

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 proved the important result that $M(z,n_0)$ determines the sequences a^2, b. In fact, we have proved the slightly stronger result:

Theorem 2.27. *One of the following set of data*
(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* $a(n_0)^2$
for one fixed $n_0\in\mathbb{Z}$ *uniquely determines the sequences* a^2 *and* b.

Remark 2.28. (i) Let me emphasize that the two diagonal elements $g(z,n_0)$ and $g(z,n_0+1)$ alone plus $a(n_0)^2$ are sufficient to reconstruct $a(n)^2$, $b(n)$. This is in contradistinction to the case of one-dimensional Schrödinger operators, where the diagonal elements of the Weyl matrix determine the potential only up to reflection.

You might wonder how the Weyl matrix of the operator H_R associated with the (at n_0) reflected coefficients a_R, b_R (cf. Lemma 1.7) look like. Since reflection at n_0 exchanges $m_\pm(z,n_0)$ (i.e., $m_{R,\pm}(z,n_0)=m_\mp(z,n_0)$) we infer

$$\begin{aligned} g_R(z,n_0) &= g(z,n_0),\\ h_R(z,n_0) &= -h(z,n_0)+2(z-b(n_0))g(z,n_0),\\ g_R(z,n_0+1) &= \frac{a(n_0)^2}{a(n_0-1)^2}g(z,n_0+1)+\frac{z-b(n_0)}{a(n_0-1)^2}\Big(h(z,n_0)\\ &\quad +(z-b(n_0))g(z,n_0)\Big), \end{aligned} \tag{2.190}$$

in obvious notation.
(ii) Remark 6.3(ii) will show 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

$$G(z,n+k,n)=g(z,n)\prod_{j=n}^{n+k-1}\frac{1+h(z,j)}{2a(j)g(z,j)},\quad k>0, \tag{2.191}$$

and we remark

$$\begin{aligned} a(n)^2 g(z,n+1)-a(n-1)^2 g(z,n-1)+(z-b(n))^2 g(z,n)\\ =(z-b(n))h(z,n). \end{aligned} \tag{2.192}$$

A similar procedure works for H_+. The asymptotic expansion

$$m_+(z,n) = -\frac{1}{z} - \frac{b(n+1)}{z^2} - \frac{a(n+1)^2 + b(n+1)^2}{z^3} + O(z^{-4}) \tag{2.193}$$

shows that $a(n+1)^2, b(n+1)$ can be recovered from $m_+(z,n)$. In addition, (2.11) shows that $m_+(z,n_0)$ determines $a(n)^2$, $b(n)$, $m_+(z,n)$, $n > n_0$. Similarly, (by reflection) $m_-(z,n_0)$ determines $a(n-1)^2$, $b(n)$, $m_-(z,n-1)$, $n < n_0$. Hence both $m_\pm(z,n_0)$ determine $a(n)^2, b(n)$ except for $a(n_0-1)^2$, $a(n_0)^2$, $b(n_0)$. However, since $a(n_0-1)^2$, $a(n_0)^2$, $b(n_0)$, and $m_-(z,n_0)$ can be computed from $\tilde{m}_-(z,n_0)$ we conclude:

Theorem 2.29. *The quantities $\tilde{m}_+(z,n_0)$ and $\tilde{m}_-(z,n_0)$ uniquely determine $a(n)^2$ and $b(n)$ for all $n \in \mathbb{Z}$.*

Next, we recall the function $\gamma^\beta(z,n)$ introduced in (1.107) with asymptotic expansion

$$\gamma^\beta(z,n) = -\frac{\beta}{a(n)} - \frac{1+\beta^2}{z} - \frac{b(n+1) + 2\beta a(n) + \beta^2 b(n)}{z^2} + O(\frac{1}{z^3}). \tag{2.194}$$

Our goal is to prove

Theorem 2.30. *Let $\beta_1, \beta_2 \in \mathbb{R} \cup \{\infty\}$ with $\beta_1 \neq \beta_2$ be given. Then $\gamma^{\beta_j}(.,n_0)$, $j = 1,2$, for one fixed $n_0 \in \mathbb{Z}$ uniquely determine $a(n)^2, b(n)$ for all $n \in \mathbb{Z}$ (set $\gamma^\infty(z,n) = g(z,n)$) unless $(\beta_1,\beta_2) = (0,\infty),(\infty,0)$. In the latter case $a(n_0)^2$ is needed in addition. More explicitly, we have*

$$\begin{aligned} g(z,n) &= \frac{\gamma^{\beta_1}(z,n) + \gamma^{\beta_2}(z,n) + 2R(z)}{(\beta_2-\beta_1)^2}, \\ g(z,n+1) &= \frac{\beta_2^2\gamma^{\beta_1}(z,n) + \beta_1^2\gamma^{\beta_2}(z,n) + 2\beta_1\beta_2 R(z)}{(\beta_2-\beta_1)^2}, \\ h(z,n) &= \frac{\beta_2\gamma^{\beta_1}(z,n) + \beta_1\gamma^{\beta_2}(z,n) + (\beta_1+\beta_2)R(z)}{(-2a(n))^{-1}(\beta_2-\beta_1)^2}, \end{aligned} \tag{2.195}$$

where $R(z)$ is the branch of

$$R(z) = \left(\frac{(\beta_2-\beta_1)^2}{4a(n)^2} + \gamma^{\beta_1}(z,n)\gamma^{\beta_2}(z,n)\right)^{1/2} = \frac{\beta_1+\beta_2}{2a(n)} + O(\frac{1}{z}), \tag{2.196}$$

which is holomorphic for $z \in \mathbb{C}\backslash\sigma(H)$ and has asymptotic behavior as indicated. If one of the numbers β_1, β_2 equals ∞, one has to replace all formulas by their limit using $g(z,n) = \lim_{\beta\to\infty} \beta^{-2}\gamma^\beta(z,n)$.

Proof. Clearly, if $(\beta_1,\beta_2) \neq (0,\infty),(\infty,0)$, we can determine $a(n)$ from equation (2.194). Hence by Theorem 2.27 it suffices to show (2.195). Since the first equation follows from (2.187) and the other two, it remains to establish the last two equations in (2.195). For this we prove that the system

$$(g^+)^2 + 2\frac{\beta_j}{2a(n)}hg^+ + \frac{\beta_j^2}{4a(n)^2}(h^2-1) = g^+\gamma^{\beta_j}(z,n), \quad j = 1,2, \tag{2.197}$$

has a unique solution $(g^+,h) = (g(z,n+1),h(z,n))$ for $|z|$ large enough which is holomorphic with respect to z and satisfies the asymptotic requirements (2.185).

Chapter 12

The Toda system

This chapter is devoted to the Toda hierarchy. The first section gives an informal introduction and is mainly for background and motivation. The following sections contain a rigorous treatment based on the Lax pair formalism. The basic existence and uniqueness theorem for solutions of the initial value problem is proven and the connection with hyperelliptic Riemann surfaces is established.

12.1. The Toda lattice

The Toda lattice is a simple model for a nonlinear one-dimensional crystal. It describes the motion of a chain of particles with nearest neighbor interaction. The equation of motion for such a system is given by

$$m\frac{d^2}{dt^2}x(n,t) = V'(x(n+1,t)-x(n,t)) - V'(x(n,t)-x(n-1,t)), \tag{12.1}$$

where m denotes the mass of each particle, $x(n,t)$ is the displacement of the n-th particle from its equilibrium position, and $V(r)$ ($V'(r) = \frac{dV}{dr}(r)$) is the interaction potential. As discovered by M. Toda, this system gets particularly interesting if one chooses an exponential interaction,

$$V(r) = \frac{m\rho^2}{\tau^2}\Big(\mathrm{e}^{-r/\rho} + \frac{r}{\rho} - 1\Big) = \frac{m\rho^2}{\tau^2}\Big(\big(\frac{r}{\rho}\big)^2 + O\big(\frac{r}{\rho}\big)^3\Big), \quad \tau,\rho\in\mathbb{R}. \tag{12.2}$$

This model is of course only valid as long as the relative displacement is not too large (i.e., at least smaller than the distance of the particles in the equilibrium position). For small displacements it is equal to a harmonic crystal with force constant $\frac{m}{\tau^2}$ (cf. Section 1.5).

After a scaling transformation, $t\mapsto t/\tau$, $x\mapsto x/\rho$, we can assume $m=\tau=\rho=1$. If we suppose $x(n,t)-x(n-1,t)\to 0$, $\dot{x}(n,t)\to 0$ sufficiently fast as $|n|\to\infty$, we can introduce the Hamiltonian ($q=x$, $p=\dot{x}$)

$$\mathcal{H}(p,q) = \sum_{n\in\mathbb{Z}}\Big(\frac{p(n,t)^2}{2} + (\mathrm{e}^{-(q(n+1,t)-q(n,t))} - 1)\Big) \tag{12.3}$$

and rewrite the equations of motion in the Hamiltonian form

$$\begin{aligned}\frac{d}{dt}p(n,t) &= -\frac{\partial\mathcal{H}(p,q)}{\partial q(n,t)}\\ &= \mathrm{e}^{-(q(n,t)-q(n-1,t))} - \mathrm{e}^{-(q(n+1,t)-q(n,t))},\\ \frac{d}{dt}q(n,t) &= \frac{\partial\mathcal{H}(p,q)}{\partial p(n,t)} = p(n,t).\end{aligned} \tag{12.4}$$

We remark that these equations are invariant under the transformation

$$p(n,t) \to p(n,t) + p_0 \quad \text{and} \quad q(n,t) \to q(n,t) + q_0 + p_0 t, \quad (p_0, q_0) \in \mathbb{R}^2, \tag{12.5}$$

which reflects the fact that the dynamics remains unchanged by a uniform motion of the entire crystal.

The fact which makes the Toda lattice particularly interesting is the existence of soliton solutions. These are pulslike waves traveling through the crystal without changing their shape. Such solutions are rather special since from a generic linear equation one would expect spreading of wave packets (see Section 1.5) and from a generic nonlinear wave equation one would expect that solutions only exist for a finite time (breaking of waves).

The simplest example of such a solitary wave is the one-soliton solution

$$q_1(n,t) = q_0 - \ln\frac{1+\gamma\exp(-2\kappa n \pm 2\sinh(\kappa)t)}{1+\gamma\exp(-2\kappa(n-1) \pm 2\sinh(\kappa)t)}, \quad \kappa,\gamma > 0. \tag{12.6}$$

It describes a single bump traveling trough the crystal with speed $\pm\sinh(\kappa)/\kappa$ and width proportional to $1/\kappa$. That is, the smaller the soliton the faster it propagates. It results in a total displacement

$$\lim_{n\to\infty}\Big(q_1(n,t) - q_1(-n,t)\Big) = 2\kappa \tag{12.7}$$

of the crystal, which can equivalently be interpreted as the total compression of the crystal around the bump. The total moment and energy are given by

$$\begin{aligned}\sum_{n\in\mathbb{Z}} p_1(n,t) &= 2\sinh(\kappa),\\ \mathcal{H}(p_1,q_1) &= 2(\sinh(\kappa)\cosh(\kappa) - \kappa).\end{aligned} \tag{12.8}$$

Existence of such solutions is usually connected to complete integrability of the system which is indeed the case here. To see this, we introduce Flaschka's variables

$$a(n,t) = \frac{1}{2}\mathrm{e}^{-(q(n+1,t)-q(n,t))/2}, \qquad b(n,t) = -\frac{1}{2}p(n,t) \tag{12.9}$$

and obtain the form most convenient for us

$$\begin{aligned}\dot{a}(n,t) &= a(n,t)\Big(b(n+1,t) - b(n,t)\Big),\\ \dot{b}(n,t) &= 2\Big(a(n,t)^2 - a(n-1,t)^2\Big).\end{aligned} \tag{12.10}$$

The inversion is given by

$$\begin{aligned} p(n,t) &= -2b(n,t), \\ q(n,t) &= q(n,0) - 2\int_0^t b(n,s)ds \\ &= q(0,0) - 2\int_0^t b(0,s)ds - 2\sum_{j=0}^{n-1}{}^{*}\ \ln(2a(j,t)) \\ &= q(0,0) - 2\int_0^t b(n,s)ds - 2\sum_{j=0}^{n-1}{}^{*}\ \ln(2a(j,0)). \end{aligned} \tag{12.11}$$

To show complete integrability it suffices to find a so-called Lax pair, that is, two operators $H(t)$, $P(t)$ such that the Lax equation

$$\frac{d}{dt}H(t) = P(t)H(t) - H(t)P(t) \tag{12.12}$$

is equivalent to (12.10). One can easily convince oneself that the choice

$$\begin{aligned} H(t):\ \ell^2(\mathbb{Z}) &\to \ell^2(\mathbb{Z}) \\ f(n) &\mapsto a(n,t)f(n+1) + a(n-1,t)f(n-1) + b(n,t)f(n) \end{aligned}, \\ \begin{aligned} P(t):\ \ell^2(\mathbb{Z}) &\to \ell^2(\mathbb{Z}) \\ f(n) &\mapsto a(n,t)f(n+1) - a(n-1,t)f(n-1) \end{aligned} \tag{12.13}$$

does the trick. Now the Lax equation implies that the operators $H(t)$ for different $t \in \mathbb{R}$ are all unitarily equivalent and that

$$\operatorname{tr}\Big(H(t)^j - H_0^j\Big), \quad j \in \mathbb{N}, \tag{12.14}$$

are conserved quantities, where H_0 is the operator corresponding to the constant solution $a_0(n,t) = \frac{1}{2}$, $b_0(n,t) = 0$ (it is needed to make the trace converge). For example,

$$\begin{aligned} \operatorname{tr}\Big(H(t) - H_0\Big) &= \sum_{n\in\mathbb{Z}} b(n,t) = -\frac{1}{2}\sum_{n\in\mathbb{Z}} p(n,t) \text{ and} \\ \operatorname{tr}\Big(H(t)^2 - H_0^2\Big) &= \sum_{n\in\mathbb{Z}} b(n,t)^2 + 2(a(n,t)^2 - \frac{1}{4}) = \frac{1}{2}\mathcal{H}(p,q) \end{aligned} \tag{12.15}$$

correspond to conservation of the total momentum and the total energy, respectively.

This reformulation of the Toda equations as a Lax pair is the key to methods of solving the Toda equations based on spectral and inverse spectral theory for the Jacobi operator H.

Using these methods one can find the general N-soliton solution

$$q_N(n,t) = q_0 - \ln\frac{\det(\mathbb{1} + C_N(n,t))}{\det(\mathbb{1} + C_N(n-1,t))}, \tag{12.16}$$

where
(12.17)
$$C_N(n,t) = \left(\frac{\sqrt{\gamma_i \gamma_j}}{1 - \mathrm{e}^{-(\kappa_i + \kappa_j)}} \mathrm{e}^{-(\kappa_i + \kappa_j)n - (\sigma_i \sinh(\kappa_i) + \sigma_j \sinh(\kappa_j))t} \right)_{1 \le i,j \le N}$$
with $\kappa_j, \gamma_j > 0$ and $\sigma_j \in \{\pm 1\}$. One can also find (quasi-)periodic solutions using techniques from Riemann surfaces (respectively algebraic curves). Each such solution is associated with an hyperelliptic curve of the type

$$w^2 = \prod_{j=0}^{2g+2} (z - E_j), \quad E_j \in \mathbb{R}, \tag{12.18}$$

where E_j, $0 \le j \le 2g+1$, are the band edges of the spectrum of H (which is independent of t and hence determined by the initial conditions). One obtains

$$q(n,t) = q_0 - 2(t\tilde{b} + n\ln(2\tilde{a})) - \ln \frac{\theta(\underline{z}_0 - 2n\underline{A}_{p_0}(\infty_+) - 2t\underline{c}(g))}{\theta(\underline{z}_0 - 2(n-1)\underline{A}_{p_0}(\infty_+) - 2t\underline{c}(g))}, \tag{12.19}$$

where $\underline{z}_0 \in \mathbb{R}^g$, $\theta : \mathbb{R}^g \to \mathbb{R}$ is the Riemann theta function associated with the hyperelliptic curve (12.18), and $\tilde{a}, \tilde{b} \in \mathbb{R}$, $\underline{A}_{p_0}(\infty_+), \underline{c}(g) \in \mathbb{R}^g$ are constants depending only on the curve (i.e., on E_j, $0 \le j \le 2g+1$). If $q(n,0)$, $p(n,0)$ are (quasi-) periodic with average 0, then $\tilde{a} = \frac{1}{2}$, $\tilde{b} = 0$.

The rest of this monograph is devoted to a rigorous mathematical investigation of these methods.

12.2. Lax pairs, the Toda hierarchy, and hyperelliptic curves

In this section we introduce the Toda hierarchy using a recursive approach for the standard Lax formalism and derive the Burchnall-Chaundy polynomials in connection with the stationary Toda hierarchy.

We let the sequences a, b depend on an additional parameter $t \in \mathbb{R}$ and require

Hypothesis H. 12.1. Suppose $a(t)$, $b(t)$ satisfy

$$a(t), b(t) \in \ell^\infty(\mathbb{Z}, \mathbb{R}), \quad a(n,t) \neq 0, \ (n,t) \in \mathbb{Z} \times \mathbb{R}, \tag{12.20}$$

and let $t \in \mathbb{R} \mapsto (a(t), b(t)) \in \ell^\infty(\mathbb{Z}) \oplus \ell^\infty(\mathbb{Z})$ be differentiable.

We introduce the corresponding operator $H(t)$ as usual, that is,

$$\begin{array}{rccl} H(t): & \ell^2(\mathbb{Z}) & \to & \ell^2(\mathbb{Z}) \\ & f(n) & \mapsto & a(n,t)f(n+1) + a(n-1,t)f(n-1) + b(n,t)f(n) \end{array}. \tag{12.21}$$

The idea of the Lax formalism is to find a finite, skew-symmetric operator $P_{2r+2}(t)$ such that the **Lax equation**

$$\frac{d}{dt} H(t) - [P_{2r+2}(t), H(t)] = 0, \quad t \in \mathbb{R}, \tag{12.22}$$

(here $[.\,,\,..]$ denotes the commutator, i.e., $[P,H] = PH - HP$) holds. More precisely, we seek an operator $P_{2r+2}(t)$ such that the commutator with $H(t)$ is a symmetric difference operator of order at most two. Equation (12.22) will then give an evolution equation for $a(t)$ and $b(t)$. Our first theorem tells us what to choose for $P_{2r+2}(t)$.

Theorem 12.2. *Suppose $P(t)$ is of order at most $2r+2$ and the commutator with $H(t)$ is of order at most 2. Then $P(t)$ is of the form*

$$P(t) = \sum_{j=0}^{r} \Big(c_{r-j} \tilde{P}_{2j+2}(t) + d_{r-j} H(t)^{j+1} \Big) + d_{r+1} \mathbb{1}, \tag{12.23}$$

where $c_j, d_j \in \mathbb{C}$, $0 \le j \le r$, $d_{r+1} \in \ell(\mathbb{Z})$, and

$$\tilde{P}_{2j+2}(t) = [H(t)^{j+1}]_+ - [H(t)^{j+1}]_- \tag{12.24}$$

(cf. the notation in (1.11)) is called homogeneous Lax operator. Moreover, denote by $P_{2r+2}(t)$ the operator $P(t)$ with $c_0 = 1$ and $d_j = 0$, $0 \le j \le r+1$. Then we have

$$P_{2r+2}(t) = -H(t)^{r+1} + \sum_{j=0}^{r} (2a(t) g_j(t) S^+ - h_j(t)) H(t)^{r-j} + g_{r+1}(t), \tag{12.25}$$

where $(g_j(n,t))_{0 \le j \le r+1}$ and $(h_j(n,t))_{0 \le j \le r+1}$ are given by

$$\begin{aligned} g_j(n,t) &= \sum_{\ell=0}^{j} c_{j-\ell} \langle \delta_n, H(t)^\ell \delta_n \rangle, \\ h_j(n,t) &= 2a(n,t) \sum_{\ell=0}^{j} c_{j-\ell} \langle \delta_{n+1}, H(t)^\ell \delta_n \rangle + c_{j+1} \end{aligned} \tag{12.26}$$

and satisfy the recursion relations

$$\begin{aligned} g_0 = 1,\ h_0 &= c_1, \\ 2g_{j+1} - h_j - h_j^- - 2b g_j &= 0, \quad 0 \le j \le r, \\ h_{j+1} - h_{j+1}^- - 2(a^2 g_j^+ - (a^-)^2 g_j^-) - b(h_j - h_j^-) &= 0, \quad 0 \le j < r. \end{aligned} \tag{12.27}$$

For the commutator we obtain

$$\begin{aligned} [P_{2r+2}(t), H(t)] &= a(t)(g_{r+1}^+(t) - g_{r+1}(t)) S^+ + a^-(t)(g_{r+1}(t) - g_{r+1}^-(t)) S^- \\ &\quad + (h_{r+1}(t) - h_{r+1}^-(t)). \end{aligned} \tag{12.28}$$

Proof. By Lemma 1.2 we can write

$$P(t) = -h_{-1}(t) H(t)^{r+1} + \sum_{j=0}^{r} (2a(t) g_j(t) S^+ - h_j(t)) H(t)^{r-j} + g_{r+1}(t), \tag{12.29}$$

where $g_{r+1}(t)$ is only added for convenience and hence can be chosen arbitrarily. Now we insert this ansatz into $[P, H]$. Considering the term $(S^-)^{r+2}$ we see that $h_{-1}(t)$ must be independent of n, say $h_{-1}(t) = c_0 - d_0$. Next, we obtain after a long but straightforward calculation

$$\begin{aligned} [P, H] &= 2a(g_0^+ - g_0) S^+ H^{r+1} - (h_0 - h_0^-) H^{r+1} \\ &\quad - \sum_{j=0}^{r-1} a \Big(\partial (2g_{j+1} - h_j - h_j^- - 2b g_j) \Big) S^+ H^{r-j} \\ &\quad - \sum_{j=0}^{r-1} \Big(h_{j+1} - h_{j+1}^- - 2(a^2 g_j^+ - (a^-)^2 g_j^-) - b(h_j - h_j^-) \Big) H^{r-j} \\ &\quad + a(g_{r+1}^+ - g_{r+1}) S^+ + S^- a(g_{r+1}^+ - g_{r+1}) + (h_{r+1} - h_{r+1}^-), \end{aligned} \tag{12.30}$$

where g_{r+1}, h_{r+1} have been chosen according to

$$\partial(2g_{r+1} - h_r - h_r^- - 2bg_r) \,=\, 0,$$
$$h_{r+1} - h_{r+1}^- - 2(a^2 g_r^+ - (a^-)^2 g_r^-) - b(h_r - h_r^-) \,=\, 0. \tag{12.31}$$

(Recall $\partial f = f^+ - f$.) But (12.30) is of order 2 if and only if (compare Lemma 1.2)

$$g_0 = c_0,\; h_0 = c_1 - d_1,$$
$$2g_{j+1} - h_j - h_j^- - 2bg_j = 2d_{j+1}, \quad 0 \le j \le r-1,$$
$$h_{j+1} - h_{j+1}^- - 2(a^2 g_j^+ - (a^-)^2 g_j^-) - b(h_j - h_j^-) = 0, \quad 0 \le j < r-2, \tag{12.32}$$

where c_0, c_1, d_j, $1 \le j \le r$, are constants. By Lemma 6.4

$$\tilde{g}_j(n,t) = \langle \delta_n, H(t)^j \delta_n \rangle, \quad \tilde{h}_j(n,t) = 2a(n,t)\langle \delta_{n+1}, H(t)^j \delta_n \rangle \tag{12.33}$$

is a solution of this system for $c_0 = 1$, $c_j = d_j = 0$, $1 \le j \le r$. It is called the homogeneous solution for if we assign the weight one to a and b, then $\tilde{g}_j(n,t)$, $\tilde{h}_j(n,t)$ are homogeneous of degree j, $j+1$, respectively. The general solution of the above system (12.32) is hence given by $g_j = \sum_{\ell=0}^{j} c_\ell \tilde{g}_{j-\ell}$, $1 \le j \le r$, and $h_j = \sum_{\ell=0}^{j} c_\ell \tilde{h}_{j-\ell} + c_{j+1} - d_{j+1}$, $1 \le j \le r-1$. Introducing another arbitrary sequence d_{r+1} it is no restriction to assume that the formula for h_j also holds for $j = r$.

It remains to verify (12.24). We use induction on r. The case $r = 0$ is easy. By (12.25) we need to show

$$\tilde{P}_{2r+2} = \tilde{P}_{2r} H + \big(2a\tilde{g}_r S^+ - \tilde{h}_r\big) - \tilde{g}_r H + \tilde{g}_{r+1}. \tag{12.34}$$

This can be done upon considering $\langle \delta_m, \tilde{P}_{2r+2}\delta_n \rangle$ and making case distinctions $m < n-1, m = n-1, m = n, m = n+1, m > n+1$. Explicitly, one verifies, for instance, in the case $m = n$,

$$\begin{aligned}
&\langle \delta_n, \tilde{P}_{2r+2}\delta_n \rangle \\
&\quad = \langle \delta_n, \tilde{P}_{2r}(a\delta_{n-1} + a^-\delta_{n+1} + b\delta_n) \rangle - \tilde{h}_r(n) - b(n)\tilde{g}_r(n) + \tilde{g}_{r+1}(n) \\
&\quad = \langle \delta_n, ([H^r]_+ - [H^r]_-)(a\delta_{n-1} + a^-\delta_{n+1} + b\delta_n) \rangle - \tilde{h}_r(n) - b(n)\tilde{g}_r(n) + \tilde{g}_{r+1}(n) \\
&\quad = \langle \delta_n, [H^r]_+\, a^-\delta_{n+1} \rangle - \langle \delta_n, [H^r]_-\, a\delta_{n-1} \rangle - \tilde{h}_r(n) - b(n)\tilde{g}_r(n) + \tilde{g}_{r+1}(n) \\
&\quad = a(n)\langle \delta_n, H^r\delta_{n+1} \rangle - a(n-1)\langle \delta_n, H^r\delta_{n-1} \rangle - \tilde{h}_r(n) - b(n)\tilde{g}_r(n) + \tilde{g}_{r+1}(n) \\
&\quad = -\frac{\tilde{h}_r(n) + \tilde{h}_r(n-1)}{2} - b(n)\tilde{g}_r(n) + \tilde{g}_{r+1}(n) = 0
\end{aligned} \tag{12.35}$$

using (12.27),

$$\langle \delta_m, [H^j]_\pm \delta_n \rangle = \begin{cases} \langle \delta_m, H^j \delta_n \rangle, & \pm(m-n) > 0 \\ 0, & \pm(m-n) \le 0 \end{cases}, \tag{12.36}$$

and $H\delta_m = a(m)\delta_{m+1} + a(m-1)\delta_{m-1} + b(m)\delta_m$. This settles the case $m = n$. The remaining cases are settled one by one in a similar fashion. □

Remark 12.3. It is also easy to obtain (12.28) from (12.23) and (12.24). In fact, simply evaluate

$$\begin{aligned}
\langle \delta_m, [\tilde{P}_{2j+2}, H]\delta_n \rangle \,=\, &\langle H\delta_m, [H^{j+1}]_+\delta_n \rangle + \langle H\delta_n, [H^{j+1}]_+\delta_m \rangle \\
&- \langle H\delta_m, [H^{j+1}]_-\delta_n \rangle - \langle H\delta_n, [H^{j+1}]_-\delta_m \rangle
\end{aligned} \tag{12.37}$$

as in the proof of Theorem 12.2.

Since the self-adjoint part of $P(t)$ does not produce anything interesting when inserted into the Lax equation, we will set $d_j = 0$, $0 \le j \le r+1$, and take

$$P_{2r+2}(t) = \sum_{j=0}^{r} c_{r-j} \tilde{P}_{2j+2}(t) \tag{12.38}$$

as our **Lax operator** in (12.22). Explicitly we have

$$\begin{aligned} P_2(t) &= a(t)S^+ - a^-(t)S^- \\ P_4(t) &= a(t)a^+(t)S^{++} + a(t)(b^+(t) + b(t))S^+ - a^-(t)(b(t) + b^-(t))S^- \\ &\quad - a^-(t)a^{--}(t)S^{--} + c_1(a(t)S^+ - a^-(t)S^-) \\ &\quad \text{etc. .} \end{aligned} \tag{12.39}$$

Clearly, $H(t)$ and $\mathrm{i}P_{2r+2}(t)$ are bounded, self-adjoint operators.

Even though the expression (12.25) for $P_{2r+2}(t)$ looks much more complicated and clumsy in comparison to (12.24), we will see that this ruse of expanding $P_{2r+2}(t)$ in powers of $H(t)$ will turn out most favorable for our endeavor. But before we can see this, we need to make sure that the Lax equation is well-defined, that is, that $H(t)$ is differentiable.

First of all, please recall the following facts. Denote by $\mathfrak{B}(\ell^2(\mathbb{Z}))$ the C^*-algebra of bounded linear operators. Suppose $A, B : \mathbb{R} \to \mathfrak{B}(\ell^2(\mathbb{Z}))$ are differentiable with derivative $\dot{A}$, $\dot{B}$, respectively, then we have

- $A + B$ is differentiable with derivative $\dot{A} + \dot{B}$,
- AB is differentiable with derivative $\dot{A}B + A\dot{B}$,
- A^* is differentiable with derivative $\dot{A}^*$,
- A^{-1} (provided A is invertible) is differentiable with derivative $-A^{-1}\dot{A}A^{-1}$.

In addition, $f : \mathbb{R} \to \ell^\infty(\mathbb{Z})$ is differentiable if and only if the associated multiplication operator $f : \mathbb{R} \to \mathfrak{B}(\ell^2(\mathbb{Z}))$ is (since the embedding $\ell^\infty(\mathbb{Z}) \hookrightarrow \mathfrak{B}(\ell^2(\mathbb{Z}))$ is isometric).

For our original problem this implies that $H(t)$ and $P_{2r+2}(t)$ are differentiable since they are composed of differentiable operators. Hence the Lax equation (12.22) is well-defined and by (12.30) it is equivalent to

$$\begin{aligned} \mathrm{TL}_r(a(t), b(t))_1 &= \dot{a}(t) - a(t)\big(g^+_{r+1}(t) - g_{r+1}(t)\big) = 0, \\ \mathrm{TL}_r(a(t), b(t))_2 &= \dot{b}(t) - \big(h_{r+1}(t) - h^-_{r+1}(t)\big) = 0, \end{aligned} \tag{12.40}$$

where the dot denotes a derivative with respect to t. Or, in integral form we have

$$\begin{aligned} a(t) &= a(0) \exp\Big(\int_0^t \big(g^+_{r+1}(t) - g_{r+1}(t)\big) ds \Big), \\ b(t) &= b(0) + \int_0^t \big(h_{r+1}(t) - h^-_{r+1}(t)\big) ds. \end{aligned} \tag{12.41}$$

Varying $r \in \mathbb{N}_0$ yields the **Toda hierarchy** (TL hierarchy)

$$\mathrm{TL}_r(a, b) = (\mathrm{TL}_r(a, b)_1, \mathrm{TL}_r(a, b)_2) = 0, \quad r \in \mathbb{N}_0. \tag{12.42}$$

Notice that multiplying $P_{2r+2}(t)$ with $c_0 \neq 0$ gives only a rescaled version of the Toda hierarchy which can be reduced to the original one by substituting $t \to t/c_0$. Hence our choice $c_0 = 1$.

Explicitly, one obtains from (12.27),

$$
\begin{aligned}
g_1 &= b + c_1,\\
h_1 &= 2a^2 + c_2,\\
g_2 &= a^2 + (a^-)^2 + b^2 + c_1 b + c_2,\\
h_2 &= 2a^2(b^+ + b) + c_1 2a^2 + c_3,\\
g_3 &= a^2(b^+ + 2b) + (a^-)^2(2b + b^-) + b^3\\
&\quad + c_1(a^2 + (a^-)^2 + b^2) + c_2 b + c_3,\\
h_3 &= 2a^2((a^+)^2 + a^2 + (a^-)^2 + b^2 + b^+ b + (b^+)^2)\\
&\quad + c_1 2a^2(b^+ + b) + c_2 2a^2 + c_4,\\
&\quad \text{etc.}
\end{aligned}
\tag{12.43}
$$

and hence

$$
\begin{aligned}
\mathrm{TL}_0(a,b) &= \begin{pmatrix} \dot a - a(b^+ - b)\\ \dot b - 2(a^2 - (a^-)^2)\end{pmatrix},\\
\mathrm{TL}_1(a,b) &= \begin{pmatrix} \dot a - a((a^+)^2 - (a^-)^2 + (b^+)^2 - b^2)\\ \dot b - 2a^2(b^+ + b) + 2(a^-)^2(b + b^-)\end{pmatrix}\\
&\quad - c_1 \begin{pmatrix} a(b^+ - b)\\ 2(a^2 - (a^-)^2)\end{pmatrix},\\
\mathrm{TL}_2(a,b) &= \begin{pmatrix} \dot a - a((a^+)^2(b^{++} + 2b^+) + a^2(2b^+ + b) + (b^+)^3 - a^2(b^+ + 2b) - (a^-)^2(2b + b^-) - b^3)\\ \dot b + 2((a^-)^4 + (a^{--} a^-)^2 - a^2(a^2 + (a^+)^2 + (b^+)^2 + bb^+ + b^2) + (a^-)^2(b^2 + b^- b + (b^-)^2))\end{pmatrix}\\
&\quad - c_1 \begin{pmatrix} a((a^+)^2 - (a^-)^2 + (b^+)^2 - b^2)\\ 2a^2(b^+ + b) - 2(a^-)^2(b + b^-)\end{pmatrix} - c_2 \begin{pmatrix} a(b^+ - b)\\ 2(a^2 - (a^-)^2)\end{pmatrix},\\
&\quad \text{etc.}
\end{aligned}
\tag{12.44}
$$

represent the first few equations of the Toda hierarchy. We will require $c_j \in \mathbb{R}$ even though c_j could depend on t. The corresponding **homogeneous Toda equations** obtained by taking all summation constants equal to zero, $c_\ell \equiv 0$, $1 \le \ell \le r$, are then denoted by

$$
\widetilde{\mathrm{TL}}_r(a,b) = \mathrm{TL}_r(a,b)\Big|_{c_\ell \equiv 0,\ 1 \le \ell \le r}. \tag{12.45}
$$

We are interested in investigating the **initial value problem** associated with the Toda equations, that is,

$$
\mathrm{TL}_r(a,b) = 0, \quad \big(a(t_0), b(t_0)\big) = (a_0, b_0), \tag{12.46}
$$

where (a_0, b_0) are two given (bounded) sequences. Since the Toda equations are autonomous, we will choose $t_0 = 0$ without restriction.

In order to draw a number of fundamental consequences from the Lax equation (12.22), we need some preparations.

Let $P(t)$, $t \in \mathbb{R}$, be a family of bounded skew-adjoint operators in $\ell^2(\mathbb{Z})$. A two parameter family of operators $U(t,s)$, $(t,s) \in \mathbb{R}^2$, is called a **unitary propagator** for $P(t)$, if

1. $U(t,s)$, $(s,t) \in \mathbb{R}^2$, is unitary.
2. $U(t,t) = 1\!\!1$ for all $t \in \mathbb{R}$.
3. $U(t,s)U(s,r) = U(t,r)$ for all $(r,s,t) \in \mathbb{R}^3$.

4. The map $t \mapsto U(t,s)$ is differentiable in the Banach space $\mathfrak{B}(\ell^2(\mathbb{Z}))$ of bounded linear operators and

$$\frac{d}{dt}U(t,s) = P(t)U(t,s), \quad (t,s) \in \mathbb{R}^2. \tag{12.47}$$

Note $U(s,t) = U(t,s)^{-1} = U(t,s)^*$ and $d/dt\, U(s,t) = -U(s,t)P(t)$.

With this notation the following well-known theorem from functional analysis holds:

Theorem 12.4. *Let $P(t)$, $t \in \mathbb{R}$, be a family of bounded skew-adjoint operators such that $t \mapsto P(t)$ is differentiable. Then there exists a unique unitary propagator $U(t,s)$ for $P(t)$.*

Proof. Consider the equation $\dot{U}(t) = P(t)U(t)$. By standard theory of differential equations, solutions for the initial value problem exist locally and are unique (cf., e.g., Theorem 4.1.5 of [**1**]). Moreover, since $\|P(t)\|$ is uniformly bounded on compact sets, all solutions are global. Hence we have a unique solution $U(t,s)$, $(t,s) \in \mathbb{R}^2$ such that $U(s,s) = \mathbb{1}$. It remains to verify that this propagator $U(t,s)$ is unitary. Comparing the adjoint equation

$$\frac{d}{dt}U(t,s)^* = (\frac{d}{dt}U(t,s))^* = (P(t)U(t,s))^* = -U(t,s)^*P(t) \tag{12.48}$$

and

$$\frac{d}{dt}U(t,s)^{-1} = -U(t,s)^{-1}\Big(\frac{d}{dt}U(t,s)\Big)U(t,s)^{-1} = -U(t,s)^{-1}P(t) \tag{12.49}$$

we infer $U(t,s)^* = U(t,s)^{-1}$ by unique solubility of the initial value problem and $U(s,s)^* = U(s,s)^{-1} = \mathbb{1}$. □

If $P(t) = P$ is actually time-independent (stationary solutions), then the unitary propagator is given by Stone's theorem, that is, $U(t,s) = \exp((t-s)P)$.

The situation for unbounded operators is somewhat more difficult and requires the operators $P(t)$, $t \in \mathbb{R}$, to have a common dense domain (cf. [**218**], Corollary on page 102, [**193**], Theorem X.69).

Now we can apply this fact to our situation.

Theorem 12.5. *Let $a(t), b(t)$ satisfy $\mathrm{TL}_r(a,b) = 0$ and (H.12.1). Then the Lax equation (12.22) implies existence of a unitary propagator $U_r(t,s)$ for $P_{2r+2}(t)$ such that*

$$H(t) = U_r(t,s)H(s)U_r(t,s)^{-1}, \quad (t,s) \in \mathbb{R}^2. \tag{12.50}$$

Thus all operators $H(t)$, $t \in \mathbb{R}$, are unitarily equivalent and we might set

$$\sigma(H) \equiv \sigma(H(t)) = \sigma(H(0)), \quad \rho(H) \equiv \rho(H(t)) = \rho(H(0)). \tag{12.51}$$

(Here $\sigma(.)$ and $\rho(.) = \mathbb{C}\backslash\sigma(.)$ denote the spectrum and resolvent set of an operator, respectively.)

In addition, if $\psi(s) \in \ell^2(\mathbb{Z})$ solves $H(s)\psi(s) = z\psi(s)$, then the function

$$\psi(t) = U_r(t,s)\psi(s) \tag{12.52}$$

fulfills

$$H(t)\psi(t) = z\psi(t), \qquad \frac{d}{dt}\psi(t) = P_{2r+2}(t)\psi(t). \tag{12.53}$$

Proof. Let $U_r(t,s)$ be the unitary propagator for $P_{2r+2}(t)$. We need to show that $\tilde{H}(t) = U_r(t,s)^{-1}H(t)U_r(t,s)$ is equal to $H(s)$. Since $\tilde{H}(s) = H(s)$ it suffices to show that $\tilde{H}(t)$ is independent of t, which follows from

$$\frac{d}{dt}\tilde{H}(t) = U_r(t,s)^{-1}\Big(\frac{d}{dt}H(t) - [P_{2r+2}(t), H(t)]\Big)U_r(t,s) = 0. \tag{12.54}$$

The rest is immediate from the properties of the unitary propagator. □

To proceed with our investigation of the Toda equations, we ensure existence and uniqueness of global solutions next. To do this, we consider the Toda equations as a flow on the Banach space $M = \ell^\infty(\mathbb{Z}) \oplus \ell^\infty(\mathbb{Z})$.

Theorem 12.6. *Suppose $(a_0, b_0) \in M$. Then there exists a unique integral curve $t \mapsto (a(t), b(t))$ in $C^\infty(\mathbb{R}, M)$ of the Toda equations, that is, $\mathrm{TL}_r(a(t), b(t)) = 0$, such that $(a(0), b(0)) = (a_0, b_0)$.*

Proof. The r-th Toda equation gives rise to a vector field X_r on M, that is,

$$\frac{d}{dt}(a(t), b(t)) = X_r(a(t), b(t)) \quad \Leftrightarrow \quad \mathrm{TL}_r(a(t), b(t)) = 0. \tag{12.55}$$

Since this vector field has a simple polynomial dependence in a and b it is differentiable and hence (cf. again [**1**], Theorem 4.1.5) solutions of the initial value problem exist locally and are unique. In addition, by equation (12.50) we have $\|a(t)\|_\infty + \|b(t)\|_\infty \le 2\|H(t)\| = 2\|H(0)\|$ (at least locally). Thus any integral curve $(a(t), b(t))$ is bounded on finite t-intervals implying global existence (see, e.g., [**1**], Proposition 4.1.22). □

Let $\tau(t)$ denote the differential expression associated with $H(t)$. If $\mathrm{Ker}(\tau(t)-z)$, $z \in \mathbb{C}$, denotes the two-dimensional nullspace of $\tau(t) - z$ (in $\ell(\mathbb{Z})$), we have the following representation of $P_{2r+2}(t)$ restricted to $\mathrm{Ker}(\tau(t) - z)$,

$$P_{2r+2}(t)\Big|_{\mathrm{Ker}(\tau(t)-z)} = 2a(t)G_r(z,t)S^+ - H_{r+1}(z,t), \tag{12.56}$$

where $G_r(z,n,t)$ and $H_{r+1}(z,n,t)$ are monic (i.e. the highest coefficient is one) polynomials given by

$$\begin{aligned} G_r(z,n,t) &= \sum_{j=0}^{r} g_{r-j}(n,t) z^j, \\ H_{r+1}(z,n,t) &= z^{r+1} + \sum_{j=0}^{r} h_{r-j}(n,t) z^j - g_{r+1}(n,t). \end{aligned} \tag{12.57}$$

One easily obtains

$$\begin{aligned} \dot{a} &= a\Big(H_{r+1}^+ + H_{r+1} - 2(z-b^+)G_r^+\Big), \\ \dot{b} &= 2\Big(a^2 G_r^+ - (a^-)^2 G_r^-\Big) + (z-b)^2 G_r - (z-b)H_{r+1}. \end{aligned} \tag{12.58}$$

As an illustration we record a few of the polynomials G_r and H_{r+1},

$$\begin{aligned}
G_0 &= 1 = \tilde{G}_0,\\
H_1 &= z - b = \tilde{H}_1,\\
G_1 &= z + b + c_1 = \tilde{G}_1 + c_1\tilde{G}_0,\\
H_2 &= z^2 + a^2 - (a^-)^2 - b^2 + c_1(z-b) = \tilde{H}_2 + c_1\tilde{H}_1,\\
G_2 &= z^2 + bz + a^2 + (a^-)^2 + b^2 + c_1(z+b) + c_2 = \tilde{G}_2 + c_1\tilde{G}_1 + c_2\tilde{G}_0,\\
H_3 &= z^3 + 2a^2 z - 2(a^-)^2 b - b^3 + a^2 b^+ - (a^-)^2 b^-\\
&\quad + c_1(z^2 + a^2 - (a^-)^2 - b^2) + c_2(z-b) = \tilde{H}_3 + c_1\tilde{H}_2 + c_2\tilde{H}_1,
\end{aligned}$$

$$\text{etc. .} \tag{12.59}$$

Here $\tilde{G}_r(z,n)$ and $\tilde{H}_{r+1}(z,n)$ are the homogeneous quantities corresponding to $G_r(z,n)$ and $H_{r+1}(z,n)$, respectively. By (12.38) we have

$$G_r(z,n) = \sum_{\ell=0}^{r} c_{r-\ell}\tilde{G}_\ell(z,n), \quad H_{r+1}(z,n) = \sum_{\ell=0}^{r} c_{r-\ell}\tilde{H}_{\ell+1}(z,n). \tag{12.60}$$

Remark 12.7. (i). Since, by (12.27), $a(t)$ enters quadratically in $g_j(t)$, $h_j(t)$, respectively $G_r(z,.,t)$, $H_{r+1}(z,.,t)$, the Toda hierarchy (12.42) is invariant under the substitution

$$a(n,t) \to \varepsilon(n)a(n,t), \tag{12.61}$$

where $\varepsilon(n) \in \{+1,-1\}$. This result should be compared with Lemma 1.6.
(ii). If $a(n_0,0) = 0$ we have $a(n_0,t) = 0$ for all $t \in \mathbb{R}$ (by (12.41)). This implies $H = H_{-,n_0+1} \oplus H_{+,n_0}$ with respect to the decomposition $\ell^2(\mathbb{Z}) = \ell^2(-\infty, n_0+1) \oplus \ell^2(n_0,\infty)$. Hence $P_{2r+2} = P_{-,n_0+1,2r+2} \oplus P_{+,n_0,2r+2}$ decomposes as well and we see that the Toda lattice also splits up into two independent parts $\mathrm{TL}_{\pm,n_0,r}$. In this way, the half line Toda lattice follows from our considerations as a special case. Similarly, we can obtain Toda lattices on finite intervals.

12.3. Stationary solutions

In this section we specialize to the stationary Toda hierarchy characterized by $\dot{a} = \dot{b} = 0$ in (12.42) or, equivalently, by commuting difference expressions

$$[P_{2r+2}, H] = 0 \tag{12.62}$$

of order $2r+2$ and 2, respectively. Equations (12.58) then yield the equivalent conditions

$$\begin{aligned}
(z-b)(H_{r+1} - H_{r+1}^-) &= 2a^2 G_r^+ - 2(a^-)^2 G_r,\\
H_{r+1}^+ + H_{r+1} &= 2(z-b^+)G_r^+.
\end{aligned} \tag{12.63}$$

Comparison with Section 8.3 suggests to define

$$R_{2r+2} = (H_{r+1}^2 - 4a^2 G_r G_r^+). \tag{12.64}$$

A simple calculation using (12.63)

$$\begin{aligned}
&(z-b)(R_{2r+2} - R_{2r+2}^-)\\
&\quad = (z-b)\big((H_{r+1} + H_{r+1}^-)(H_{r+1} - H_{r+1}^-) - 4G_r(a^2 G_r^+ - (a^-)^2 G_r^-)\big)\\
&\quad = 2\big(H_{r+1} + H_{r+1}^- - 2(z-b)G_r\big)\big(a^2 G_r^+ - (a^-)^2 G_r^-\big) = 0
\end{aligned} \tag{12.65}$$

then proves that R_{2r+2} is independent of n. Thus one infers

$$R_{2r+2}(z) = \prod_{j=0}^{2r+1} (z - E_j), \quad \{E_j\}_{0 \le j \le 2r+1} \subset \mathbb{C}. \tag{12.66}$$

The resulting hyperelliptic curve of (arithmetic) genus r obtained upon compactification of the curve

$$w^2 = R_{2r+2}(z) = \prod_{j=0}^{2r+1} (z - E_j) \tag{12.67}$$

will be the basic ingredient in our algebro-geometric treatment of the Toda hierarchy in Section 13.1.

Equations (12.63), (12.64) plus Theorem 2.31 imply

$$g(z,n) = \frac{G_r(z,n)}{R^{1/2}_{2r+2}(z)}, \quad h(z,n) = \frac{H_{r+1}(z,n)}{R^{1/2}_{2r+2}(z)}, \tag{12.68}$$

where $g(z,n) = \langle \delta_n, (H-z)^{-1}\delta_n \rangle$, $h(z,n) = 2a(n)\langle \delta_{n+1}, (H-z)^{-1}\delta_n \rangle - 1$ as usual.

Despite these similarities we need to emphasize that the numbers E_m, $0 \le m \le 2r+1$, do not necessarily satisfy (8.54). This is no contradiction but merely implies that there must be common factors in the denominators and numerators of (12.68) which cancel. That is, if the number of spectral gaps of H is $s+2$, then there is a monic polynomial $Q_{r-s}(z)$ (independent of n) such that $G_r(z,n) = Q_{r-s}(z) G_s(z,n)$, $H_{r+1}(z,n) = Q_{r-s}(z) H_{s+1}(z,n)$, and $R^{1/2}_{2r+2}(z) = Q_{r-s}(z)^2 R^{1/2}_{2s+2}(z)$.

We have avoided these factors in Section 8.3 (which essentially correspond to closed gaps (cf. Remark 7.6)). For example, in case of the constant solution $a(n,t) = 1/2$, $b(n,t) = 0$ of $\mathrm{TL}_r(a,b) = 0$ we have for $r = 0, 1, \dots$

$$\begin{aligned} &G_0(z) = 1, \quad H_1(z) = z, \quad R_2(z) = z^2 - 1, \\ &G_1(z) = z + c_1, \quad H_2(z) = (z + c_1) z, \quad R_4(z) = (z + c_1)^2 (z^2 - 1), \\ &\text{etc. } . \end{aligned} \tag{12.69}$$

Conversely, any given reflectionless finite gap sequences (a,b) satisfy (12.63) and hence give rise to a stationary solution of some equation in the Toda hierarchy and we obtain

Theorem 12.8. *The stationary solutions of the Toda hierarchy are precisely the reflectionless finite-gap sequences investigated in Section 8.3.*

In addition, with a little more work, we can even determine which equation (i.e., the constants c_j). This will be done by relating the polynomials $G_r(z,n)$, $H_{r+1}(z,n)$ to the homogeneous quantities $\tilde{G}_r(z,n)$, $\tilde{H}_{r+1}(z,n)$. We introduce the constants $c_j(\underline{E})$, $\underline{E} = (E_0, \dots, E_{2r+1})$, by

$$R^{1/2}_{2r+2}(z) = -z^{r+1} \sum_{j=0}^{\infty} c_j(\underline{E}) z^{-j}, \quad |z| > \|H\|, \tag{12.70}$$

implying

$$c_0(\underline{E}) = 1, \quad c_1(\underline{E}) = -\frac{1}{2}\sum_{j=0}^{2r+1} E_j, \quad \text{etc. .} \tag{12.71}$$

Lemma 12.9. *Let $a(n)$, $b(n)$ be given reflectionless finite-gap sequences (see Section 8.3) and let $G_r(z,n)$, $H_{r+1}(z,n)$ be the associated polynomials (see (8.66) and (8.70)). Then we have (compare (12.60))*

$$G_r(z,n) = \sum_{\ell=0}^{r} c_{r-\ell}(\underline{E})\tilde{G}_\ell(z,n), \quad H_{r+1}(z,n) = \sum_{\ell=0}^{r} c_{r-\ell}(\underline{E})\tilde{H}_{\ell+1}(z,n). \tag{12.72}$$

In addition, $\tilde{g}_\ell(n)$ can be expressed in terms of E_j and $\mu_j(n)$ by

$$\tilde{g}_1(n) = b^{(1)}(n), \quad \tilde{g}_\ell(n) = \frac{1}{\ell}\Big(b^{(\ell)}(n) + \sum_{j=1}^{\ell-1}\frac{j}{\ell}\tilde{g}_{\ell-j}(n)b^{(j)}(n)\Big), \quad \ell > 1, \tag{12.73}$$

where

$$b^{(\ell)}(n) = \frac{1}{2}\sum_{j=0}^{2r+1} E_j^\ell - \sum_{j=1}^{r}\mu_j(n)^\ell. \tag{12.74}$$

Proof. From (8.96) we infer for $|z| > \|H\|$, using Neumann's expansion for the resolvent of H and the explicit form of $\tilde{g}, \tilde{h}$ given in Theorem 12.2, that

$$\begin{aligned} G_r(z,n) &= -\frac{R_{2r+2}^{1/2}(z)}{z}\sum_{\ell=0}^{\infty}\tilde{g}_\ell(n)z^{-\ell}, \\ H_{r+1}(z,n) &= R_{2r+2}^{1/2}(z)\Big(1 - \frac{1}{z}\sum_{\ell=0}^{\infty}\tilde{h}_\ell(n)z^{-\ell}\Big). \end{aligned} \tag{12.75}$$

This, together with (12.70), completes the first part. The rest follows from (6.59) and Theorem 6.10. □

Corollary 12.10. *Let $a(n)$, $b(n)$ be given reflectionless finite-gap sequences with corresponding polynomial $R_{2s+2}^{1/2}(z)$. Then (a,b) is a stationary solution of* TL_r *if and only if there is a constant polynomial $Q_{r-s}(z)$ of degree $r-s$ such that $c_j = c_j(\underline{E})$, where $\underline{E}$ is the vector of zeros of $R_{2r+2}^{1/2}(z) = Q_{r-s}(z)^2 R_{2s+2}^{1/2}(z)$.*

It remains to show how all stationary solutions for a given equation of the Toda hierarchy can be found. In fact, up to this point we don't even know whether the necessary conditions (12.63) can be satisfied for arbitrary choice of the constants $(c_j)_{1\le j\le r}$.

Suppose $(c_j)_{1\le j\le r}$ is given and define $d_0 = c_0 = 1$,

$$d_j = 2c_j + \sum_{\ell=1}^{j-1} c_\ell c_{j-\ell}, \quad 1 \le j \le r. \tag{12.76}$$

Choose $d_j \in \mathbb{R}$, $r+1 \le j \le 2r+2$, and define $(E_j)_{0\le j\le 2r+1}$ by

$$R_{2r+2}(z) = \sum_{j=0}^{2r+2} d_{2r+2-j}z^j = \prod_{j=0}^{2r+1}(z - E_j). \tag{12.77}$$

Note that our choice of d_j implies $c_j(\underline{E}) = c_j$, $1 \le j \le r$, which is a necessary condition by Lemma 12.9. Since $g(z,n)$ cannot be meromorphic, $R_{2r+2}(z)$ must not be a complete square. Hence those choices of $d_j \in \mathbb{R}$, $r+1 \le j \le 2r+2$, have to be discarded. For any other choice we obtain a list of band edges satisfying (8.54) after throwing out all closed gaps. In particular, setting

$$\Sigma(\underline{d}) = \bigcup_{j=0}^{r} [E_{2j}, E_{2j+1}] \tag{12.78}$$

any operator in $\mathrm{Iso}_R(\Sigma(\underline{d}))$ (see Section 8.3) produces a stationary solution. Thus, the procedure of Section 8.3 can be used to compute all corresponding stationary gap solutions.

Theorem 12.11. *Fix* TL_r, *that is, fix* $(c_j)_{1\le j\le r}$ *and* r. *Let* $(d_j)_{1\le j\le r}$ *be given by (12.76). Then all stationary solutions of* TL_r *can be obtained by choosing* $(d_j)_{r+1\le j\le 2r+2}$ *such that* $R_{2r+2}(z)$ *defined as in (12.77) is not a complete square and then choosing any operator in the corresponding isospectral class* $\mathrm{Iso}_R(\Sigma(\underline{d}))$.

Remark 12.12. The case where $R_{2r+2}(z)$ is a complete square corresponds to stationary solutions with $a(n) = 0$ for some n. For instance, $G_0(n) = 1$, $H_1(n) = z - b(n)$, $R_{2r+2}(z) = (z - b(n))^2$ corresponds to $a(n) = 0$, $n \in \mathbb{Z}$.

Finally, let us give a further interpretation of the polynomial $R_{2r+2}(z)$.

Theorem 12.13. *The polynomial* $R_{2r+2}(z)$ *is the* **Burchnall-Chaundy polynomial** *relating* P_{2r+2} *and* H, *that is,*

$$P_{2r+2}^2 = R_{2r+2}(H) = \prod_{j=0}^{2r+1} (H - E_j). \tag{12.79}$$

Proof. Because of (12.62) one computes

$$\begin{aligned} \Big(P_{2r+2}\Big|_{\mathrm{Ker}(\tau-z)}\Big)^2 &= \Big((2aG_r S^+ - H_{r+1})\Big|_{\mathrm{Ker}(\tau-z)}\Big)^2 \\ &= \Big(2aG_r(2(z-b^+)G_r^+ - H_{r+1}^+ - H_{r+1})S^+ + H_{r+1}^2 - 4a^2 G_r G_r^+\Big)\Big|_{\mathrm{Ker}(\tau-z)} \\ &= R_{2r+2}(z)\Big|_{\mathrm{Ker}(\tau-z)} \end{aligned} \tag{12.80}$$

and since $z \in \mathbb{C}$ is arbitrary, the rest follows from Corollary 1.3. □

This result clearly shows again the close connection between the Toda hierarchy and hyperelliptic curves of the type $M = \{(z,w) | w^2 = \prod_{j=0}^{2r+2}(z - E_j)\}$.

12.4. Time evolution of associated quantities

For our further investigations in the next two chapters, it will be important to know how several quantities associated with the Jacobi operator $H(t)$ vary with respect to t.

First we will try to calculate the time evolution of the fundamental solutions $c(z,.,t)$, $s(z,.,t)$ if $a(t)$, $b(t)$ satisfy $\mathrm{TL}_r(a,b) = 0$. For simplicity of notation we will not distinguish between $H(t)$ and its differential expression $\tau(t)$. To emphasize that a solution of $H(t)u = zu$ is not necessarily in $\ell^2(\mathbb{Z})$ we will call such solutions **weak solutions**. Similarly for $P_{2r+2}(t)$.

First, observe that (12.22) implies

$$(H(t) - z)(\frac{d}{dt} - P_{2r+2}(t))\Phi(z,.,t) = 0, \tag{12.81}$$

where $\Phi(z,n,t)$ is the transfer matrix from (1.30). But this means

$$(\frac{d}{dt} - P_{2r+2}(t))\Phi(z,.,t) = \Phi(z,.,t)C_r(z,t) \tag{12.82}$$

for a certain matrix $C_r(z,t)$. If we evaluate the above expression at $n = 0$, using $\Phi(z,0,t) = \mathbb{1}$, we obtain

$$\begin{aligned} C_r(z,t) &= \big(P_{2r+2}(t)\Phi(z,.,t)\big)(0) \\ &= \begin{pmatrix} -H_{r+1}(z,0,t) & 2a(0,t)G_r(z,0,t) \\ -2a(0,t)G_r(z,1,t) & 2(z-b(1,t))G_r(z,1,t) - H_{r+1}(z,1,t) \end{pmatrix}. \end{aligned} \tag{12.83}$$

The time evolutions of $c(z,n,t)$ and $s(z,n,t)$ now follow from

$$\dot{\Phi}(z,.,t) = P_{2r+2}\Phi(z,.,t) + \Phi(z,.,t)C_r(z,t) \tag{12.84}$$

or more explicitly

$$\begin{aligned} \dot{c}(z,n,t) &= 2a(n,t)G_r(z,n,t)c(z,n+1,t) - \big(H_{r+1}(z,n,t) \\ &\quad + H_{r+1}(z,0,t)\big)c(z,n,t) - 2a(0,t)G_r(z,1,t)s(z,n,t), \\ \dot{s}(z,n,t) &= 2a(n,t)G_r(z,n,t)s(z,n+1,t) - (H_{r+1}(z,n,t) + H_{r+1}(z,1,t) \\ &\quad - 2(z-b(1,t))G_r(z,1,t))s(z,n,t) + 2a(0,t)G_r(z,0,t)c(z,n,t). \end{aligned} \tag{12.85}$$

Remark 12.14. In case of periodic coefficients, this implies for the time evolution of the monodromy matrix $M(z,t)$

$$\frac{d}{dt}M(z,t) = [M(z,t), C_r(z,n,t)], \tag{12.86}$$

where

$$C_r(z,n,t) = \begin{pmatrix} -H_{r+1} & 2aG_r \\ -2aG_r & 2(z-b^+)G_r^+ - H_{r+1} \end{pmatrix}. \tag{12.87}$$

This shows (take the trace) that the discriminant is time independent and that $\{E_j\}_{j=1}^{2N}$, A, and B (cf. Section 7.1) are time independent.

Evaluating (12.86) explicitly and expressing everything in terms of our polynomials yields (omitting some dependencies)

$$\begin{aligned} &\frac{d}{dt}\begin{pmatrix} -H/2 & aG \\ aG^+ & H/2 \end{pmatrix} = \\ &\begin{pmatrix} 4a^2(G_rG^+ - G_r^+G) & 2aG_rH + (z-2b^+)G_r^+G \\ -2aG_r^+H - a(z-2b^+)G_r^+G^+) & -4a^2(G_rG^+ - G_r^+G) \end{pmatrix}. \end{aligned} \tag{12.88}$$

Equation (12.84) enables us to prove

Lemma 12.15. *Assume (H.12.1) and suppose* $\mathrm{TL}_r(a,b) = 0$. *Let* $u_0(z,n)$ *be a weak solution of* $H(0)u_0 = zu_0$. *Then the system*

$$H(t)u(z,n,t) = zu(z,n,t), \quad \frac{d}{dt}u(z,n,t) = P_{2r+2}(t)u(z,n,t) \tag{12.89}$$

has a unique weak solution fulfilling the initial condition

$$u(z,n,0) = u_0(z,n). \tag{12.90}$$

If $u_0(z,n)$ is continuous (resp. holomorphic) with respect to z, then so is $u(z,n,t)$.

Furthermore, if $u_{1,2}(z,n,t)$ both solve (12.89), then

$$\begin{aligned} W(u_1(z),u_2(z)) &= W_n(u_1(z,t),u_2(z,t)) = \\ & a(n,t)\Big(u_1(z,n,t)u_2(z,n+1,t) - u_1(z,n+1,t)u_2(z,n,t)\Big) \end{aligned} \tag{12.91}$$

depends neither on n nor on t.

Proof. Any solution $u(z,n,t)$ of the system (12.89) can be written as

$$u(z,n,t) = u(z,0,t)c(z,n,t) + u(z,1,t)s(z,n,t) \tag{12.92}$$

and from (12.84) we infer that (12.89) is equivalent to the ordinary differential equation

$$\begin{pmatrix} \dot u(z,0,t) \\ \dot u(z,1,t) \end{pmatrix} = -C_r(z,t)\begin{pmatrix} u(z,0,t) \\ u(z,1,t) \end{pmatrix}, \quad \begin{pmatrix} u(z,0,0) \\ u(z,1,0) \end{pmatrix} = \begin{pmatrix} u_0(z,0) \\ u_0(z,1) \end{pmatrix}, \tag{12.93}$$

which proves the first assertion. The second is a straightforward calculation using (12.56) and (12.58). □

The next lemma shows that solutions which are square summable near $\pm\infty$ for one $t \in \mathbb{R}$ remain square summable near $\pm\infty$ for all $t \in \mathbb{R}$, respectively.

Lemma 12.16. *Let $u_{\pm,0}(z,n)$ be a solution of $H(0)u = zu$ which is square summable near $\pm\infty$. Then the solution $u_\pm(z,n,t)$ of the system (12.89) with initial data $u_{\pm,0}(z,n) \in \ell^2_\pm(\mathbb{Z})$ is square summable near $\pm\infty$ for all $t \in \mathbb{R}$, respectively.*

Denote by $G(z,n,m,t)$ the Green function of $H(t)$. Then we have ($z \in \rho(H)$)

$$G(z,m,n,t) = \frac{1}{W(u_-(z),u_+(z))}\begin{cases} u_+(z,n,t)u_-(z,m,t) & \text{for } m \le n \\ u_+(z,m,t)u_-(z,n,t) & \text{for } n \le m \end{cases}. \tag{12.94}$$

Especially, if $z < \sigma(H)$ and $a(n,t) < 0$ we can choose $u_{\pm,0}(z,n) > 0$, implying $u_\pm(z,n,t) > 0$.

Proof. We only prove the u_- case (the u_+ case follows from reflection) and drop z for notational simplicity. By Lemma 12.15 we have a solution $u(n,t)$ of (12.89) with initial condition $u(n,0) = u_{+,0}(n)$ and hence

$$S(n,t) = S(n,0) + 2\int_0^t \mathrm{Re} \sum_{j=-n}^{0} \overline{u(j,s)} P_{2r+2}(s)u(j,s)ds, \tag{12.95}$$

where $S(n,t) = \sum_{j=-n}^{0} |u(j,t)|^2$. Next, by boundedness of $a(t)$, $b(t)$, we can find a constant $C > 0$ such that $4|H_{r+1}(n,t)| \le C$ and $8|a(n,t)G_r(n,t)| \le C$. Using (12.56) and the Cauchy-Schwarz inequality yields

$$\Big|\sum_{j=-n}^{0} \overline{u(j,s)} P_{2r+2}(s)u(j,s)\Big| \le \frac{C}{2}\Big(|u(1,s)|^2 + S(n,s)\Big). \tag{12.96}$$

Invoking Gronwall's inequality shows

$$S(n,t) \le \Big(S(n,0) + C\int_0^t |u(1,s)|^2 \mathrm{e}^{-Cs} ds\Big)\mathrm{e}^{Ct} \tag{12.97}$$

and letting $n \to \infty$ implies that $u(z,.,t) \in \ell^2_-(\mathbb{Z})$.

Since $u(z,n,t) = 0$, $z < \sigma(H)$, is not possible by Lemma 2.6, positivity follows as well and we are done. □

Using the Lax equation (12.22) one infers ($z \in \rho(H)$)

$$\frac{d}{dt}(H(t)-z)^{-1} = [P_{2r+2}(t), (H(t)-z)^{-1}]. \tag{12.98}$$

Furthermore, using (12.94) we obtain for $m \le n$

$$\begin{aligned} &\frac{d}{dt}G(z,n,m,t) = \\ &= \frac{u_-(z,m)(P_{2r+2}u_+(z,.))(n) + u_+(z,n)(P_{2r+2}u_-(z,.))(m)}{W(u_-(z),u_+(z))}. \end{aligned} \tag{12.99}$$

As a consequence (use (12.56) and (12.58)) we also have

$$\begin{aligned} \frac{d}{dt}g(z,n,t) &= 2\big(G_r(z,n,t)h(z,n,t) - g(z,n,t)H_{r+1}(z,n,t)\big), \\ \frac{d}{dt}h(z,n,t) &= 4a(n,t)^2\big(G_r(z,n,t)g(z,n+1,t) \\ &\qquad - g(z,n,t)G_r(z,n+1,t)\big) \end{aligned} \tag{12.100}$$

and

$$\begin{aligned} \frac{d}{dt}\tilde{g}_j(t) &= -2\tilde{g}_{r+j+1}(t) + 2\sum_{\ell=0}^{r}\big(g_{r-\ell}(t)\tilde{h}_{\ell+j}(t) - \tilde{g}_{\ell+j}(t)h_{r-\ell}(t)\big) \\ &\quad + 2g_{r+1}(t)\tilde{g}_j(t), \\ \frac{d}{dt}\tilde{h}_j(t) &= 4a(t)^2\sum_{\ell=0}^{r}\big(g_{r-\ell}(t)\tilde{g}^+_{\ell+j}(t) - \tilde{g}_{\ell+j}(t)g^+_{r-\ell}(t)\big). \end{aligned} \tag{12.101}$$